Interplay Between Charge, Spin, and Phonons in Low Dimensional
Strongly Interacting Systems

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Dedication

To my parents, Zinat Habibi and Karim Soltaniedyhha, who passed on a love of reading and respect for education. Without their caring support and sacrifice, this would not have been possible.
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Abstract

Interacting one-dimensional electron systems are generally referred to as “Luttinger liquids”, after the effective low-energy theory in which spin and charge behave as separate degrees of freedom with independent energy scales. The “spin-incoherent Luttinger liquid” describes a finite-temperature regime that is realized when the temperature is very small relative to the Fermi energy, but larger than the characteristic spin energy scale, and it is realized for instance in the strongly interacting Hubbard chain (with $U \to \infty$). Similar physics can take place in the ground-state, when a Luttinger Liquid is coupled to a spin bath, which effectively introduces a “spin temperature” through its entanglement with the spin degree of freedom. We show that the spin-incoherent state can be exactly written as a factorized wave-function, with a spin wave-function that can be described within a valence bond formalism. This enables us to calculate exact expressions for the momentum distribution function and the entanglement entropy. This picture holds not only for two antiferromagnetically coupled $t-J$ chains, but also for the $t-J$-Kondo chain with strongly interacting conduction electrons. In chapter 3 we argue that this theory is quite universal and may describe a family of problems that could be dubbed “spin-incoherent”.

This crossover to the spin-incoherent regime at finite temperatures can be understood by means of Ogata and Shiba’s factorized wave-function, where charge and spin are totally decoupled, and assuming that the charge remains in the ground state, while the spin is thermally excited and at an effective “spin temperature”. In chapter 4 we use the time-dependent density matrix renormalization group method (tDMRG) to calculate the dynamical contributions of the spin, to reconstruct the single-particle spectral function of the electrons. The crossover is characterized by a redistribution of spectral weight both in frequency and momentum, with an apparent shift by $k_F$ of the minimum of the dispersion.

In chapter 5, we calculate the spectral function of the one-dimensional Hubbard-Holstein model using the tDMRG, focusing on the regime of large local Coulomb repulsion, and away from electronic half-filling. We argue that, from weak to intermediate electron-phonon coupling, phonons interact only with the electronic charge, and not with the spin degrees of freedom. For strong electron-phonon interaction, spinon and holon bands are not discernible anymore and the system is well described by a spinless polaronic liquid. In this regime, we observe multiple peaks in the spectrum with an energy separation corresponding to the energy of the lattice vibrations (i.e. phonons). We support the numerical results by introducing a well controlled analytical approach based on Ogata-Shiba’s factorized wave-function, showing that the spectrum can be understood as a convolution of three contributions, originating from charge, spin, and lattice sectors. We recognize and interpret these signatures in the spectral properties and discuss the experimental implications.
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<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>SCS</td>
<td>Spin Charge Separation</td>
</tr>
<tr>
<td>LL</td>
<td>Luttinger Liquid</td>
</tr>
<tr>
<td>1D</td>
<td>1 Dimension(al)</td>
</tr>
<tr>
<td>DMRG</td>
<td>Density Matrix Renormalization Group</td>
</tr>
<tr>
<td>tDMRG</td>
<td>time-dependent Density Matrix Renormalization Group</td>
</tr>
<tr>
<td>ED</td>
<td>Exact Diagonalization</td>
</tr>
<tr>
<td>SILL</td>
<td>Spin Incoherent Luttinger Liquid</td>
</tr>
<tr>
<td>GS</td>
<td>Ground State</td>
</tr>
<tr>
<td>PES</td>
<td>PhotoEmission Spectroscopy</td>
</tr>
<tr>
<td>IPES</td>
<td>Inverse PhotoEmission Spectroscopy</td>
</tr>
<tr>
<td>ARPES</td>
<td>Angle-Resolved PhotoEmission Spectroscopy</td>
</tr>
<tr>
<td>LHB</td>
<td>Lower Hubbard Band</td>
</tr>
<tr>
<td>UHB</td>
<td>Upper Hubbard Band</td>
</tr>
<tr>
<td>el-el</td>
<td>electron-electron</td>
</tr>
<tr>
<td>el-ph</td>
<td>electron-phonon</td>
</tr>
<tr>
<td>HH</td>
<td>Hubbard Holstein</td>
</tr>
<tr>
<td>CDW</td>
<td>Charge Density Wave</td>
</tr>
<tr>
<td>AFM</td>
<td>Anti-FerroMagnet</td>
</tr>
<tr>
<td>ZFA</td>
<td>Zheng Feinberg Avignon (Zheng et al., 1989)</td>
</tr>
<tr>
<td>CPT</td>
<td>Cluster Perturbation Theory</td>
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Chapter 1

Introduction

1.1 Interacting systems in one dimension

The physics of correlated low dimensional systems is quite different than that of their higher dimensional counterparts. In three-dimensions, the physics can be described within the Fermi liquid theory, where there is a one-to-one correspondence between the excitations of a weakly interacting Fermi system, so-called quasi-particles, and the excitations of a non-interacting one. Quasi-particles preserve the same quantum numbers as the original excitations in the original system. This scenario breaks down in one dimension (1D): in this case, the Fermi surface reduces to two points in momentum space, at $k = \pm k_F$, and the resulting nesting, pervasive at all densities, prevents the application of perturbation theory. This leads to a new paradigm: the Luttinger liquid [1, 2, 3]. In the next section we will give an overview of this theory.

Such systems of correlated particles have been studied theoretically for over 50 years, and have been the driving force behind the Luttinger liquid theory, bosonization, and conformal field theory. In some cases one might be able to obtain a complete and exact solution of a problem using Bethe ansatz [4].
We began to see experimental realizations of the one-dimensional behavior in isolated 1D and also bulk materials in the 1970’s with polymers and organic compounds. Some of them are organic superconductors [5], ladder compounds [6], quantum wires [7], carbon nanotubes [8], edge states in quantum hall systems [3, 9, 10] to mention a few. TTF-TCNQ (Tetrathiafulvalene-tetracyanoquinodimethane) is a quasi-1D organic conductor that has been studied in depth experimentally. The crystal structure of this organic conductor is shown in Figure 1.1 from Ref. [11]. Another example of a 1D-type material representing spin-charge separation is SrCuO$_2$, the crystal structure of which is shown in Figure 1.2 [12].

In the following sections of this introduction, we will illustrate the phenomenon spin-charge separation (where we see in some materials that the spin and charge of an electron propagate independently, as if they were separate excitations with different quantum numbers) in the absence of electron-phonon interaction. In particular, we will discuss how angle-resolved photoemission spectroscopy has been the main tool to probe this phenomenon experimentally. First, we give a general introduction of this experimental technique and then we consider the case of one-dimensional systems. Next, we will introduce the Hubbard model, its $t - J$ limit, and discuss the impact of spin-charge
separation on the electronic ground state wave-function. In the final section we discuss the effect of the phonons on a strongly correlated system from the experimental and theoretical standpoint.

1.1.1 Luttinger liquid theory

Tomonaga-Luttinger liquid (Tomonaga, 1950) [1, 2, 3], or more often known as simply Luttinger liquid (LL), is a theoretical model describing interacting fermions in one-dimensional systems, such as organic conductors, carbon nanotubes, nanowires as well as the examples introduced in the previous section.

Landau’s Fermi liquid theory, which described weakly interacting fermions in higher dimensions, breaks down in 1D. In this theory, excitations in the solid can be described as free quasi-particles, which carry the same quantum numbers as the original fermions, but with a renormalized mass and finite life-time. In 1D, as opposed to individual excitations in the Fermi liquid picture, excitations become collective (bosonic), and do not carry the
same quantum numbers as the original fermions. This is definitely a major difference between the world in 1D and higher dimensions. In a Luttinger liquid, the natural excitations are collective density fluctuations, that carry either spin (“spinons”), or charge (“holons”). These excitations have different dispersions, and obviously, do not carry the same quantum numbers as the original fermions. This leads to the spin-charge separation (SCS) picture, in which a fermion injected into the system breaks down into excitations carrying different quantum numbers, each with a characteristic energy scale and velocity (one for the charge, one for the spin).

One can understand the origin of this discrepancy by using perturbation theory to calculate for instance the susceptibility:

$$\chi(q, \omega) = \frac{1}{\Omega} \sum_k \frac{f(\epsilon(k)) - f(\epsilon(k+q))}{\omega + \epsilon(k) - \epsilon(k+q) + i\delta}$$

We find that some points in the Brillouin zone may introduce a singularity. This, in general happens when we have nesting \([3]\)

$$\epsilon(k + Q) = \epsilon(k)$$

where \(\epsilon(k)\) is the energy of the electron at momentum \(k\). In high dimensions, this singularity gets smoothed out or regularized when summing over many other terms. This does not occur in 1D since we always have nesting \((Q = 2k_F)\) and the singularity is dominant. The fact that perturbation theory diverges shows that the ground state of our interacting system is completely different than the non-interacting ground state, which indicates that a new theory is needed to understand this physics. Luttinger liquid theory solves this problem by postulating that the natural excitations are free density fluctuations carrying the charge and spin degrees of freedom. In fact, the density fluctuations can be described by a superposition of particle-hole excitations (we omit the spin index for now):

$$\rho^\dagger(q) = \sum_k c^\dagger_{k+q} c_k.$$
It can be seen that this is a well defined excitation with a well defined energy. Since they are build from pairs of fermionic operators, these excitations are bosonic.

1.2 Angle-resolved photoemission spectroscopy

Angle-resolved photoemission spectroscopy, ARPES, is an experimental technique to detect the density of single-particle electronic states in the Bravais lattice of solids. This approach is an improvement to ordinary photoemission spectroscopy, PES (shown in Figure 1.7 schematically), where the measurement is done on the energy spectrum of the electrons emitted from the solid. PES is a general term referred to “photoelectric effect” based techniques originally observed by Hertz in 1887 and later in 1905 explained by Einstein in the language of quantum mechanics. Einstein realized that light can be absorbed

![Diagram of electronic energy distribution in PES. From Hüfner, 1995.](image)

**Figure 1.3:** Electronic energy distribution in PES. From Hüfner, 1995.
Figure 1.4: Angle-resolved photoemission spectroscopy: (a) geometry of an ARPES experiment. (b) Momentum-resolved one-electron removal and addition spectra for a noninteracting electronic system (free electrons). Also on the top, the momentum distribution is shown; the occupation $n_k$ has a discontinuity of magnitude 1 at the Fermi surface. (c) The same spectra for an interacting Fermi-liquid system (Sawatzky, 1989; Meinders, 1994). Momentum distribution has still a discontinuity with a reduced magnitude $Z_k < 1$, where $Z_k$ is the quasiparticle weight. (c) Lower right, photoelectron spectrum of gaseous hydrogen and the ARPES spectrum of solid hydrogen developed from the gaseous one, where we see the replica due to the lattice vibrations and their coupling with electrons (Sawatzky, 1989). From Damascelli et al., 2003.

In a sample by an electron which can escape from the material with a maximum kinetic energy of $h\nu - \phi$ (where $\nu$ is the photon frequency and $\phi$ the material’s work function, usually around a few eV).

In addition to energy, ARPES gives information on the direction and speed of valence band electrons in the material that is being studied. The momentum-resolved (k-space) information combined with the energy spectrum results in a detailed picture of the band dispersion and Fermi surface.

In the past few decades ARPES has been the leading experimental method for studying the electronic structure of solids, understanding the physics of interacting systems and, more recently, studying high-$T_c$ superconductivity (see [13], for instance). Starting from a microscopic Hamiltonian and calculating the single-particle Green’s function, ARPES is the ultimate experimental tool to confirm theory and guide new searches. Since ARPES provides this connection between a measurable experiment and a microscopic analysis of the system, it has been widely studied in different many-body theories.
In Figure 1.3 (from Ref. [14]) the electron energy distribution produced by the incoming photons is shown as a function of kinetic energy $E_{\text{kin}}$ on the right, and on the left in terms of binding energy $E_B$ versus the density of states. Figure 1.4 (a) (from Ref. [15]) shows the ARPES experiment schematically, where the emission direction of the photoelectron is specified by the polar $\theta$ and azimuthal $\phi$ angles. Photo-emitted electrons are collected by the analyzer, where kinetic energy $E_{\text{kin}}$ and emission angle $\theta$ are determined (the entire system is in high vacuum at pressures lower than $5 \times 10^{-11}$ torr). Momentum-resolved one-electron removal and addition spectra for a noninteracting electron system and for an interacting Fermi-liquid system are shown in Figure 1.4 (b) and (c) [15, 16, 17]. For the noninteracting case (b), the ARPES spectrum is given by delta-function peaks at the Hartree-Fock orbital energies, and the momentum distribution function shows a step function behavior at the Fermi momentum $k_F$. In this ideal case where the effect of interactions is negligible the quasi-particle weight is $Z_F = 1$ and one can consider these noninteracting electrons to be a free electron gas obeying Fermi-Dirac statistics. This quasi-particle weight $Z_F$ gets smaller once we turn on the interactions (as shown in Figure 1.4 (c) inset), and the system follows the Fermi liquid theory. The contributions in the spectra come from several different terms and the peaks are in general evaluated from delta functions due to the el-el interactions.

1.3 The single-band Hubbard model

In this section we introduce the single-band Hubbard model (or simply Hubbard model), a paradigm to understand strongly correlated electrons, and later focus on the one-dimensional case to see how spin-charge separation emerges from the theory. The Hubbard model is probably the simplest model of interacting particles in a lattice, containing a kinetic term allowing the particles to tunnel through the lattice sites (hopping), and a potential energy term consisting of an on-site interaction (Coulomb repulsion) [18].
In two dimensions (2D), the one-band Hubbard model reads as:

$$H = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow},$$  \hspace{1cm} (1.1)

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (destroys) an electron of spin $\sigma$ at site $i$ of a square lattice, and $n_{i,\sigma}$ is the particle number operator. $\langle ij \rangle$ denotes the nearest neighbor lattice sites on a given square lattice, $t$ is the hopping amplitude parametrizing the kinetic energy (or the bandwidth) and $U$ the on-site Coulomb repulsion.

This Hamiltonian has been assumed for decades to be the minimal model that can explain high-temperature superconductivity, and has acquired even more relevance recently in view of the current efforts to realize it in cold atom systems.

Despite its apparent simplicity, this model cannot be solved exactly, except in the 1D case that we will discuss on the next section. However, this model spawned some remarkable theoretical “technologies”, as well as some of the most important computational advances in the field. Some mean-field theory approaches [19], Green’s function decoupling schemes, variational methods and other techniques have been used to study the model. Quantum Monte Carlo[20], the Density Matrix Renormalization Group (DMRG) [21, 22], Gutzwiller approximation (GA) based calculations [23, 24, 25], and Dynamical Mean-Field Theory are computational methods that conceived with the Hubbard model as a main motivation[20].

The one-band Hubbard model on bi-partite lattices has particle-hole symmetry, or invariance under a particle-hole transformation. This means that at half-filling the upper Hubbard band (UHB) and the lower Hubbard band (LHB) are symmetric, as shown in Figure 1.5; this is also seen on the phase diagram of the Hubbard model on a bi-partite lattice about half-filling (not true in general when long-range hopping is considered).
The Hubbard model is an extension of the so-called tight-binding model

$$H = -t \sum_{(i,j),\sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right).$$

(1.2)

“The tight-binding model evinces the quantum-mechanical quintessence of electrons in a solid: the emergence of an electronic band structure — intervals of allowed and forbidden energies — lying at the heart of present-day semiconductor technology”[26].

Electrons with opposite spin would not see each other since we have turned off the interaction term $U$. Since this is a trivial non-interacting problem, the Hamiltonian can be readily diagonalized in this limit by Fourier transforming the operators to momentum space, where it reads

$$H = \sum_{k,\sigma} \epsilon(k) c_{k\sigma}^\dagger c_{k\sigma},$$

(1.3)

where the momentum $k$ is defined in the corresponding Brillouin zone.

### 1.3.1 Hubbard model in 1D

The one-dimensional Hubbard Hamiltonian is a paradigmatic model in condensed matter, not only for its relative simplicity, but mainly because it contains the basic ingredients
to understand the physics emerging from strong interactions. However, it turned out to be a “mathematically hard” problem.

Let us first consider an isolated chain of strongly interacting fermions, described by a Hubbard Hamiltonian in 1D

\[
H = -t \sum_{i,\sigma} \left( c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \tag{1.4}
\]

Here, \( c_{i\sigma}^\dagger \) (\( c_{i\sigma} \)) creates (destroys) an electron of spin \( \sigma \) on the \( i \)th site along a chain of length \( L \), \( n_{i,\sigma} \) is the particle number operator.

The 1D model can be exactly solved by Bethe Ansatz, and its low energy physics can be understood in terms of Luttinger liquid (LL) theory [1]. In a Luttinger liquid, the natural excitations are collective density fluctuations, that carry either spin (“spinons”), or charge (“holons”). This leads to the spin-charge separation picture, in which a fermion injected into the system breaks down into excitations carrying different quantum numbers, each with a characteristic energy scale and velocity (one for the charge, one for the spin). For more details on Luttinger liquid we encourage the reader to see Refs.[2, 3].

To illustrate this, Figure 1.6 shows results of simulations by A. E. Feiguin (unpublished): when a particle is destroyed at the center of a half-filled Hubbard chain, the spin and charge light cones have different slopes, demonstrating that the corresponding excitations have different velocities, and propagate ballistically. The simulation has been done for \( L = 160 \) and \( U = 4 \) using tDMRG with 300 DMRG states (\( m = 300 \)).

Spin-charge separation is present for all finite values of the interaction \( U \neq 0 \). In the \( U/t \to 0 \) limit, the Hamiltonian basically describes free fermions on the lattice.

1.3.2 \( U \gg t \) regime and the mapping to the \( t - J \) model

In the large \( U \) regime, configurations with doubly occupied orbitals are energetically unfavorable. One can project these states out, and obtain an effective low energy theory
that has support on this reduced Hilbert space. The resulting Hamiltonian is the so-called $t - J$ model (Appendix A)

$$H = -t \sum_{\langle ij \rangle, \sigma} \left( c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + J \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j),$$

(1.5)

where $\vec{S}_i$ is the spin operator, and we consider the implicit constraint of forbidden double-occupancy. This means that the hopping term cannot create a particle on an orbital that is occupied by a fermion with the opposite spin. The exchange energy between spins is parametrized by $J$, where $J = 4t^2/U$. Unless otherwise specified, we express all energies in units of the hopping parameter $t$. Notice that at half-filling, the system becomes a Mott insulator with one particle per site, and the model reduces to the Heisenberg Hamiltonian

$$H = \sum_{\langle ij \rangle} \sum_{\alpha = x,y,z} \tilde{J}^\alpha (S_i^\alpha S_j^\alpha - \frac{1}{4} \delta_{\alpha,z}),$$

(1.6)

with $\tilde{J}^\alpha = 4t^2/U$.

**Figure 1.6:** Spin and charge wave propagations through time on a strongly interacting Hubbard chain with $L = 160$ where one electron at site = 80 and time = 0 has been destroyed. The simulation has been done for $U/t = 4$ by DMRG ($m = 300$).
1.4 Spin-charge separation and Ogata-Shiba’s wave-function

In the strong coupling regime of the Hubbard model \((U \to \infty)\) or equivalently \(J \to 0\) limit in the \(t - J\) model, double occupancy is strictly forbidden, and the spin flip term in the Hamiltonian vanishes. Formally, the Hamiltonian can be written as:

\[
H = -t \sum_{\langle ij \rangle, \sigma} P \left( c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) P^\dagger,
\]

where the operator \(P\) is an operator that projects out all configuration with double occupied sites.

In the one-dimensional case, spin and charge excitations are described separately and they become collective \textit{bosonic} fluctuations. For instance as illustrated in Figure 1.7 removing a

\[\text{Figure 1.7: Schematic photoemission on an antiferromagnetic Hubbard chain with } U \to \infty. \text{ As shown there is no more individual excitations and we observe separate collective spin and charge excitations.}\]
\( \downarrow\)-electron from an antiferromagnetic ground-state results in propagating charge excitation (holon) and spin excitation (spinon) in different directions with different energy scales and velocities.

In this particular limit \((U \to \infty)\), one can easily define independent charge and spin excitations within the framework of the Bethe Ansatz. Since \(J = 0\), all spin configurations are in principle degenerate in this limit. The ground-state of Hamiltonians (1.4 and 1.5) can be reconstructed as a product of a spinless fermionic wave-function \(|\phi\rangle\) and a spin wave-function \(|\chi\rangle\). Described by Ogata and Shiba’s factorized wave-function [27], this multiplication can be written as

\[
|\text{g.s.}\rangle = |\phi\rangle \otimes |\chi\rangle. \tag{1.8}
\]

The first piece, \(|\phi\rangle\), describes the charge degree of freedom, and is simply the ground-state of a one-dimensional tight-binding chain of \(N\) non-interacting spinless fermions [Eq. 1.3]. The spin wave-function \(|\chi\rangle\) corresponds to a “squeezed” chain of \(N\) spins, where all the unoccupied sites have been removed. In this limit, the charge and the spin are governed by independent Hamiltonians. For \(J = 0\) the spin states are degenerate, and the charge dispersion becomes that of a non-interacting band \(\epsilon(k) = -2t \cos(k)\). However, any finite value of \(J\) will lift this degeneracy and give the spin excitations a finite bandwidth. Notice that in finite systems with periodic boundary conditions, the spin degree of freedom affects the charge through an effective magnetic flux [28, 29, 30].

This factorization also applies to a given excited state \(|\psi(P)\rangle\)

\[
|\psi(P)\rangle = |\phi^{N}_{L,Q}(I)\rangle \otimes |\chi^{N}_{N}(Q,M)\rangle, \tag{1.9}
\]

where for a system with \(N\) electrons on a chain with \(L\) sites, \(I\) labels a combination of \(N\) wave-vectors \(k_{i}L = 2\pi i + Q\), with \(i = -L/2, -L/2 + 1, \cdots, L/2 - 1\), that are compatible with the total fermionic momentum \(P\). The index \(M\) labels all possible configurations of momenta compatible with the total momentum of the spin wave-function \(Q = 2\pi j/N\),
with \( j = 0, 1, \ldots, N - 1 \). The fermionic part stays coupled to the spin part only by a phase \( Q \) introduced at the boundaries, resulting in twisted boundary conditions for the fermions, which ensures momentum conservation for the original problem.

### 1.4.1 Spin-charge separation evidence in ARPES experiments

As illustrated in Figure 1.7 the removal of an electron creates a hole in the lattice. Under the right conditions where we have spin-charge separation, the hole decays into a spinon and a holon. When the electron fractionalizes into two particles, a continuum of excited states with a double-edge structure (referred to as spinon and holon branches) is expected as shown in Figure 1.8 \cite{12}. Thus, having these two branches in an ARPES spectrum would be the most direct evidence of spin-charge separation.

In Figure 1.9 \( SrCuO_2 \) ARPES measurements are shown. From Figure 1.8 (a) the 1D nature of \( SrCuO_2 \) is clear; as the intensity modulates along \( k_\parallel \) there is almost no change

![Figure 1.8](image)

**Figure 1.8:** (left) Existence of a single branch in the excitation spectrum where we have no spin-charge separation. (right) Two branches with edge singularities are expected within spin-charge separation. One can also expect that the ratio between the width of the spinon band and holon band is proportional to \( J/t \). From Kim et al., 2006.
Figure 1.9: ARPES data for SrCuO$_2$. (a) intensity distribution as a function of momentum at a constant energy. (b) Raw ARPES data with $k_\perp = 0.7$ Å$^{-1}$. (c) Second derivatives are plotted to trace the peaks. From Kim et al., 2006.

when $k_\perp$ varies. In the part (b) of the same figure we see that the low-energy features are being repeated due to the periodicity in the crystal. The two bands due to spinon and holon stand out in this picture, although Figure 1.9 (c) provides derivatives of the raw data and a clearer picture of these bands.

The ARPES spectrum of TTF-TCNQ is shown in Figure 1.10. One can see the spinon band is clearly separated from the holon band, another experimental signature of spin-charge separation [11]. The bandwidth of the spinon band is proportional to $J$ and the holon band to $t$.

Comparing this picture coming from the ARPES experiments, the two separate bands
resulting from spin-charge separation show a lot of similarities with the single-band Hubbard model $U/t \to \infty$. In fact, as shown in Ref. [11], these results can be explained by the 1D Hubbard model, even quantitatively. In Figure 1.10 (a) a schematic electron removal on a doped 1D Hubbard chain is shown, and in part (b) a comparison of the conduction band of a 1D Hubbard $U$ with the experimental result of TTF-TCNQ are shown on top of each other, and proving the agreement with theory.

1.5 The spin-incoherent Luttinger Liquid regime

Recently, a previously overlooked regime at finite temperature in one-dimensional systems has come to light: the “spin-incoherent Luttinger liquid” (SILL) [31, 32, 33, 34, 35, 36]. Due to the fact that the holons and spinons have independent energy scales, their behavior at finite temperature will be quite different. If the spinon bandwidth is much smaller than the holon bandwidth, a small temperature relative to the Fermi energy may actually be
felt as a very large temperature by the spins. In fact, the charge will remain very close to the charge ground-state, but the spins will become totally incoherent, effectively at infinite temperature. This regime is characterized by universal properties in the transport, tunneling density of states, and the spectral functions \[35\], and will occupy a great deal of our attention in the rest of our discussion.

In Ref.\[37\], it was shown how this crossover from spin-coherent to spin-incoherent is characterized by a transfer of spectral weight. Remarkably, the photoemission spectrum of the SILL can be understood by assuming that after the spin is thermalized, the charge becomes spinless, with a shift of the Fermi momentum from \(k_F\) to \(2k_F\). In a follow-up paper \[38\], it was shown that a coupling to a spin bath can have a similar effect as temperature, but in the ground-state. We will elaborate this idea on chapter 3, where we see the SILL behavior on a \(t - J\) chain coupled to a spin bath. The “spin-incoherent” ground-state will have the same qualitative features as the SILL at finite temperature.

In Figure 1.11 (a) from \[39\] we see the PES results achieved by tDMRG showing the momentum shift and transferring of the spectral weight due to the spin-incoherent behavior. This is in a good qualitative agreement with the experiments in nanowires \[40\] (shown in Figure 1.11 (c)).
In the next few chapters we formalize this conjecture into a unified theory that describes the spin-incoherent ground-state for a variety of model Hamiltonians, such as the $t - J - Kondo$ chain and $t - J$ ladders [41]. The main ingredient for the validity of this theory is to have a very flat spinon dispersion, which corresponds to the limit in which spin and charge completely decouple from each other, as it can be seen from the Bethe ansatz solution. This formalism is exact in this limit, and provides a new theoretical framework to understand spin-incoherent physics, including the structure of the Kondo lattice ground-state and entanglement.

1.6 Electron-phonon interactions and The Holstein model

Electron-phonon (el-ph) interaction in metallic systems has been studied for many years but still some of the fundamental problems remain with no answer. It is an important mechanism that determines ground-state properties in a solid by renormalizing the mass of the charge carrier and in some cases explains superconductivity and charge density waves [42, 43]. In the presence of electron-electron (el-el) interactions the physics is even more complex. There are many examples of systems where el-el as well as el-ph interactions are present and important. For instance, in alkali metal doped compounds, high critical superconducting temperatures have been observed [44, 45] and are known to have strong el-ph and el-el interactions. The relevance of these interactions has been supported by other observations such as inelastic scattering [46] and high-resolution angle resolved photoemission spectroscopy (ARPES) experiments [47, 48]. Also ARPES experiments indicate strong el-ph coupling in the cuprate high-temperature superconductors [13]. There is a clear need of theoretical techniques to tackle these problems in the strong-coupling regime.

One interesting question that arises naturally in this context whether phonons will have any effect on the spin-charge separation phenomenon. The dynamical vibration of the
lattice degrees of freedom is unavoidable in low dimensional solids and can give new interesting effects that cannot be explained with a frozen lattice. One can see a phonon as a quantum harmonic oscillator that interacts with the electronic density fluctuations on a given lattice orbital. These density fluctuations give rise to a local lattice deformation that can attract the electron while it is hopping through the lattice. If the phonon frequency is large compared to the electronic bandwidth, the electron can absorb and emit phonons while moving through the lattice, carrying almost instantaneously the deformation of the lattice with itself and eventually slowing its motion. In the case of small electronic correlations, this new quasi-particle (carrying the same quantum number as the original electron) is called polaron. In the chapter 5 of this thesis, we will investigate the physics of these quasi-particles in the presence of spin-charge separation.

In this section, we will first briefly introduce the Hamiltonian for the Holstein model which will be followed by the Hubbard-Holstein Hamiltonian.

1.6.1 Holstein Hamiltonian in 1D

Here we will discuss the Hamiltonian for the Holstein model that describes electrons moving almost freely on a one-dimensional lattice without interacting with each other, lattice vibrations (phonons), and the interactions between electrons and the lattice (el-ph interactions). The Holstein model describes Einstein phonons locally coupled to free electrons and in the second quantization language the form of the Hamiltonian reads

$$H = -t \sum_{i,\sigma} (c_{i, \sigma}^\dagger c_{i+1, \sigma} + \text{h.c.}) + \omega_0 \sum_i a_i^\dagger a_i + g \omega_0 \sum_{i,\sigma} n_{i,\sigma} (a_i + a_i^\dagger) - \mu_0 \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma},$$

where $t$ is the hopping amplitude between nearest neighbor sites, the total number of lattice sites is $L$, $\omega_0$ is the phonon frequency, $g$ is the el-ph coupling constant, $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) is the standard electron creation (annihilation) operator on site $i$ with spin $\sigma = \uparrow, \downarrow$, $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ is the electronic occupation operator, and $a_i^\dagger$ ($a_i$) is the phonon creation
(annihilation) operator. The Planck constant is set to $\hbar = 1$, the lattice parameter $a = 1$, and all of the energies are in units of the hopping $t$.

Analysis of Holstein ground states was accomplished decades ago\cite{49}, however, without taking into account the repulsive Coulomb interactions. In the next section we will add the el-el interaction to the Hamiltonian.

### 1.6.2 The 1D Hubbard-Holstein model

Seeing the weakly connected spinon and holon branches for TTF-TCNQ (as shown in Figure 1.10) and comparing the ARPES experiment with the results coming from the numerical calculation considering the phonon effect in the Hamiltonian (Hubbard-Holstein)\cite{50}, Ning et al. conclude in their paper that the ARPES results are not very well explained with the Hubbard model as a stand alone model, but el-ph interactions should be included in order to get a better understanding of the physics of the system.

Several other experiments performed using the ARPES technique\cite{51, 52} as well as resonant inelastic x-ray scattering (RIXS\footnote{For a clear review on RIXS we refer the reader to Ref.\cite{53}})\cite{54} show a clear image of phonon effects on the band structure. For instance, the ARPES experiment shown in Figure 1.12\cite{51} on the material $\text{Bi}_2\text{Sr}_2\text{Ca}_{0.92}\text{Y}_{0.08}\text{Cu}_2\text{O}_{8+\delta}$ (Bi-2212) presents the observation of some kinks at low binding energies. This has been observed in other types of cuprates as well and we believe these kinks are a consequence of el-ph coupling existing in these materials. In Chapter 5 we consider a similar problem by means of tDMRG and Ogata-Shiba’s factorized wave-function and extend it to strong el-ph coupling where these kinks turn into replicas.

As a straightforward generalization of the Holstein model one can include el-el interaction (Hubbard) which will result in the so-called Hubbard-Holstein (HH) Hamiltonian. In 1D
Figure 1.12: Calculated (upper panels) and measured (lower panels) ARPES spectra for Bi$_2$Sr$_2$Ca$_{0.92}$Y$_{0.08}$Cu$_2$O$_{8+\delta}$ (Bi-2212) in the normal (a1,b1,c1 — a3,b3,c3) and superconducting (a2,b2,c2 — a4,b4,c4) states. The red bar is indicating the Fermi level $k_F$. From Devereaux et al., 2004.

It can be written as

$$H = -t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c.) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \omega_0 \sum_i a_i^\dagger a_i + g \omega_0 \sum_{i,\sigma} n_{i\sigma} (a_i + a_i^\dagger), \quad (1.11)$$

where $U$ is the on-site Coulomb repulsion and other parameters and operators are the same as the ones defined in Eq. 1.10.

It is well known that the HH model is extremely complicated and impossible to solve analytically. Its phase diagram and ground-state static properties[55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66] have been thoroughly studied in the literature, using different numerical techniques, including DMRG [67, 68, 69]. The main difficulty consists of handling the phononic degrees of freedom, that need to be described in principle by an infinite-dimensional Hilbert space at every lattice site. Different truncation schemes for the phononic Hilbert space have been proposed, including the possibility of using optimal phonon bases[70, 71, 72]. Still, solving the problem numerically remains remarkably time consuming, especially for the calculation of the dynamical properties such as the spectral function. We remark that a semiclassical treatment of the lattice degrees of freedom has been recently adopted for the study of spectral and transport properties of organic semiconductors [73, 74] and the transport properties of suspended carbon nanotubes[75, 76].
This model is one of the simplest to incorporate both el-el and el-ph interactions. By varying the parameters several different phases will result, which will also depend on the spatial dimensionality.

For the case of half filling and in 1D, the Holstein el-ph coupling \( g \) promotes on-site pairs of electrons and a Peierls charge-density wave, while the Hubbard on-site Coulomb repulsion \( U \) promotes antiferromagnetic (AFM) correlations and a Mott insulating state [55]. Numerical studies have found a possible third intermediate metallic phase between Peierls and Mott states [77].

As showed in Figure 1.13 taken from Ref.[55], these three phases compete with each other.

**Figure 1.13:** Phase diagram of the half-filling Hubbard-Holstein model with \( \omega = 0.5 \), \( \omega = 1 \), and \( \omega = 5 \). The three phases shown are Mott, (I)ntermediate, and Peierls. The Mott/I and I/Peierls boundaries merge into a single first-order Mott/Peierls boundary indicated by a solid line for \( U \gtrsim 4 \) for \( \omega = 0.5 \) and \( U \gtrsim 5 \) for \( \omega = 1 \). This calculation has been done by the stochastic series expansion quantum Monte Carlo (SSE-QMC) method. From Hardikar et al., 2007.
in the presence of $U$ and $g$. Peierls state has both charge and spin gaps. For Holstein phonons that couple to the local charge, the local charge density is modulated in a charge density wave (CDW) ground state. Also, the Hubbard on-site interaction term in 1D has a well-known effect; the ground state is a Mott insulator for a positive $U$ at half filling, with short ranged AFM spin correlations. At half filling CDW and AFM cannot coexist together so they are competing phases.
Chapter 2

Numerical techniques

2.1 Exact diagonalization method

One can calculate the eigenenergies and eigenstates of the full Hamiltonian matrix of a finite-size quantum system by numerical tools such as exact diagonalization. For instance considering the Hubbard Hamiltonian (1.4), it is transferable into a matrix form for a finite system size that can be solved in order to find the energies and eigenfunctions. The Hilbert space and as a result the corresponding matrix grows exponentially with the system size \( L \) and specifically for this model as \( 4^L \), since there exist four possible states for each given site. Without applying any symmetries one can achieve numerical results up to maximum systems sizes around \( L = 16 \) (depending on the electronic density) by current technology. Each site can be in one of the four possible states

- \( |0\rangle \) no electron on site \( i \),
- \( c_{i\uparrow}^\dagger |0\rangle \) one \( \uparrow \)-electron on site \( i \),
- \( c_{i\downarrow}^\dagger |0\rangle \) one \( \downarrow \)-electron on site \( i \),
- \( c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger |0\rangle \) two electrons on site \( i \).
Table 2.1: Basis states for a Hubbard model with $L = 4$, $\uparrow$-spin= 2 and $\downarrow$-spin= 1.

<table>
<thead>
<tr>
<th>i</th>
<th>$\uparrow$-spin</th>
<th>j</th>
<th>$\downarrow$-spin</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0011$\uparrow$</td>
<td>0</td>
<td>0001$\downarrow$</td>
</tr>
<tr>
<td>1</td>
<td>0101$\uparrow$</td>
<td>1</td>
<td>0010$\downarrow$</td>
</tr>
<tr>
<td>2</td>
<td>0110$\uparrow$</td>
<td>2</td>
<td>0100$\downarrow$</td>
</tr>
<tr>
<td>3</td>
<td>1001$\uparrow$</td>
<td>3</td>
<td>1000$\downarrow$</td>
</tr>
<tr>
<td>4</td>
<td>1010$\uparrow$</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1100$\uparrow$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The basis is constructed by specifying the configuration of each orbital of the system. One can then construct the Hamiltonian matrix by applying $H$ on every state to get all the matrix elements.

$$ H_{\alpha,\beta} = \langle \alpha | H | \beta \rangle. $$

The Hubbard Hamiltonian has two contributions: the on-site interaction which is diagonal, and an off-diagonal hopping. In order to illustrate with an example let us consider a given arbitrary state $|\psi\rangle$ on a lattice with $L = 4$ sites and $N = 3$ particles

$$ |\psi\rangle = |\uparrow 2 0 0\rangle = c_{3\uparrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle, $$

In which $|0\rangle$ represents the vacuum. We can also represent this state by two up and down states in a bit representation as

$$ |\uparrow 2 0 0\rangle = |\uparrow \uparrow 0 0\rangle \times |0 \downarrow 0 0\rangle = |1100\rangle_{\uparrow} \times |0100\rangle_{\downarrow}, $$

where the first integer represents $\uparrow$-spins and the second one $\downarrow$-spins.

In order to build the other states we need to consider all of the possible four-bit integers with two bits set to 1 and one bit set to 1 for $\uparrow$ and $\downarrow$ spins respectively. We can label these states according to Table 2.1 and show each set of states with a pair of indices $(i, j)$, or just simply show them by one mixed overall index $n = 4i + j$, where 4 is coming from the fact that there are only 4 states for spin $\downarrow$. 
Minus signs are possible when hopping over the boundaries while working with periodic boundary conditions. Basically anytime an electron goes around the boundary and the number of electrons the operator passes through is odd, a minus sign is added to the given state. Here is how different terms of Hamiltonian (1.4) act on the aforementioned $|\psi\rangle$

$\uparrow$-hopping: $-t\sum_i (c_{i+1\uparrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i-1\uparrow}) |1100\rangle_{\uparrow} \times |0100\rangle_{\downarrow} = -t (|1010\rangle_{\uparrow} - |0101\rangle_{\uparrow}) \times |0100\rangle_{\downarrow}$, 

$\downarrow$-hopping: $-t\sum_i (c_{i+1\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i-1\downarrow}) |1100\rangle_{\uparrow} \times |0100\rangle_{\downarrow} = -t \left( |1100\rangle_{\uparrow} \times (|1000\rangle_{\downarrow} + |0010\rangle_{\downarrow}) \right)$,

U-term(diagonal): $U \sum_i n_{i\uparrow} n_{i\downarrow} |1100\rangle_{\uparrow} \times |0100\rangle_{\downarrow} = U |1100\rangle_{\uparrow} \times |0100\rangle_{\downarrow}$.

Using the combined index $|n\rangle$ one can rewrite these terms in a more compact way

$\uparrow$-hopping: $-t\sum_i (c_{i+1\uparrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i-1\uparrow}) |22\rangle = -t(|18\rangle - |6\rangle)$, 

$\downarrow$-hopping: $-t\sum_i (c_{i+1\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i-1\downarrow}) |22\rangle = -t(|23\rangle + |21\rangle)$,

U-term(diagonal): $U \sum_i n_{i\uparrow} n_{i\downarrow} |22\rangle = U |22\rangle$.

Acting the full Hubbard Hamiltonian (1.4) on our sample state, $|22\rangle$, gives

$$H_{Hubbard} |22\rangle = -t(|18\rangle - |6\rangle + |23\rangle + |21\rangle) + U |22\rangle.$$ 

Having calculated all the matrix elements, we end up with a $24 \times 24$ matrix for $L = 4$, $\uparrow$-spin= 2 and $\downarrow$-spin= 1. For this specific example we have fixed the number of up and down electrons, resulting in a much smaller matrix. Not using this conservation, the total number of basis states becomes much larger, equal to $4^L = 256$ leaving a much larger matrix to deal with ($256 \times 256$).

The brute force approach to this problem, without using any symmetry, would be to solve (diagonalize) a $4^L \times 4^L$ matrix which is certainly not the most efficient method for doing it. Just by applying the particle symmetry one can convert this matrix into smaller ones
which will optimize the problem since compact matrices get solved faster and require less computer memory. If one is still interested to solve the big matrix for all of the particle numbers, considering this symmetry will result in having a Hamiltonian matrix with a block structure in which each block can be done individually. Having this block structure helps us to increase the system size, as well as the possibility of parallelizing the problem which was not a trivial task for the large matrix with no symmetries.

One should mention that one can use additional symmetries to reduce the problem into even smaller matrices with well defined quantum numbers, such as translations (using linear momentum), rotations, and reflections [78].

2.1.1 The Lanczos method

The main idea of the Lanczos (Lanczos 1950; Pettifor and Weaire, 1985) method is that a special set of bases can be constructed to represent the Hamiltonian as a tridiagonal matrix. This is an iterative method and the big advantage in using it is that one can get to very accurate answers by only a few iterations (∼ 100) which computationally, and specially compared to the method described above, is very efficient. But with this technique only the energy, wave-function of the ground-state and a few excited states are achievable, making it a very affordable and productive tool for the low-energy physics problems.

For a start one needs to pick a random state \( |\phi_0\rangle \) that lies within the Hilbert space of the problem being studied. The only constraint is that this \( |\phi_0\rangle \) not be orthogonal to the ground-state \( |\psi_0\rangle \). Having any information about the ground-state of the system helps us to choose a smart initial (random) state so that an accelerated convergence is guaranteed and a meaningful result is obtained in the end. We obtain a second state by applying the Hamiltonian \( H \) on \( |\phi_0\rangle \) and making sure the new state stays orthogonal to the initial
state $|\phi_0\rangle$ (Gram-Schmidt orthogonalization)

$$|\phi_1\rangle = H|\phi_0\rangle - \frac{\langle \phi_0 | H | \phi_0 \rangle}{\langle \phi_0 | \phi_0 \rangle} |\phi_0\rangle.$$  \hspace{1cm} (2.1)

This automatically satisfies the orthogonality condition $\langle \phi_0 | \phi_1 \rangle = 0$. From here on we continue constructing states iteratively by having the two previous ones, on each step we make sure that these states stay orthogonal all together. For the third state we end up with

$$|\phi_2\rangle = H|\phi_1\rangle - \frac{\langle \phi_1 | H | \phi_1 \rangle}{\langle \phi_1 | \phi_1 \rangle} |\phi_1\rangle - \frac{\langle \phi_1 | \phi_1 \rangle}{\langle \phi_0 | \phi_0 \rangle} |\phi_0\rangle.$$  \hspace{1cm} (2.2)

The generalization of the approach for making these orthogonal states would be

$$|\phi_{n+1}\rangle = H|\phi_n\rangle - a_n|\phi_n\rangle - b_n^2|\phi_{n-1}\rangle,$$  \hspace{1cm} (2.3)

where $n = 0, 1, 2, \ldots$ and the coefficients $a_n$ and $b_n^2$ are given by

$$a_n = \frac{\langle \phi_n | H | \phi_n \rangle}{\langle \phi_n | \phi_n \rangle}, \quad b_n^2 = \frac{\langle \phi_n | \phi_n \rangle}{\langle \phi_{n-1} | \phi_{n-1} \rangle},$$  \hspace{1cm} (2.4)

with the initial conditions of $b_0 = 0$ and $|\phi_{-1}\rangle = 0$.

In our new basis the Hamiltonian matrix becomes a tridiagonal matrix

$$H = \begin{pmatrix}
a_0 & b_1 & 0 & 0 & \cdots \\
b_1 & a_1 & b_2 & 0 & \cdots \\
0 & b_2 & a_2 & b_3 & \cdots \\
0 & 0 & b_3 & a_3 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}.$$  \hspace{1cm} (2.5)

The matrix in this tridiagonal form can be diagonalized using standard routines very easily. Details of this is not a goal of this work and we refer the reader to Ref. [78]. As mentioned above the size of this matrix is a function of the accuracy needed for the
solution. We may keep this relatively small and still get a suitable outcome that describes the physics.

### 2.2 Density Matrix Renormalization Group Method

The Density Matrix Renormalization Group (DMRG) is one of the most accurate and efficient numerical methods to describe the low-energy physics of strongly correlated systems. DMRG is a variational technique for precisely estimating the ground state and the first low-lying excited states of strongly interacting low-dimensional quantum lattice systems, such as the Hubbard and Heisenberg models. The formalism was invented by Steve White [21, 79] in 1992 as a development of Wilson’s Numerical Renormalization Group, NRG [80].

As we have previously seen, the size of the Hilbert space of quantum many-body systems grows exponentially with the size of the system. Just as in exact diagonalization techniques, the DMRG targets one specific state, mainly the ground-state of the system or one of the first excited states, and minimizes the number of effective degrees of freedom or basis states needed to represent it. The method has full control over the accuracy and can provide results that are essentially exact, also referred to as quasi-exact. It is able to treat very large systems in order of hundreds of sites and give a very precise description of the ground-state, first excited-states and gaps in low dimensional systems.

#### 2.2.1 Ground-state algorithm

Let us split our 1D lattice consisting of $L$ sites into two parts $A$ and $B$ with the length $L_A$ and $L_B$ respectively. Hamiltonian $H_S$ describes a single site; let $d$ be the number of possible configurations on any site. Ignoring symmetries, the size of the Hilbert space for each of the subsystems becomes $d_A = d^{L_A}$ and $d_B = d^{L_B}$. The basis set of Hilbert space is given by $\{|i\rangle_A\}$ with $d_A$ members for sublattice $A$ and $\{|i\rangle_B\}$ with $d_B$ members.
for sublattice $B$. A decomposition of a given quantum wave-function $|\psi\rangle$ is given by

$$|\psi\rangle = \sum_i \sum_j \psi_{i,j} (|i\rangle_A \otimes |j\rangle_B).$$  \hfill (2.6)$$

This matrix $\psi_{i,j}$ contains all the information about the state $\psi$. It is possible to reduce the number of coefficients in this wave-function by recognizing that $\psi$ is actually a matrix, and taking advantage of a well studied problem in machine learning –so-called matrix rank-reduction. Using a singular value decomposition we get

$$\psi_{i,j} = USV^\dagger,$$  \hfill (2.7)$$

where $U$ is a column unitary and $V^\dagger$ a row unitary matrix. $S$ is a diagonal matrix, where its diagonal elements are placed in a descending order; these values for $S$ are real and positive: $s_1 \geq s_2 \geq \cdots \geq s_r > 0$, $r$ being the rank of $s$. Replacing this in Eq. 2.6 one gets

$$|\psi\rangle = \sum_i \sum_j \sum_\alpha U_{i,\alpha} s_\alpha V^*_{\alpha j} (|i\rangle_A \otimes |j\rangle_B)$$

$$\equiv \sum_\alpha s_\alpha (|\alpha\rangle_A \otimes |\alpha\rangle_B).$$  \hfill (2.8)$$

This final step is known as the “Schmidt decomposition” of the state and the bases $|\alpha\rangle_A$ and $|\alpha\rangle_B$ as “Schmidt bases”. Here we have defined $|\alpha\rangle_A$ and $|\alpha\rangle_B$ as

$$|\alpha\rangle_A \equiv \sum_i U_{i,\alpha} |i\rangle_A,$$

$$|\alpha\rangle_B \equiv \sum_j V^*_{\alpha j} |j\rangle_B.$$
DMRG truncates the basis by keeping the $m$ largest singular values and throwing away the rest of them. The number of DMRG states is determined by the value of $m$.

$$|\psi^m\rangle = \sum_\alpha s_\alpha (|\alpha\rangle_A \otimes |\alpha\rangle_B),$$  

(2.9)

This new state is not exact anymore (for $m < r$). The variation of $|\psi_m\rangle$ from the original state is given by

$$\delta_\rho \equiv ||\psi\rangle - |\psi^m\rangle||^2 = \sum_{\alpha=m+1}^r s_\alpha (|\alpha\rangle_A \otimes |\alpha\rangle_B) = \sum_{\alpha=m+1}^r s_\alpha^2 = 1 - \sum_\alpha s_\alpha^2.$$  

(2.10)

By changing the number of states kept ($m$) we have control over the accuracy, where one can optimize it by its computation cost, which is a well-known problem called the “low rank approximation”.

We will now move this into a density matrix picture

$$\rho^m = |\psi^m\rangle \langle \psi^m| = \sum_\alpha \sum_\beta s_\alpha s_\beta (|\alpha\rangle_A \otimes |\alpha\rangle_B) (A\langle \beta| \otimes_B \langle \beta|),$$  

(2.11)
resulting in two reduced density matrices that share the spectrum

\[
\rho_A^m = Tr_B \rho^m = \sum_\alpha s_\alpha^2 \langle \alpha | A \langle \alpha |,
\]

(2.12)

\[
\rho_B^m = Tr_A \rho^m = \sum_\beta s_\beta^2 \langle \beta | B \langle \beta |.
\]

(2.13)

Minimizing the Frobenius distance (Eq. 2.10) between the two matrices for a fixed \( m \) is obtained if the optimal basis is given by the eigenvectors of the reduced density matrix with the \( m \) largest eigenvalues.

A DMRG algorithm works by adding sites to a lattice and applying the density matrix truncation when the basis size grows larger than \( m \). This process is called the infinite-size DMRG algorithm (shown in Figure 2.1). After obtaining the new blocks from the previous step, a new site is added to each one of the two blocks, then the ground-state and reduced density matrix of this super-block is calculated, in stage (d) a rotation of the basis of the eigenvectors with \( m \) largest eigenvalues is done to build the new blocks for the next step.

![Figure 2.2: Schematic illustration of the finite-size DMRG algorithm. From Feiguin, 2011.](image)
Once the desired system size is reached, one can iteratively optimize the basis by sweeping from left to right, and right to left, as shown in Figure 2.2. As mentioned above and shown in Figure 2.2, during the sweeping iterations one block grows, and the other one “shrinks”. The shrinking block is retrieved from the blocks obtained in the previous sweep in the opposite direction, which are stored in memory. A complete review of DMRG can be found at Ref. [22]

2.2.2  Adaptive time-dependent DMRG

In this section a brief review of the time-dependent DMRG (tDMRG) method is given. We refer the reader to Refs. [22, 81, 82] for details. The tDMRG method is a generalization of the DMRG to solve the time-dependent Schrödinger equation

\[ i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle, \tag{2.14} \]

with a formal solution

\[ |\psi(t)\rangle = e^{-itH} |\psi(0)\rangle, \tag{2.15} \]

where \( e^{-itH} \) is the time-evolution operator and \( |\psi(0)\rangle \) is the state of the system at \( t = 0 \).

Assuming all the eigenenergies and eigenstates of the system are known one can write any wave-function in the natural bases as

\[ |\psi(0)\rangle = \sum_n A_n |n\rangle, \tag{2.16} \]

where \( A_n \) is the appropriate coefficient for the eigenstate \( |n\rangle \). Applying the time-evolution operator gives

\[ |\psi(t)\rangle = \sum_n A_n e^{-itE_n} |n\rangle. \tag{2.17} \]

If we had the complete solution to the full Hamiltonian (by ED, for instance) our work is done right here. The problem rises in situations where we are dealing with larger
systems, and we cannot solve the entire Hamiltonian. In that case we need to use the DMRG instead. In DMRG, matrix product states (MPS) are used to approximate the time evolving state. We are also working in a truncated space where all the Hilbert space is not reachable. The time evolution of the wave-function $|\psi\rangle$ might explore some regions of the Hilbert space that have been truncated in the previous steps of the DMRG. We now need to adapt our basis at every new time step.

The execution of the algorithm is very straightforward if we are already using a ground-state DMRG code that implements the ground-state prediction. Initially the ground-state of the Hamiltonian is calculated. A perturbation is applied to the calculated state: for instance by changing a parameter in the Hamiltonian or adding extra terms. Another possibility is to alter the state by applying an operator on it. Next, the diagonalization is turned off, and we start the sweeping process by applying the bond evolution operator ($U_{i,j} = e^{-i H_x \delta t}$, where $H_x$ includes only the interaction terms acting on site $x$ and $x + 1$ and $\delta t$ is our imaginary time) on the single sites as shown in Figure 2.3, where we can see a half-sweep. On each taken step we add one site to the growing block (left here) and apply the truncation, similar to the ground-state DMRG. After one sweep is completed,
we repeat it a few more times (varies according to the decomposition we are using) and then we do a final sweep without evolving in time to do the measurements. The initial state and the perturbation applied will depend on the problem of interest. Details and a complete picture of the method are described in depth in Ref. [22].
Chapter 3

Class of variational ansätze for the spin-incoherent ground state of a Luttinger Liquid coupled to a spin bath

At finite temperatures, 1D systems undergo a crossover to a regime known as “spin-incoherent Luttinger liquid” (SILL) [31, 32, 33, 34, 35, 36]. Since holons and spinons have independent energy scales, their behavior at finite temperature is quite different. If the spinon bandwidth is much smaller than the holon bandwidth, a small temperature relative to the Fermi energy may actually be felt as a very large temperature by the spins. In fact, the charge will remain very close to the charge ground-state, but the spins will become totally incoherent, effectively at infinite temperature.

This crossover from spin-coherent to spin-incoherent is characterized by a transfer of spectral weight [37]. Remarkably, the photoemission spectrum of the SILL can be understood by assuming that after the spin is thermalized, the charge becomes spinless, with a shift of the Fermi momentum from $k_F$ to $2k_F$. In a follow-up paper [38], it was shown that a
coupling to a spin bath also can have a similar effect as temperature, but in the ground-state. The “spin-incoherent” (SI) ground-state will have the same qualitative features as the SILL at finite temperature.

We formalize this conjecture into a unified theory that describes the spin-incoherent ground-state for a variety of model Hamiltonians, such as the $t - J - Kondo$ chain and $t - J$ ladders [41]. The main ingredient for the validity of this theory is to have a very flat spinon dispersion, which corresponds to the limit in which spin and charge completely decouple from each other.

As described in section 1.4 in the Hubbard $U \to \infty$ limit or equivalently $J \to 0$ for the $t - J$ model (Eqs. 1.4 and 1.5), the ground-state of these two Hamiltonians can be described by the Ogata and Shiba’s factorized wave-function (Eq. 1.8) [27], which is the product of a fermionic wave-function $|\phi\rangle$, and a spin wave-function. $|\phi\rangle$ marks out the charge degree of freedom, and is simply the ground-state of a one-dimensional tight-binding chain of $N$ non-interacting spinless fermions. The spin wave-function $|\chi\rangle$ corresponds to a “squeezed” chain of $N$ spins, where all the unoccupied sites have been removed. In this limit, the charge and the spin are governed by independent Hamiltonians. Since the spin energy scale is determined by $J$, for $J = 0$ the spin states are degenerate, and the charge dispersion becomes that of a non-interacting band $\epsilon(k) = -2t \cos(k)$. However, any finite value of $J$ will lift this degeneracy and give the spin excitations a finite bandwidth. Notice that in finite systems, the spin degree of freedom affects the charge through an effective magnetic flux [28, 29, 30].

Similar physics can take place in the ground-state, when a Luttinger Liquid is coupled to a spin bath, which effectively introduces a “spin temperature” through its entanglement with the spin degree of freedom. We show that the SI state can be exactly written as a factorized wave-function, where our numerical results for two different models each consisting of a $t - J$ chain coupled to a spin bath back up this variational ansatz. The first model we study is two antiferromagnetically coupled $t - J$ chains, and next a $t - J - Kondo$ chain with strongly interacting conduction electrons. We also argue that this theory
is quite universal and may describe a family of problems that could be dubbed spin-incoherent.

In order to show that the spin incoherent regime at infinite spin temperature can be described exactly using a pure state we start by establishing an analogy between (i) a thermal mixed state and (ii) a pure state in an enlarged Hilbert space. This is the key idea behind the so-called thermofield formalism [83]. Assuming the dimension of Hilbert space is \( d \), we need \( d \times d \) elements to define an operator \( A \) (where \( A = \sum_{i,j} A_{i,j} |i\rangle \langle j| \)).

Now we define an “ancillary” space, which is a duplicate of our Hilbert space

\[ \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H} \]

For any state \( |x\rangle \) in the original Hilbert space we define a “tilde” state in the ancillary space \( (|\tilde{x}\rangle) \), which is an identical copy. Then we rewrite the operator \( A \) as a wave-function \( |\psi_A\rangle = \sum_{i,j} A_{i,j} |i,\tilde{j}\rangle \). The advantage of this formalism is that now operators are wave-functions and super-operators become conventional operators, hence we can apply all the zero-temperature many-body tools on the system with the price of working in a larger Hilbert space. We can now introduce the thermal density matrix \( \rho = \exp ( -\beta H ) \) as a pure state wave-function \( |\rho\rangle = \sum_{i,j} \rho_{i,j} |i,\tilde{j}\rangle \). This gives us the framework for our analogy: If a thermal density matrix can be represented as a pure state in an enlarged Hilbert-space, all we need to do is find a parent Hamiltonian for this state. The ground-state of such Hamiltonian will then describe a finite-temperature density matrix, at zero-temperature.

For illustration purposes, let us first assume that we have two spins \( S = 1/2 \), that we put into a maximally entangled state

\[ |I_0\rangle = \frac{1}{\sqrt{2}} \left[ |\uparrow,\tilde{\downarrow}\rangle \pm |\downarrow,\tilde{\uparrow}\rangle \right], \tag{3.1} \]

where the sign is irrelevant in the following treatment. We shall assume the first spin is our “physical” spin, while the one with a tilde is the ancilla, or impurity spin. It is straightforward to see that the reduced density matrix of the physical spin, after tracing
over the ancillary degrees of freedom, is the identity matrix. Thus, if we assume that the ancilla acts as some sort of effective thermal bath, the physical spin is at infinite temperature.

The maximally mixed state for a number of spins can be rewritten as: \( |I\rangle = \prod_i |I_{0i}\rangle \), defining the maximally entangled state \( |I_{0i}\rangle \) of spin \( i \) with its ancilla, as in Eq.(3.1). This construction allows one to represent a mixed state of a quantum system as a pure state in an enlarged Hilbert space and lies at the core of the imaginary-time DMRG [84].

Now it is easy to construct a generalization of the Ogata-Shiba wave-function to describe the system at \textit{infinite spin temperature}. All we have to do is to add spin ancillas, and replace the spin component in Eq.(1.8), by the corresponding maximally entangled state, \( |I\rangle = \prod_i |I_{0i}\rangle \), \( |\psi_{SILL}\rangle = |\phi\rangle \otimes |I\rangle \). Thus, the charge will remain at zero temperature, while the spin component will be effectively at infinite temperature! This state is describing the spin-incoherent regime.

### 3.1 Applying the factorized wave-function on different Hamiltonian models

Since the SILL regime can be described by a pure state, it is natural to wonder if there is a parent Hamiltonian for this state. Or at least, we would like to find a model whose ground-state can be associated to a thermal state at finite spin temperature. Let us assume that we antiferromagnetically couple our 1D chain to a bath of spins in the \( J = 0 \) limit. Regardless of the internal structure and dynamics of the bath, it is easy to realize that the charge will be in principle unaffected by it, while the spin degree of freedom will get entangled into a many-body state with the spins from the bath. If we trace over the bath, we expect the spins of the chain to be at an effective finite temperature, parametrized by the magnitude of the system-bath coupling (even though the entire chain plus bath are in a pure state: the ground state of the Hamiltonian). Therefore, the spins
of the chain can be driven incoherent by this interaction, while the charge remains in the ground-state. This physics is completely analogous to the SILL physics at finite temperature. In Ref.[38] it was numerically shown that this physics is indeed realized in the $t - J$–Kondo chain with strongly correlated conduction electrons, where the Kondo impurities act as an effective spin bath. Later in this work we calculate the exact ground-state of this system in this limit, and also coupled $t - J$ chains, and we show that the structure of the ground-state is quite universal, and indicates the path toward a unified formalism to describe spin-incoherent behavior at zero and finite temperatures.

### 3.1.1 Two coupled $t - J$ chains

Let us assume two chains governed by the Hamiltonian (1.5), and we take the limit $J \to 0$. In the limit in which the chains are independent, the exact ground-state will be that of two decoupled factorized wave-functions of the form (1.8):

$$ |g.s.) = |g.s.)_1 \otimes |g.s.)_2 = |\phi)_{1} \otimes |\phi)_{2} \otimes |\chi)_{1} \otimes |\chi)_{2}, \quad (3.2) $$

where the subindex $\lambda = 1, 2$ refers to the chain index. Now we introduce a small but finite antiferromagnetic interaction between the chains (as shown in Figure 3.1) of the form

$$ H' = J' \sum_{i=1}^{L} \vec{s}_{i,1} \cdot \vec{s}_{i,2}, \quad (3.3) $$

Figure 3.1: Schematic $t - J$ ladder and the model parameters. In this work we consider $J = 0$ and all energies in units of the hopping $t$. 
where $J'$ parametrizes the interaction perpendicular to the direction of the chains, along the rungs of a ladder. This is equivalent to a $t-J$ ladder without inter-chain hopping. We acknowledge that this is a very idealized scenario, since the presence of exchange always implies the existence of a hopping, since $J' \sim t'$. Still, this could be considered a model for a two band problem with a Hund coupling, as studied in Ref.[85]. One expects that this interaction will couple the spin pieces of the wave-function $|\chi\rangle_1$ and $|\chi\rangle_2$, leaving the charge unaltered:

$$|\text{g.s.}\rangle = |\phi\rangle_1 \otimes |\phi\rangle_2 \otimes |S\rangle,$$

(3.4)

where $|S\rangle$ represents the many-body state of the spins for the two coupled chains, once they become entangled by action of the Hamiltonian $H'$. It is also expected that this state $|S\rangle$ will be a singlet. However, the exact structure of this singlet is not necessarily trivial.

Without attempting to deduce the exact effective Hamiltonian for the spin sector, we shall propose a variational ansatz for the wave-function, that we later prove to be exact by numerical means. We argue that every time two spins interact on a rung via $H'$, they will become entangled forming a singlet. Since the interaction along the chain is set to $J = 0$, these spins will remain entangled as they move apart from each other by action of the hopping term even in the absence of interactions between sites $i$ and $j$.

Therefore, this entanglement persists at infinite distance. If we consider a system with periodic boundary conditions, it is expected that eventually all spins from one chain will interact with all the spins on the second chain. In a one-dimensional system, they
cannot hop past each other, but in a chain with periodic boundary conditions, they can wind around the boundaries and come from the other side. Therefore, we will have a superposition of singlets that connect all possible pairs of spins on both chains, and at all distances, with the same amplitude. In order to describe this wave-function it is useful to resort to a valence bond (VB) picture [86, 87, 88, 89]. Let us assume that each chain corresponds to a sublattice. Then, our wave-function is the equal superposition of all possible valence-bond coverings connecting the two sublattices, as shown in Figure 3.2 for the particular case of three electrons per chain.

In order to prove that our guess accurately describes the physics, we have numerically computed the overlap between the exact ground-state and the variational ansatz on small systems with periodic boundary conditions. We assume $S_{\text{Total}} = 0$ and take the number of particles on each chain ($N$) not a multiple of 2, to avoid degeneracies. We show the results in Figure 3.3(a), for different values of $J'$. The overlap is 1 within numerical precision for a range of small values of $J'$. As $J'$ increases, we observe how this overlap becomes smaller, but still remains higher than 0.9 for $J' < 0.1$. This range depends only on the number of conduction electrons $N$, and tends to get smaller as $N$ increases.

Having shown that the ansatz is a good description of the spin-incoherent regime for $J' \to 0$, we proceed to derive some straightforward exact results that can be obtained using the variational form of the wave-function. For a start, the entanglement between chains originates from the spin, and the charge does not contribute to it. One might feel inclined to think that spins are in a maximally entangled state. However, we should not forget that the VB basis is overcomplete, and in fact, the entanglement entropy is not $S = N \log 2$, as one might expect for a state with $N$ singlets. Using the exact wavefunction it is relatively easy to obtain a closed expression for $S$, as shown in the Appendix B:

$$ S = \log(N + 1). $$

Looking at this expression more closely, one realizes that this is equivalent to two spins $S = N/2$ in a maximally entangled state, instead of $N$ spins $1/2$ in a maximally entangled
Figure 3.3: Exact diagonalization results for small ladders of length $L$, and $N$ electrons per chain: (a) overlap with variational wave-function, and (b) entanglement entropy between chains, normalized by the exact value for $J' \rightarrow 0$.

In Figure 3.3(b) we show the entanglement entropy, normalized by the exact value for $J' = 0$. Just as found for the overlap, the expression holds for a range of $J'$, and $S$ increases as the charge becomes also entangled with the spin.

It is enlightening to calculate the momentum distribution function (MDF) for the fermions:

$$n(k) = (1/L) \sum_{l,\sigma} \exp(ikl) \langle c_{1,\sigma}^\dagger c_{l,\sigma} \rangle.$$  \hspace{1cm} (3.5)

In order to estimate this quantity, we follow Ref.[29] and break the fermionic operators $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ into spinless fermionic operators $f_{i}^\dagger, f_{i}$ acting on the (spinless) charge part of the wave-function, and new operators $Z_{i,\sigma}^\dagger$ and $Z_{i,\sigma}$ acting on the spin part of the wave-function. These spin operators have a very peculiar behavior: $Z_{i,\sigma}^\dagger$ inserts a spin $\sigma$ to the spin chain after skipping the first $i - 1$ spins and makes it $N + 1$ sites long, while $Z_{i,\sigma}$ has the opposite effect, shortening the chain. For instance, for the first site of the chain, we have:

$$c_{1,\sigma}^\dagger = Z_{1,\sigma} f_{1}^\dagger \quad \text{and} \quad c_{1,\sigma} = Z_{1,\sigma} f_{1}.$$  \hspace{1cm} (3.6)

The generic expression for the operators can become more complicated, since to act with the $Z$ operators on the spin chain, we need to count the number of charges on the spinless
fermion chain. We refer the reader to Refs. [29, 90, 91, 92] for details. The action of the operators $c_{1,\sigma}^\dagger c_{l,\sigma}$ is to move a fermion from site $l$ to site 1. If there are no particles in between, the spin wave-function will remain unchanged. If there is one or more particles in between, it is quite easy to realize that since the spin wave-function is the equal sum of all singlet coverings, it will also remain so after moving one of the ends of a singlet across any number of sites. Therefore, the momentum distribution function reduces to

$$n(k) = (1/L) \sum_{l,\sigma} \exp(ikl) \langle f_{1}^\dagger f_{l} \rangle,$$

which is nothing else but the MDF for spinless fermions. Since the charge wave-function is that of non-interacting particles, we find that the excitations are free spinless fermions with quasi-particle weight $z = 1$, and Fermi momentum $2k_F$. In Figure 3.7(a) we show the MDF calculated for large systems using the density matrix renormalization group (DMRG) method [21, 79], indicating that the quasi-particle weight may remain finite for a range of $J'$. We have to concede that since the calculations are on finite-systems with $L = 30$ sites and $N = 15$ electrons per chain, we cannot argue with full certainty that the discontinuity at $k = 2k_F$ is not actually a singularity, and this remains an interesting problem to pursue.

### 3.1.2 $t - J$–Kondo chains

We consider a Kondo chain in which the conduction electrons strongly interact, and are described by Hamiltonian (1.5). At the same time, the electrons are antiferromagnetically coupled to localized impurities via an exchange $J_K$:

$$H_K = J_K \sum_{i=1}^{L} \vec{s}_i \cdot \vec{S}_i,$$

where $\vec{s}_i$ describes the conduction spins and $\vec{S}_i$ the localized spins. It is easy to see that this is equivalent to the two coupled chains, in which one of them is at half-filling.
Curiously, this model has not received much attention in the literature. It has been shown that in the limit of $J \to 0$, any infinitesimal $J_K$ will yield a ferromagnetic ground-state\cite{93}, in which the localized impurities are underscreened: the $N$ conduction spins will screen $N$ impurity spins, and the remaining “unpaired” impurities will be in a ferromagnetic state with maximum spin $S_{\text{Total}} = (L - N)/2$. Notice that this means that the paramagnetic state with a large Fermi surface is totally suppressed in this regime.

This state will be a multiplet, and for convenience we focus on the configuration with projection $S_{\text{Total}}^z = S_{\text{Total}}$. Following a similar reasoning as in the previous part, we argue that the $N$ conduction electrons will form the same VB state as the one described before, while the unpaired impurities will all point in the same direction. The polarized spins can sit on any site of the lattice with equal probability. Therefore, our ansatz can be written as:

$$|\text{g.s.}\rangle = |\phi\rangle \otimes |S\rangle \otimes |\sigma\rangle,$$

(Figure 3.4).
Figure 3.6: Exact diagonalization results for small $t − J$–Kondo chains of length $L$, and $N$ conduction electrons: (a) overlap with variational wave-function, and (b) entanglement entropy between chains, normalized by the exact value for $J_K \to 0$.

where $|S\rangle$ is the VB wave-function, and $|\sigma\rangle$ indicates the positions of the unpaired polarized spins:

$$|\sigma\rangle = \sum_x |x\rangle,$$

This wave-function is the sum with equal amplitude of all the configurations $|x\rangle$ of $L − N$ particles in $L$ sites. Figure 3.6(a) shows the overlap between the exact and variational ground-states, and we again observe identical behavior as the $t − J$ ladder.

The VB basis for this problem is overcomplete, and we also have to account for the unpaired polarized spins, as shown schematically in Figure 3.5. This generalization can be easily carried out [94], and it is still straightforward to obtain a closed expression for the entropy, which is slightly different than the one for the coupled chains. We show results in Figure 3.6(b), which have strong resemblance with those for the ladder.

The calculation of the MDF is strictly the same as before and the results are identical for $J_K = J' = 0$. Notice however, that unlike the $t − J$ ladder, the MDF for up and down spins will be different, and only the sum of the two will be the same. This is shown in Figure 3.7(b), (c), and (d). In particular, there is a striking difference between the MDF for the majority up and minority down electrons. The up electrons present a clear discontinuity at the Fermi level, while the down electrons display the behavior of a Luttinger liquid with zero quasi-particle weight. The sum of the two, shown in Figure 3.7(b) of course
Figure 3.7: Momentum distribution function for (a) coupled $t - J$ chains as a function of the inter-chain coupling $J'$, and (b),(c),(d) the Kondo lattice, as a function of the Kondo coupling $J_K$. The two lower panels show the results for different spin orientations. Calculations were done with DMRG for a system of size $L = 30$ and $N = 15$ conduction electrons, and periodic boundary conditions.

hides these interesting features. This resembles the behavior of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) polarized paired state in one dimension[95, 96, 97, 98, 99, 100, 101]. However, the physics of our problem is quite different, since only the spin entangles, and not the charge. We would rather call this state a “half-Fermi-liquid”, or “half-Luttinger-liquid”. Whether these are finite-size artifacts or not, undoubtedly, it is a problem that requires further study. We point out again that the shift to a larger momentum in the MDF should not be confused with a large Fermi surface, that is a feature of the paramagnetic phase of the Kondo lattice.

### 3.2 Conclusions

In this chapter we presented a ground-state ansatz for antiferromagnetically coupled $t - J$ chains, and the $t - J$–Kondo chain that is numerically exact in the limit of $J = 0$ (corresponding to infinite–$U$ Hubbard chains), and coupling to the bath $J', J_K \to 0$, as
tested on small systems. Our DMRG results indicate that the variational wave-functions describe the physics of the problem in a range of $J'$ and $J_K$. In this regime, the charge and the spin can be considered to a good extent as separate degrees of freedom with independent dynamics: the charge can be described as non-interacting spinless fermions in the ground-state, while the spin is entangled into a VB-like state where all valence bond coverings have the same weight. The inter-chain coupling $J'$ and the Kondo interaction $J_K$ parametrize an effective spin temperature. If we trace over the bath, the spins of an isolated chain will be in equilibrium at a certain “quasi-spin temperature”. This spin temperature is not infinite, since we have proven that the spin is not maximally entangled. However, this state seems to correspond to a fine-tuned point in which excitations can be described as free spinless fermions.

The introduced wave-functions establish a framework to study spin-incoherent behavior in systems with spin-charge separation. Normally considered a finite-temperature scenario, this physics can also be realized at zero temperature, once the system is coupled to external spin degrees of freedom. It is not restricted to the models used in this work for illustration, but the theory can be easily extended and generalized to other cases, such as an arbitrary number of coupled $t - J$ chains, for instance [19, 102].

We point out that even though our study applies to systems with periodic boundary conditions, the same ideas apply to problems with open boundary conditions. In that case, we expect the VB wave-function to be quite different, with only the first kind of configurations shown in Figure 3.2 carrying most of the weight, and a consequent entanglement entropy $S = N \log 2$ corresponding to infinite effective spin temperature [38].

Contrary to other problems studied with VB-type variational wave-functions [103], the accuracy of our ansatz seems to depend primarily on the number of particles $N$, and not the size of the chains $L$, which may suggest that our description will still be valid for large systems, as long as the density is sufficiently small. Yet, our DMRG results a
quarter-filling still display the same physics. In any case, one has to keep in mind that our considerations are strictly valid in the limit $J', J_K \to 0$. 
Chapter 4

Spectral function of the $U \to \infty$ one-dimensional Hubbard model at finite temperature and the crossover to the spin-incoherent regime

As seen above, the factorized wave-function contains already all the ingredients to qualitatively, and even quantitatively, understand the phenomenon of spin-charge separation. This phenomenon is an important problem in strongly correlated systems, and has intrigued physicists for decades. Even though these concepts are well established, we keep finding new surprises in unexplored parameter ranges that escaped previous scrutiny. Recently, a previously overlooked regime at finite temperature has come to light: the “spin-incoherent Luttinger liquid” (SILL) [31, 32, 33, 34, 35, 36, 104]. If the spinon bandwidth is much smaller than the holon bandwidth, a small temperature relative to the Fermi energy may actually be felt as a very large temperature by the spins. In fact, the charge will remain very close to the charge ground-state, but the spins will become totally incoherent, effectively at infinite temperature. This regime is characterized by universal properties in the transport, tunneling density of states, and the spectral functions [35].
We are particularly interested in the effects of temperature on the spectral function of the Hubbard model in the large $U$ limit. In this limit, the spinon band is non-dispersive, and an infinitesimally small temperature will drive them effectively incoherent, leading to the SILL paradigm.

This crossover from spin-coherent to spin-incoherent is characterized by a transfer of spectral weight. Remarkably, the photoemission spectrum of the SILL can be understood by assuming that after the spin is thermalized, the charge becomes spinless, with a shift of the Fermi momentum from $k_F$ to $2k_F$ [38]. Clearly, this behavior defies our intuition, since the excitation spectrum of the problem is completely determined by the Hamiltonian, at finite temperature (and in the absence of phase transitions) we only expect a redistribution of spectral weight. This paradox can be reconciled in the context of spin-charge separation. If we assume that spin and charge degrees of freedom are completely decoupled, the single-particle spectral function of the electrons can be understood as the convolution of the charge and spin dynamical correlation functions.

In this chapter, we use Ogata and Shiba’s factorized wave-function [27], complemented by tDMRG calculations at finite spin temperature, to obtain the spectral function of strongly interacting Hubbard chains ($U \rightarrow \infty$) in the crossover between spin-coherent and spin-incoherent regimes.

4.1 Spectral functions with Ogata-Shiba’s formalism

In a lot of scenarios containing spin-charge separation, one can take advantage of the wave-function factorization for finding the ground-state, excited states, and spectral functions. In order to calculate the spectral functions of the Hamiltonian (1.4), we follow the formalism developed in Refs.[29, 90, 91, 92, 105, 106, 107], described in great detail in Ref.[29]. We sketch the main ideas, avoiding technicalities and directing the reader to the aforementioned references. Let us focus on an antiferromagnetic Hubbard chain with $U \rightarrow \infty$ for the time being. The Ogata-Shiba factorization originates from the exact
solution of the 1D Hubbard model in this limit. Since in most of this work we use this solution for finite $U$ as well, it should be considered as a (very good!) approximation, or a variational approach. In other parts of this work, we will introduce generalizations of this idea for other model Hamiltonians. As obtained with the Bethe ansatz and mentioned in the previous chapter Ogata and Shiba demonstrated that the exact solution of the ground-state can be factorized and split into two parts

$$|\psi_{L,GS}^{N}\rangle = |\phi\rangle \otimes |\chi\rangle,$$

(4.1)

where $|\phi\rangle$ describes the charge and is comprised by spinless fermionic degrees of freedom, and $|\chi\rangle$ is consistent with a “squeezed” chain of $N$ spins, where all the empty sites have been removed. $|\phi\rangle$ is simply the ground-state of a one-dimensional tight-binding chain of $N$ non-interacting spinless fermions on a lattice with $L$ sites. The factorization applies also to excited states as

$$|\psi(P)\rangle = |\phi_{L,Q}^{N}(I)\rangle \otimes |\chi_{N}^{N}(Q, M)\rangle,$$

(4.2)

where $I$ labels a combination of $N$ wave-vectors $k_{i}L = 2\pi i + Q$, with $i = -L/2, -L/2 + 1, \cdots, L/2 - 1$, that are compatible with the total fermionic momentum $P$. The index $M$ labels all possible configurations of momenta compatible with the total momentum of the spin wave-function $Q = 2\pi j/N$, with $j = 0, 1, \cdots, N - 1$. The fermionic part stays coupled to the spin part only by a phase $Q$ introduced at the boundaries, resulting in twisted boundary conditions for the fermions, which ensures momentum conservation for the original problem. This phase is $Q = \pi$ for the ground-state $|\psi_{L,GS}^{N}\rangle$, and we would fill up the Fermi sea by minimizing the energy with the combination of momenta \{-N/2, -N/2 + 1, ..., N/2 - 1\} [92].

The dynamics of the spinless fermions are governed by a tight-binding Hamiltonian, with an energy dispersion $\epsilon(k) = -2t \cos(k)$, while the spin degrees of freedom are in principle non-interacting. For finite but large $U \gg t$, the physics of the spins can be approximated
by that of a Heisenberg spin chain, with $J = 4nt^2[1 - \sin(2\pi n)/(2\pi n)]/U$, where $n = N/L$ is the density $[29, 108]$. 

In order to calculate the Green’s function for the electrons, we start by noticing that destroying an electron in the original Hubbard chain would translate into the annihilation of a fermion in the charge wave-function, and a spin in the spin chain (and the opposite effect for the creation operator). As discussed above one can write down any state of the system in this strong coupling regime by introducing the decoupled spin and charge wave-functions. Having the spin fluctuations separated from the spinless fermionic (charge) ones, enables one to break down the operators $c_{i,\sigma}^\dagger$ and $c_{i,\sigma}$ into spinless fermionic operators $f_{i}^\dagger$, $f_{i}$ acting on the (spinless) charge part of the wave-function, and the new operators $Z_{l(i),\sigma}^\dagger$ and $Z_{l(i),\sigma}$ acting on the spin part of it. This is achieved by introducing new operators such that

$$c_{i,\sigma} = f_{i}Z_{l(i),\sigma}, \quad (4.3)$$

where $f_{i}$ is a fermionic annihilation operator without spin, acting at position $i$ on the fermionic wave-function, and $Z_{l(i),\sigma}$ removes a spin $\sigma$ at position $l(i)$ from the spin chain. The operator $Z$ has a peculiar behavior, since it destroys the spin and the site itself, making the spin chain $N - 1$ sites long. The index function $l(i)$ indicates the position of the spin that belongs to site $i$ of the original chain, after squeezing the wave-function and removing all the holes.

The generic expression for the operators can become more complicated, since to act with the $Z$ operators on the spin chain, we need to count the number of charges on the spinless fermion chain. We refer the reader to Refs.$[29, 90, 91, 92]$ for more details. The action of the operators $c_{l,\sigma}^\dagger c_{l,\sigma}$ is to move a fermion from site $l$ to site 1.

The zero-temperature one-particle spectral function is obtained from the imaginary part of the Green’s function. We focus only on the contribution from the occupied levels, corresponding to the photoemission spectrum. In order to do this we start from the Green’s function

$$G(t) = -i\langle T_t \, c(t)c^+(0) \rangle \quad (4.4)$$

53
where the expectation value is evaluated on the ground state of the problem. The factorized representation of the wave-functions and operators will introduce a great simplification.

The imaginary part of the Fourier transform of this Green’s function gives the spectral function, which is associated with the angle-resolved photoemission spectrum of the problem as (for $\omega < \mu$)

$$B(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega).$$

(4.5)

In the Lehmann representation we write it as

$$B(k, \omega) = \sum_{f,\sigma} |\langle f, N - 1 | c_{k,\sigma} | GS, N \rangle|^2 \delta(\omega - E_{GS} + E_{f}^{N-1}),$$

(4.6)

$f$ is the final state with $N - 1$ particles and $N$ is the total number of electrons. In order to use the factorized wave-function in the calculation, and working in the real space for more convenience, one can re-write this expression as

$$B(k, \omega) = L \sum_{f, \sigma} |\langle f, N - 1 | c_{0,\sigma} | GS, N \rangle|^2 \times \delta(\omega - E_{GS} + E_{f}^{N-1}) \delta_{k,P_{GS}^{N} - P_{f}^{N-1}},$$

(4.7)

where we have imposed momentum conservation with the term $\delta_{k,P_{GS}^{N} - P_{f}^{N-1}}$ and used the definition $c_{j,\sigma} = \frac{1}{\sqrt{L}} \sum_{k'} e^{ik'j} c_{k',\sigma}$.

By using both spin-charge separation and splitting the operators (for $i = 0$) we get

$$B(k, \omega) = \sum_{Q, \omega', \sigma} D_{\sigma}(Q, \omega') B_{Q}(k, \omega - \omega').$$

(4.8)

where in

$$B_{Q}(k, \omega) = L \sum_{I} |\langle \phi_{L=0}^{N-1}(\{I\}) | f_{0} | \phi_{L=\pi}^{N,GS} \rangle|^2 \times \delta(\omega - E_{GS,ch}^{N} + E_{f,ch}^{N-1}) \times \delta_{k,P_{GS}^{N} - P_{f}^{N-1}},$$

$$D_{\sigma}(Q, \omega) = \sum_{M} |\langle \chi_{N-1}(Q, M) | Z_{0,\sigma} | \chi_{N}^{GS} \rangle|^2 \times \delta(\omega - E_{GS,s}^{N} + E_{f,s}^{N-1}),$$

(4.9)
Figure 4.1: Momentum distribution function obtained using the factorized wave-function, for $J = 0.05$, $L = 56$ sites, and $N = 42$ fermions, and different values of the spin temperature.

$B_Q(k, \omega)$ is the charge part of the spectral function where energies are obtained from the tight-binding dispersion and the two delta functions guarantee momentum and energy conservation. The charge part is not entirely decoupled from the spin part, momentum $Q = 2\pi j/N$ ($j = 0, 1, 2, \ldots, N - 1$) of the spin wave-function imposes a twisted boundary condition on the spinless fermion wave-function to ensure the periodic boundary condition for the original problem [92]. $D_{\sigma}(Q, \omega)$ determines the spin portion of the spectral function. The advantage of splitting up the spectral function is that now the Hilbert space that we define our $B_Q$ on is much smaller than the original one, and we can use results for the non-interacting tight-binding chain to evaluate the electronic contributions. The same is valid for the spin part, where we are dealing with a well-known Heisenberg spin chain. This allows us to handle a larger system size with much less computation cost.

Operator $f_0$ destroys one spinless fermion on site 0 of the ground state of the system with $N$ particles. Then, the overlap between this new state and all other possible configurations with $N - 1$ particles is calculated and summed over. During this step, one has to realize that the wave-functions with $N - 1$ particles have a momentum shift $Q$ (introduced by the spins), and therefore obtaining these quantities is not straight-forward. However, it is easy to see that one can write them as Cauchy-like determinants, and follow the method detailed in Ref.[92].
Figure 4.2: Spin transfer structure factor $\Omega_\sigma(Q, \beta_\sigma)$ calculated on Heisenberg spin chain ($J = 1$), for different temperatures, obtained with the time-dependent DMRG.

One can also get the momentum distribution function by having these two separate spectral functions as

$$n_k = \sum_Q D(Q)B_Q(k),$$

where we are using the relations $B_Q(k) = \int B_Q(k, \omega)d\omega$ and $D(Q) = \int D(Q, \omega)d\omega$.

The spin contribution $D_\sigma(Q, \omega)$ is defined by the action of the spin operators $Z$:

$$D_\sigma(Q, \omega) = \sum_M |\langle \chi_{N-1}(Q, M)|Z_{0,\sigma}\chi_{N}^{GS}\rangle|^2 \times \delta(\omega - E_{GS,s}^N + E_{j,s}^{N-1}).$$

To calculate $D_\sigma(Q, \omega)$, in principle one would need to solve the spin-$\frac{1}{2}$ Heisenberg Hamiltonian to obtain the energies and the wave-functions for $N$ and $N-1$ sites. In the $U \to \infty$ or $J \to 0$ limit the excitation spectrum collapses and $D_\sigma(Q, \omega) = \Omega_\sigma(Q)\delta(\omega)$. The spin transfer structure factor $\Omega_\sigma(Q)$ can be derived by using the spin transfer function $\omega_{j' \to j,\sigma}$ defined by Ogata and Shiba [27, 109], and by Sorella and Parola [90]. This function represents the amplitude of moving the spin $\sigma$ from site $j'$, to $j$. For $j' = 0$ it is given by

$$\omega_{0 \to j,\sigma} = \langle \chi_{N}^{GS} | P_{j,j-1} \cdots P_{1,0}\delta_{\sigma,S_0}^z | \chi_{N}^{GS} \rangle,$$
where we introduced the permutation operator $P_{j,j-1} = 2\vec{S}_j \cdot \vec{S}_{j-1} + \frac{1}{2}$, that exchanges the spins at sites $j$ and $j-1$. The spin transfer structure factor is defined as

$$\Omega_\sigma(Q) = \frac{1}{N-1} \sum_{j=0}^{N-2} e^{i(Q+\pi)j} \omega_{0\rightarrow j,\sigma}. \tag{4.13}$$

This expression for $\Omega_\sigma(Q)$ can be generalized to finite spin temperatures. The problem reduces to evaluating the thermal average of $\omega_{0\rightarrow j,\sigma}$, described by Eq.4.12, for a one-dimensional Heisenberg chain.

$$\Omega_\sigma(Q,\beta_\sigma) = \frac{1}{N-1} \frac{1}{Z_s} \sum_{M} \sum_{j=0}^{N-2} \omega_{0\rightarrow j,\sigma} e^{i(Q+\pi)j} e^{-\beta_\sigma E_{M,s}}, \tag{4.14}$$

where $Z_s$ is the spin partition function. In the following, we express the spin temperature in units of $J$, and the inverse temperature as $\beta_\sigma = 1/T_\sigma$.

In order to obtain this quantity numerically, we resort to tDMRG calculations at finite temperature[84]. Since the Heisenberg chain is weakly entangled at high temperatures, $T_\sigma \gg 1$, we are able to simulate systems as large as 300 sites. We point out that the calculation of $\omega_{0\rightarrow j,\sigma}$ is not that trivial, since it involves building a string of permutations between all pairs of spins between sites 0 and $j$. In order to carry it out, we use a recipe similar to the one used to time-evolve the wave-function in tDMRG. Since the structure of the DMRG block decimation always leaves two individual single sites in the original spin basis, we apply the permutation operator between these two sites. We propagate the wave-function to the next site, and apply the next permutation. This builds a chain of permutations as the DMRG algorithm sweeps through the lattice. In order to calculate the quantum mechanical average, we need to use two target states, the original thermal state (or the ground state at $T = 0$), and the state obtained after applying the permutations. The calculation is done more efficiently if one starts from the middle of the chain. The application of $P_{1,0}$ yields the first average $\omega_{0\rightarrow 1}$. In the next left-to-right iteration we apply $P_{2,1}$ to the previous state, leading to $\omega_{0\rightarrow 2}$. We can repeat this procedure all the
way until we reach the right end of the chain, and a single DMRG sweep yields all the correlations needed to construct $\Omega_{\sigma}(Q, \beta_\sigma)$.

For the final calculation, we assume $J/t \ll 1$, and approximate $D_{\sigma}(Q, \omega, \beta_\sigma)$ by introducing the frequency dependence as [92]

$$D_{\sigma}(Q, \omega, \beta_\sigma) = \Omega_{\sigma}(Q, \beta_\sigma)\delta(\omega - E_s + \epsilon_Q),$$  \hspace{1cm} (4.15)

where $\epsilon_Q = \frac{\pi}{2}J|\sin(Q - \pi/2)|$ is the des Cloizeaux-Pearson dispersion, and $E_s = -J \ln 2$ is the ground state energy, which are obtained from the exact Bethe ansatz solution for the Heisenberg chain [110].

In order to calculate $B_Q(k, \omega)$ we need to evaluate matrix elements such as $\langle \phi_{L,Q}^{N-1}(I)|f_0|\phi_{L,\pi}^{N,GS}\rangle$. A typical overlap of this type is given by

$$\langle 0|f_{k_N} \ldots f_{k_2} f_{k_1} f_{k_1}' f_{k_2}' \ldots f_{k_N}'|0\rangle.$$  \hspace{1cm} (4.16)

This overlap is given by the following determinant [105]

$$\begin{vmatrix}
\{f_{k_1}' , f_{k_1}\} & \{f_{k_1}' , f_{k_2}\} & \ldots & \{f_{k_1}' , f_{k_N}\} \\
\{f_{k_2}' , f_{k_1}\} & \{f_{k_2}' , f_{k_2}\} & \ldots & \{f_{k_2}' , f_{k_N}\} \\
\vdots & \vdots & \ddots & \vdots \\
\{f_{k_N}' , f_{k_1}\} & \{f_{k_N}' , f_{k_2}\} & \ldots & \{f_{k_N}' , f_{k_N}\}
\end{vmatrix}.$$  \hspace{1cm} (4.17)

The momenta $k$ and $k'$ have different origins according to their phase shift introduced by the twisted boundary condition ($Q/L$ in general and $\pi/L$ for the ground-state). This results in a non-trivial anti commutator relation

$$\{f_{k'}^\dagger , f_k\} = \frac{1}{L} \sum_{j,j'} e^{i(k'-k)j} \{f_{j'}^\dagger , f_{j}\}$$  \hspace{1cm} (4.18)

$$= \frac{1}{L} e^{-i(k'-k)/2} e^{i(Q-\pi)/2} \frac{\sin(|Q|/2)}{\sin((k'-k)/2)}.$$
Replacing the anti-commutators 4.18 in the determinant 4.17 one gets

\[ L^{-N} e^{i(\pi-Q)N/2} \sin^{N} \frac{\pi}{2} \prod_{j} e^{(k'_j-k_j)/2} \]

This expression is similar to a Cauchy determinant and can be expressed as a product. The general form of the product can be summarized as

\[
\langle 0| f_k^N \cdots f_k^1|0 \rangle = \pm L^{-N} e^{i(\pi-Q)N/2} \sin^{N} \frac{\pi}{2} \prod_{j} e^{(k'_j-k_j)/2} \]

\[
\times \prod_{j>i} \frac{\sin k_j - k_i}{2} \prod_{j>i} \frac{\sin k'_j - k'_i}{2} \prod_{i,j} \frac{\sin^{-1} k'_i - k_j}{2},
\]

the sign + is for \( N = 1, 4, 5, 8, 9, \ldots \) and - for \( N = 2, 3, 6, 7, \ldots \).

We can now rewrite \( L|\langle \phi^{N-1}_{LQ}(|I\rangle|f_0|\phi^{N,GS}_{L,\pi} \rangle|^2 \) as

\[
L|\langle \phi^{N-1}_{LQ}(|I\rangle|f_0|\phi^{N,GS}_{L,\pi} \rangle|^2 = L^{-2N+2} \sin^{2N-2} \frac{\pi}{2} \prod_{j>i} \frac{\sin^2 k_j - k_i}{2} \]

\[
\times \prod_{j>i} \frac{\sin^2 k'_j - k'_i}{2} \prod_{i,j} \frac{\sin^{-2} k'_i - k_j}{2}. \tag{4.19}
\]

We are now ready to calculate the spectral function numerically. One needs to generate the quantum numbers \( \{ I \} \), evaluate the energies and momentum and the expression above.
4.2 Results

The results for \( \Omega_{\sigma}(Q,\beta_{\sigma}) \) are shown in Figure 4.2 and, for the \( \beta_{\sigma} = 0 \) limit, they are exact and can be compared to the expression

\[
\Omega_{\sigma}(Q, \beta_{\sigma} = 0) = \frac{1}{N - 10} \frac{3}{8} \cos(Q - \pi).
\]

(4.20)

As the temperature decreases the peak in \( Q = \pi \) shifts toward \( Q = \pi/2 \), as expected for an antiferromagnetic spin chain. At very low temperatures the correlation function develops a singularity at \( Q \), which introduces serious finite-size effects in our calculations. We therefore restrict our simulations to values of \( \beta_{\sigma} \) that we can trust. For \( T = 0 \) we use a fit to the values obtained with exact diagonalization.

Figure 4.3: Spectral function obtained using the factorized wave-function, for \( J = 0.05 \), \( L = 56 \) sites, and \( N = 42 \) fermions. The panels correspond to different values of the “spin temperature” (see text).
In Figure 4.3 we show the results for the electronic spectral function after the convolution, using the data for $\Omega_{\sigma}(Q, \beta_{\sigma})$ obtained with tDMRG. We choose the value of $J = 0.05$ to compare with the results from Ref.[98]. We observe identical behavior, the spectral weight shifting in momentum, with the minimum of the dispersion at the bottom of the band moving from $k = 0$ at infinite spin temperature to $k = k_F$ at zero temperature. In addition, we notice a series of discrete flat energy levels. These energy levels correspond to the convolution of a single charge excitation with $\Omega_{\sigma}(Q, \beta_{\sigma})$. The spacing between them is inversely proportional to the system size $\approx 2w/L$, where $w = 4$ is the bandwidth, and it is a finite size effect. This naturally explains the DMRG spectra reported in Ref.[98].

This behavior has an additional manifestation in the momentum distribution function, shown in Figure 5.5, obtained by integrating the spectral weight as [29]

$$n_k = \sum_{Q} \Omega_{\sigma}(Q, \beta_{\sigma}) \int_{\omega} B_Q(k, \omega) d\omega. \quad (4.21)$$

These results are in remarkable agreement with the DMRG calculations from Ref.[98], and illustrate how the Fermi momentum $k_F$ seems to shift to $2k_F$ at infinite spin temperature. This is a distinctive feature of the spin incoherent Luttinger liquid [32, 33, 34].

**Figure 4.4:** Spectral function for a finite chain with $L = 14$ sites at half-filling, with $J = 0.05$, obtained with exact diagonalization. The discrete bars show the spectrum of the Hamiltonian, illustrating that only a small fraction of states carry most of the spectral weight at $T = 0$. 
To fully understand this effect, we look at the spectral function of a finite $t - J$ chain using exact diagonalization. We follow the reasoning sketched in Ref.[111], which at the time was based on pure intuition, and was later proved to be the correct interpretation. It is easy to observe in Figure 4.4 that one could fix a spinon momentum $Q$, and draw a shifted tight-binding dispersion to trace a full holon band. This principle can be used to build the full set of branches. The figure shows that at $T = 0$ only a very small fraction of the states carry most of the spectral weight. Now, one may want to pose the following question: if the spectrum is completely determined by the Hamiltonian, and obviously does not change with the temperature, how can the spectral function shift in momentum? If that is possible, there have to be states available at those energies and momenta. Indeed, those states exist (shown with red bars in the figure) but they have vanishingly small spectral weight at $T = 0$. As the temperature increases, the spectral density shifts in such a way that they acquire a larger weight. This shift is determined by the spin transfer function $\Omega_\sigma(Q, \beta_\sigma)$, and at infinite spin temperature, makes the dispersion resemble non-interacting spinless-like particles.

4.3 Conclusions

We have generalized a formalism originally developed in Refs.[29, 90, 91, 92] to study the crossover from the spin-coherent to SILL regime in the spectral signatures of strongly correlated Hubbard chains. The main idea behind the approximation consists of convolving the spectral functions of spinless fermions at zero temperature, and a spin chain at finite temperatures, following the Bethe ansatz prescription. The finite-temperature spin correlation function can be obtained with high-accuracy using tDMRG. The theory reproduces and explains previous numerical results in a very natural way. Although the spectrum is completely determined by the Hamiltonian, the spectral weight of the spinons shifts to high momentum as the temperature increases. This translates into an apparent shift of the minimum of the electronic spectrum by $k_F$. Remarkably, in the SILL regime, the spectral function resembles that of spinless fermions at zero temperature, with a Fermi
momentum $2k_F$. Besides a conventional thermal broadening of the line shape, one would also expect to see a broadening in momentum, due to the spread of $\Omega_\sigma(Q, \beta_\sigma)$. This transfer of spectral weight does not mean that the spectrum itself changes with temperature, and it is a clear departure from the non-interacting, or Fermi-liquid picture. Even when instruments may not be able to resolve the fine details of the spectrum, this shift and momentum broadening are a distinctive signature of spin-charge separation that should be experimentally observable.
Chapter 5

Interplay of charge, spin, and lattice degrees of freedom in the spectral properties of the one-dimensional Hubbard-Holstein model

In the past two decades, we have witnessed a tremendous improvement in the energy and momentum resolution of angular-resolved photoemission spectroscopy (ARPES), which is one of the most powerful experimental tools for investigating strongly correlated materials. In particular, recent ARPES spectra of high-$T_C$ cuprates[13, 112], alkali-doped fullerides[113], and manganites[114], have shown that the interplay of electron-electron (el-el) and electron-phonon (el-ph) interactions has an important role in the qualitative and quantitative understanding of the experiments.

When considering systems of low dimensionality, the situation is even more complicated. In one dimension (1D), the low-energy states separate into spin (spinon) and charge (holon) excitations that move with different velocities and are at different energy scales [2, 3, 115]. Spin-charge separation has been observed experimentally in semiconductor
quantum wires[116], organic conductors[117], carbon nanotubes[118], atomic chains on semiconductor surfaces[119] and was recently predicted to be present in optical lattices of ultracold atoms[98, 120, 121]. A clear detection of the phenomenon has been proposed theoretically in Ref.[122] using time-resolved spin-polarised density measurements. Evidence of spin-charge separation has been observed also in photoemission experiments on quasi-1D cuprate SrCuO$_2$[12] and on organic conductor TTF-TCNQ[11]. In these quasi-1D materials, the coupling to the lattice is considered to be responsible for the unusual spectral broadening of the spin and charge peaks observed by ARPES. Recently, the interplay between spin, charge, and lattice degrees of freedom has also been investigated in the family of quasi-1D cuprates Ca$_{2+5x}$Y$_{2-5x}$Cu$_5$O$_{10}$, using high resolution resonant inelastic x-ray scattering (RIXS)[123, 124].

In 1D systems and in the absence of el-ph interaction, the spin excitations are described by a band whose curvature is proportional to the exchange energy scale $J$, while the charge excitation dispersion width is comparable to the electronic hopping ($\approx 4t$). Moreover, the collective excitation spectrum of 1D systems presents spectral weight (shadow bands) at momenta larger than the Fermi momentum $k_F$ due to their Luttinger liquid nature. It is therefore of paramount importance to study the behavior of the photoemission spectrum of materials in which it is believed that a strong interaction with the lattice degrees of freedom is present. In particular, this aspect is not entirely understood and one expects that the interplay between el-el and el-ph interactions has a profound effect on spin-charge separation and on the interpretation of the experiments.

The basic lattice model used to describe el-el and el-ph interactions in 1D is the so-called Hubbard-Holstein (HH) Hamiltonian, which contains nearest-neighbor hopping $t$, on-site Coulomb repulsion $U$ and a linear coupling between the charge density and the lattice deformation of a dispersionless phonon mode (see Sec. II). Within this model, the electronic spectral properties have been studied by Ref.[125] and [126], where the adiabatic limit (phonon frequency smaller than the electronic hopping) is mostly analyzed at half electronic filling in the regime of weak to intermediate el-ph coupling. In the first paper, the authors use dynamical Density Matrix Renormalization Group (D-DMRG) and assess
the robustness of spin-charge separation against el-ph coupling, interpreting the spectral function as a superposition spectra of spinless fermions dressed by phonons. In particular, a peak-dip-hump structure is found, where the dip energy scale is given by the phonon frequency and originated from the charge-mediated coupling of phonons and spinons. In the second paper, the authors use cluster perturbation theory (CPT) and an optimized phonon approach observing that el-ph coupling mainly gives rise to a broadening of the holon band, due to the presence of many adiabatic phonons.

In contrast to these previous studies, in this work we consider the case of a phonon frequency larger than the electronic hopping (antiadiabatic limit) and a finite hole doping (or equivalently electronic density below half-filling), a regime that could be currently accessible in the experiments[124]. We develop a controlled analytical approach for the calculation of the spectral function (photoemission spectrum, PES) which is rigorously valid in the presence of an infinitely large Coulomb repulsion, and in the anti-adiabatic limit.

In this regime, the exchange $J$ is a small energy scale (of the order of $t^2/U$) in the problem, but it is not zero as in the spinless Holstein model$^\dagger$. Our theory relies on Ogata-Shiba’s Bethe ansatz solution[27] of the $U \to \infty$ Hubbard model (1.4), combined with the Zheng, Feinberg and Avignon (ZFA) treatment[139] of the el-ph interaction. In order to support the analytical results, we numerically calculate the PES using the time-dependent DMRG[81, 140] (tDMRG) finding a quantitative and qualitative agreement with the analytical approximation for weak and strong el-ph interaction. One of the main observations is that the el-ph interaction induces a reduction of the spinon and the holon bandwidths. For strong el-ph interaction, we observe spectral side-bands separated by energy gaps with length proportional to the phonon frequency. Eventually, the separation of spin and charge spectral peaks is not appreciable anymore as spinon and holon bands merge in one main band. Therefore, in this case, the system can be described as a

$^\dagger$In the literature the strong Hubbard-$U$ ($U$ is the on-site Coulomb repulsion) limit of the HH model is usually considered as the spinless Holstein model. For this model, the dynamical properties have been thoroughly studied both analytically and numerically[127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138].
polaronic liquid, with the spectral weight extended well beyond Fermi momentum $k_F$. The tDMRG simulations show that at weak coupling spin-charge separation is robust against el-ph coupling, and spinon and holon bands are well resolved. Therefore, we argue that, from weak to intermediate el-ph coupling, phonons are mainly coupled to the charge degrees of freedom while the spinon is pretty much unaffected to a good approximation. Finally, the PES is investigated with tDMRG decreasing the phonon frequency and exploring also the adiabatic limit. In this case, we reproduce the results of Ref. [125] finding the characteristic spectral peak-dip-hump structure. We point out that throughout this chapter, the Coulomb repulsion is considered large enough to avoid competition with other phases such as the CDW Peierls state[55].

5.1 The ZFA approach

In this section we present an analytical method that allows us to calculate the photoemission part of the spectral function

$$B(k,\omega) = -\frac{1}{\pi} \text{Im} G(k,\omega) \quad \text{for} \quad \omega < \mu,$$

(5.1)

where $G(k,\omega)$ is the electronic retarded single particle Green’s function and $\mu$ is the chemical potential. The method consists of a variational canonical transformation originally proposed in Ref.[139] and then employed in Ref.[141] for calculating the spectral and optical properties of the spinless Holstein model. The starting point of the approach is the assumption that, in the limit of strong el-ph coupling, $U \to \infty$ and infinite phonon frequency $\omega_0$, the model is described by spinless polarons. Then, the ZFA approach extends the polaron formation to the intermediate el-ph coupling regime, recovering the mean field solution at zero phonon frequency. We introduce the generator of the so-called variational Lang-Firsov transformation[142], given by

$$T[f,\Delta] = e^{\sum_j [n_j f + \Delta](a_j - a_j^\dagger)},$$

(5.2)
where \( n_j = n_{j,\uparrow} + n_{j,\downarrow} \), and \( f \) and \( \Delta \) are variational parameters whose meaning will be described below. For more technical details of a unitary transformation on such systems one can study Appendix C of this dissertation where we show the Green’s function solution to Einstein model for a one and \( n \)-site problem. Going back to our Lang-Firsov transformation, the transformed Hamiltonian reads

\[
\tilde{H}[\tilde{f}, \Delta] = T^{-1}HT = -t \sum_{i,\sigma} (c_{i,\sigma}^\dagger X_i^\dagger X_{i+1} c_{i+1,\sigma} + \text{h.c.}) + (U - 2g^2 f^2 \omega_0) \sum_i n_{i,\uparrow} n_{i,\downarrow} \\
+ g\omega_0 (1 - f) \sum_i n_i (a_i + a_i^\dagger) - g\omega_0 \Delta \sum_i (a_i + a_i^\dagger) \\
+ \omega_0 \sum_i a_i^\dagger a_i + \eta \sum_i n_i + L g^2 \omega_0 \Delta^2,
\]

(5.3)

where we have defined a phonon operator \( X_i = e^{gf(a_i - a_i^\dagger)} \) and \( \eta = g^2 \omega_0 f(1 - f) + 2g^2 \omega_0 (1 - f) \Delta \). In the next subsection, we will show the actual procedure employed for the calculation of the variational parameters \( f \) and \( \Delta \). Also, it will be shown that the variational parameter \( \Delta \) can be obtained as a function of \( f \) \( (\Delta = (1 - f) N/L) \), and one is thus left with only one variational parameter. Assuming \( \tilde{f} \) is the optimal choice for \( f \), one can thus proceed by writing the transformed Hamiltonian as

\[
\tilde{H}[\tilde{f}] = \tilde{H}_0 + V,
\]

(5.4)

where \( \tilde{H}_0 \) is the unperturbed part given by strongly correlated electrons and non-interacting phonons,

\[
\tilde{H}_0[\tilde{f}] = -t e^{-g^2 \tilde{f}^2} \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) + (U - 2g^2 \tilde{f}^2 \omega_0) \sum_i n_{i,\uparrow} n_{i,\downarrow} \\
- g\omega_0 (1 - \tilde{f}) \frac{N}{L} \sum_i (a_i + a_i^\dagger) + \omega_0 \sum_i a_i^\dagger a_i + g^2 \omega_0 (1 - \tilde{f})^2 \frac{N^2}{L} + \tilde{\eta} N,
\]

(5.5)

with \( \tilde{\eta} = g^2 \omega_0 \tilde{f}(\tilde{f} - 2) - 2g^2 \omega_0 (1 - \tilde{f})^2 N/L \), while \( V \) is a many-body interaction operator

\[
V = -t \sum_{i,\sigma} [c_{i,\sigma}^\dagger X_i^\dagger X_{i+1} - e^{-g^2 \tilde{f}^2} c_{i+1,\sigma} + \text{h.c.}] + g\omega_0 (1 - \tilde{f}) \sum_i n_i (a_i + a_i^\dagger).
\]

(5.6)
The PES is now calculated approximately by neglecting the perturbation $V$. One can use perturbation theory and consider the effect of $V$ in higher orders of perturbation after the calculation of the PES, but in this work we are only taking the zeroth order into account. In fact, the determination of the optimal parameter $\tilde{f}$ is meant to minimize the error produced by neglecting the interaction term $V$ from the Hamiltonian (5.4). The unperturbed Hamiltonian $\tilde{H}_0[\tilde{f}]$ still contains information about el-ph interacting terms in the original Hamiltonian (1.11), since all the parameters of $\tilde{H}_0[\tilde{f}]$ are renormalized by our variational technique. Indeed, $\tilde{H}_0[\tilde{f}]$ consists of free phonons and a Hubbard model with a shift of $\tilde{\eta}$ in the chemical potential, a hopping $\tilde{t}$ and an on-site repulsion $\tilde{U}$ renormalized by the el-ph interaction

$$\tilde{t} = t e^{-g^2 \tilde{f}^2}, \tilde{U} = U - 2g^2 \tilde{f}^2 \omega_0.$$

(5.7)

In this limit, in the transformed space electronic and lattice degrees of freedom are governed by independent Hamiltonians

$$\tilde{H}_0[\tilde{f}] = \tilde{H}_{el} + \tilde{H}_{phonon},$$

(5.8)

and the total wave-function can be factorized in two parts

$$|\psi\rangle = |\Lambda\rangle \otimes |\{n_{ph}\}\rangle,$$

(5.9)

where $|\Lambda\rangle$ describes the electrons, and $|\{n_{ph}\}\rangle$ is given by the product of $L$ separate non-interacting phononic wave-functions, each one containing an integer number of phonons

$$|\{n_{ph}\}\rangle = |\{n_{ph}^0\}\rangle \otimes |\{n_{ph}^1\}\rangle \otimes \cdots |\{n_{ph}^{L-1}\}\rangle).$$

It is trivial to show that the PES in the original space is given by

$$B(k, \omega) = \sum_{\tilde{n}} |\tilde{n}|X_0|0\rangle|^2 B_{el}(k, \omega + \tilde{n}\omega_0),$$

(5.10)

where $B_{el}(k, \omega)$ is the PES in the transformed space and the sum is extended over all the phonon states $\tilde{n}$ of a single site phonon. $B_{el}(k, \omega)$ is now evaluated in the Lehmann
representation

\begin{equation}
B_e(k, \omega) = L \sum_{z,\sigma} |\langle z, N-1 | c_{k,\sigma} | g_s, N \rangle|^2 \times \delta(\omega - E^N_{g_s} + E^{N-1}_z),
\end{equation}

(5.11)

where \( c_{k,\sigma} \) destroys an electron with momentum \( k \) and spin \( \sigma \) \((c_{j,\sigma} = \frac{1}{\sqrt{L}} \sum_{k'} e^{ik'j} c_{k',\sigma})\), \( N \) is the total number of electrons, and \( z \) the final state with \( N - 1 \) electrons. \( E^{N-1}_z \) represents the total energy of the final state, and \( E^N_{g_s} \) describes the energy of the ground state of the original Hamiltonian (1.11) with \( N \) electrons. Since Einstein phonons carry no momentum, we can impose the momentum conservation with the term \( \delta_{k,P_{g_s}^{N-1} - P_{N-1}^{N-1}} \) to reduce Eq.(5.11) to a calculation involving only site 0 in the real space and one phonon mode at that site

\begin{equation}
B_e(k, \omega) = L \sum_{z,\sigma} |\langle z, N-1 | c_{0,\sigma} | g_s, N \rangle|^2 \times \delta(\omega - E^N_{g_s} + E^{N-1}_z) \delta_{k,P_{g_s}^{N-1} - P_{N-1}^{N-1}}.
\end{equation}

(5.12)

Up to here, no assumptions have been made on the electronic spectral function and the general form shown above is extremely complex. However, in the limit of \( \tilde{U} >> \tilde{t} \) one can use Ogata-Shiba’s factorization\[27\] to show that the electronic wave-function \(|\Lambda\rangle\) in Eq.(5.9) is split into spin and charge parts. The total wave-function \(|\psi\rangle\) can be further factorized as

\begin{equation}
|\psi\rangle = |\phi\rangle \otimes |\chi\rangle \otimes |\{n_{ph}\}\rangle,
\end{equation}

(5.13)

where \(|\phi\rangle\), describes spinless charges, \(|\chi\rangle\) is the spin wave-function that corresponds to a “squeezed” chain of \( N \) spins, where all the unoccupied sites have been removed. In this limit, charge, spin, and lattice degrees of freedom are governed by independent Hamiltonians

\begin{equation}
\tilde{H}_0[\tilde{f}] = \tilde{H}_{\text{charge}} + \tilde{H}_{\text{spin}} + \tilde{H}_{\text{phonon}}.
\end{equation}

(5.14)

Due to this simplification, we are now able to tackle the problem and calculate the PES. Indeed, operator \( c_{0,\sigma} \) after the polaron transformation will look like \( c_{0,\sigma} X_0 \). Moreover, using the Ogata-Shiba formalism\[27\] one can factorize the electronic annihilation operator
\(c_{0,\sigma} = Z_{0,\sigma} b_0\), where \(b_0\) is a spinless fermionic operator acting on the (spinless) charge part of the wave-function \(|\phi\rangle\), and \(Z_{0,\sigma}\) is acting on the spin part \(|\chi\rangle\). The \(Z_{0,\sigma}\) operator has a very peculiar behavior, destroying the spin \(\sigma\) at site \(i = 0\) as well as the site, making the chain \(N - 1\) sites long. For details about the use of the \(Z_{0,\sigma}\) operator we refer the reader to Refs.[41, 92, 143]. The spectral function can be therefore expressed as a convolution

\[
B_{\omega}(k, \omega) = \sum_{\omega', Q, \sigma} D_{\sigma}(Q, \omega') B_{Q}(k, \omega - \omega')
\]

where \(D_{\sigma}(Q, \omega)\) is the spin spectral function with momentum \(Q\), and

\[
B_{Q}(k, \omega) = L \sum_{\{I\}} |\langle \psi_{N,L,Q}^{N,gs} | b_0 | \psi_{N,L,\pi}^{N,gs} \rangle|^2 \times \delta(\omega - E_{gs}^{N} + E_{gs}^{N-1}) \delta_{k, P_{N-P N-1}},\]

(5.16)

describes the charge part. By following the approach introduced in Ref.[92], one can calculate numerically both \(D_{\sigma}(Q, \omega)\) and \(B_{Q}(k, \omega)\). In the next section the numerical method used to estimate the best value of the variational parameter \(f\) is presented.

### 5.1.1 Variational calculation of the parameter \(f\)

In this section we determine the variational parameters \(f\) and \(\Delta\) appearing in the transformed Hamiltonian (5.3) of the previous section. An effective electronic Hamiltonian, \(H_{eff}\), is used, which is obtained by averaging Eq.(5.3) on the phononic vacuum of the transformed Hilbert space, \(H_{eff}[f, \Delta] = \langle O_{ph}|\hat{H}|O_{ph}\rangle\)

\[
H_{eff}[f, \Delta] = -t e^{-g^2 f^2} \sum_{i, \sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c.)
\]

\[
+ (U - 2 g^2 f^2 \omega_0) \sum_i n_{i,\uparrow} n_{i,\downarrow} + \eta \sum_i n_i + L g^2 \omega_0 \Delta^2.
\]

(5.17)

The parameter \(\Delta\) is simply obtained by using the Hellmann-Feynman theorem

\[
\frac{\partial}{\partial \Delta} \langle gs|H_{eff}|gs\rangle = 0 \Rightarrow \Delta = (1 - f) \frac{N}{L},
\]
Figure 5.1: The parameter $\tilde{f}$ is obtained by minimizing the ground state energy of Hamiltonian (5.18) with respect to $f$. Panel (a) shows DMRG calculations for two different values of el-ph coupling $g$. Panel (b) shows $\tilde{f}$ as a function of $g$. All results are for density $N/L = 0.75$.

where $N$ is the total number of electrons, $N/L$ is the electronic density, and $|gs\rangle$ is the ground state of $H_{\text{eff}}$. One is now left only with the determination of the parameter $f$, which will be found by solving the Hamiltonian

$$H_{\text{eff}}[f] = -te^{-g^2f^2} \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c.)$$

$$+ (U - 2g^2f^2\omega_0) \sum_i n_{i,\uparrow}n_{i,\downarrow} + g^2\omega_0(1 - f)^2N^2/L + \eta N,$$

by using the static DMRG and minimizing the ground-state energy of this new Hamiltonian as a function of $f$. For each set of values $U$, $t$, $g$, and $\omega_0$, one can get an optimal polaronic parameter $\tilde{f}$. In panel (a) Fig.5.1, the ground-state energy of $H_{\text{eff}}[f]$ as a function of $f$ for two different values of el-ph coupling $g = 0.8$ and $g = 1.8$ is shown. Here $N/L = 0.75$, $U = 20$ and $\omega_0 = 2.0$. For $g = 1.8$ the value of $\tilde{f}$ obtained is close to 0.8 meaning that for these sets of parameters the system is near the polaronic regime, that ideally is expected to be reached for stronger el-ph coupling and phonon frequency.
Indeed, for \( \tilde{f} = 1 \) one has well defined polarons, while, for \( \tilde{f} = 0 \), the unitary transformation, Eq.(5.2), becomes trivially the identity. In panel (b) of Fig.5.1, the optimal polaronic parameter \( \tilde{f} \) as a function of el-ph is shown. As will become clear in the next section, \( \tilde{f} \) describes the degree of polaron formation, that is the amount of spectral weight redistribution in phonon side-bands.

### 5.1.2 Analytical results

Once the optimal \( \tilde{f} \) is determined, one can finally study and analyze the properties of the PES calculated from Eq.(5.15) and Eq.(5.10). We start by considering a phonon frequency \( \omega_0 > 1 \) (anti-adiabatic limit) and choose in particular \( \omega_0 = 2.0 \). Moreover, throughout this chapter, we consider an electronic filling equal to \( N/L = 0.75 \). Fig.5.2 shows \( B(k,\omega) \) from weak el-ph coupling \( g = 0.2 \) up to strong interaction \( g = 2.0 \). In order to interpret the results in more detail, Fig.5.3 shows three vertical cuts at \( k = 0, k = k_F \) (\( k_F = \pi N/2L = 0.375\pi \)), and \( k = 2k_F \) of the same spectrum (dashed red lines). We note that the spectrum for \( g = 0.2 \) is very similar to the \( g = 0 \) PES \([125, 126, 144]\) (not shown): the presence of spin-charge separation is very clear, with the spectral weight concentrated on the spinon and holon bands forming a triangular spectral structure between \(-k_F\) and \(+k_F\) (Fig.5.2). As expected for a Luttinger liquid, the shadow bands extend beyond \( k_F \).

At \( g = 0.6 \), phonon effects start to become appreciable with interesting features at all momenta. One can observe a reduction of the spinon and holon bandwidth, as the triangular spectral structure comprising the spinon and holon bands gets squeezed. Indeed, the reduction of the spinon and holon bandwidths is due to the fact that the el-ph coupling renormalizes the hopping parameter \( \tilde{t} = te^{-g^2j^2} \) exponentially (see Hamiltonian \( H_0[\tilde{f}] \), Eq.(5.4)). Moreover, one starts to see a replica of the entire spectrum appearing shifted below the main band by an energy amount exactly equal to the phonon frequency \( \omega_0 \).
As can be seen in Fig.5.1, for the set of parameters used in this work $\tilde{f}$ assumes a value of 0.4 for $g = 0.2$ increasing slightly up to 0.5 for $g = 1.2$, showing that strong Coulomb repulsion and the large phonon frequency already give a sizable spectral redistribution from weak to intermediate el-ph couplings.

Increasing the el-ph coupling, the spectral weight redistribution in identical replicas continues (see panels $g = 1.0$, $g = 1.2$, $g = 1.5$ of Fig.5.2), until the triangular structure is
almost collapsed into a flat line for $g = 1.5$. Moreover, for $g \leq 1.5$, the PES is broken in spectral replicas (at least 5 for $g = 1.5$) whose weight decreases from the first structure to the followings. This is not true anymore for the case of $g = 2.0$. In this case, one can observe more than 10 spectral replica lines with a Gaussian distribution of the spectral weights typical of the polaronic regime[145]. In this case, the separation between the holon and the spinon peak is not discernible anymore, suggesting that the system is in a state that can be described in terms of a spinless polaronic liquid where the spins are completely uncorrelated. It is now clear that the quantity $f$ governs the magnitude of the anti-adiabatic polaronic effect, which mainly consists in a spectral redistribution in phonon replicas. It is important to point out that it also provides a shift of the bands given by $\tilde{\eta} = g^{2}\omega_{0}\tilde{f}(\tilde{f} - 2) + 2g^{2}\omega_{0}(\tilde{f} - 1)\Delta$. All the spectra shown in Fig.5.2 are shifted by a quantity that increases quadratically as a function of the variational parameter $\tilde{f}$ as the el-ph is increased.

In the next section we present a numerical calculation of the PES with the tDMRG, which will allow us to verify and support the results of the ZFA approach.
5.2 Spectral function with the tDMRG

In order to obtain dynamical properties of 1D quantum lattice models in the presence of phonons, several techniques such as dynamical DMRG[125] and exact diagonalization combined with cluster perturbation theory have been used in the literature[126]. In contrast to these approaches, here the PES is calculated using the tDMRG with Krylov expansion of the time-evolution operator[82, 146, 147, 148, 149]. The time evolution is computed using $m = 400$ DMRG states and the bare phonon bases are truncated keeping up to 9 phonons per site. Unless otherwise stated, a lattice with $L = 32$ sites, $N = 24$ electrons and open boundary conditions is considered. In order to calculate the PES, we measure the time-dependent correlation function

$$B_{i,j}(t) = i\langle \Psi_0 | e^{iHt} c_i^\dagger e^{-iHt} c_j | \Psi_0 \rangle, \quad (5.19)$$

where $| \Psi_0 \rangle$ is the ground-state of Hamiltonian (1.11). $| \Psi_0 \rangle$ and the ground-state energy is calculated using static DMRG. Excited states $| \Psi_j \rangle = c_j | \Psi_0 \rangle$ and their time evolution $| \Psi_j(t) \rangle = e^{-iHt} | \Psi_j \rangle$ are then calculated with the tDMRG. Since the time evolution of the ground-state is trivial $\langle \Psi_0 | e^{iHt} = e^{iE_{gs}t} \langle \Psi_0 |$, Eq.(5.19) reduces to

$$B_{i,j}(t) = i e^{iE_{gs}t} \langle \Psi_0 | c_i^\dagger | \Psi_j(t) \rangle, \quad (5.20)$$

for all pairs $(i,j)$ with $i,j = 0, L−1$. Long time evolutions up to $T_{end} = 14$ with time steps of $\Delta t = 0.01$ are considered, and $B(k, \omega)$ is obtained by a space-time Fourier transform performed using a Hann window function ($H(x) = \frac{1}{2} [1 + \cos(x\pi)]$ with $x = 2t/T_{end}$), giving a broadening of the spectral peaks approximately given by $\delta \simeq 0.25$ (the details of the procedure are reported in Ref.[81]). Here, $k$ and $\omega$ are the momentum and energy of the electron.
Figure 5.4: Photoemission spectrum of the HH model calculated with tDMRG for the same frequency and el-ph coupling values considered in Fig.5.2. Here $L = 32$ sites, $U = 20$ and filling $N/L = 3/4$.

### 5.2.1 Numerical results

Fig.5.4 shows the PES calculated with the tDMRG in the anti-adiabatic regime, for the same regime of parameters of Fig.5.2. In analogy with the results obtained with the ZFA approach, we also show three vertical cuts of the spectrum at $k = 0$, $k = k_F$, $k = 2k_F$ in Fig.5.3 (solid (black) lines). It is important to point out that, even within the ZFA approach, a broadening of the spectral peaks of the order of $\delta \simeq 0.25$ has been used.
As stated in the previous section, one expects that the ZFA approach is a good approximation of the results in the regime where $\tilde{U} \gg \tilde{t}$ and $\omega_0 > \tilde{t}$. In particular, as one can see in the top row of panels of Fig.5.3, for $g = 0.2$ a very good agreement between ZFA and the tDMRG results is obtained. This characteristic is also evident at all momenta if one compares the upper left panel of Fig.5.4 and Fig.5.2.

Noticeable differences between the ZFA approach and the tDMRG results can be observed in the intermediate el-ph coupling regime ($g = 0.6, 1.0, 1.2$). In this case, the ZFA approach is qualitatively reproducing the reduction of the spinon and holon bandwidths, which are parametrized by the renormalized hopping parameter $\tilde{t} = t e^{-g^2 f^2}$ in the Hamiltonian $H_0[\tilde{f}]$, Eq.(5.4). While reproducing the correct position of the spectral side-bands, the ZFA approach provides access to their internal structure, showing that the separation between the holon and spinon peaks is still well defined.

For $g = 0.6$, tDMRG results show an apparent suppression of the spectral weight or gap that appears at $\omega - \mu \simeq -2$ with the formation of a new band ranging from $\omega - \mu \simeq -2$ to $\omega - \mu \simeq -4$, whose dispersion resembles those of the holon and shadow bands. The same characteristics are visible in Fig.5.3 for $k = 0$, where the distance between the spinon peak and the holon peak is reduced and a side-band at the left of the holon peak is formed. This new spectral feature seems to originate from the holon band, while the height of the spinon peak is practically unchanged going from $g = 0.2$ to $g = 0.6$.

At $g = 1.0$, the progressive reduction of the electronic bandwidth (both of the spinon and holon bands) is even more evident, and the triangular spectral structure has almost collapsed. The new band formed at $g = 0.6$ is now separated by a larger gap with respect to the main spectrum, while the spectral redistribution creates a newer side-band whose width is smaller, ranging from $\omega - \mu \simeq -4$ to $\omega - \mu \simeq -6.2$. As one can see, in Fig. 5.3 for $k = 0$, several side-bands separated in energy by a quantity proportional to $\omega_0$ are visible. The side-bands present no internal structure and suggest that, up to $g = 1.0$, they originate from the holon bands without contribution from the spinons. These results indicate that, from weak to intermediate $g$, spin-charge separation is robust against el-ph
Figure 5.5: Momentum distribution function for the same parameter values as in Fig. 5.4. Solid (black), dashed (red), dotted (green), dashed-dotted (blue), dashed-dotted-dashed (cyan), short-dashed (magenta), represent respectively $g = 0.2, 0.6, 1.0, 1.2, 1.5, 2.0$. Inset: Luttinger parameter $K$ as a function of $g$, extracted from the electronic density-density correlation function.

coupling: the phonons couple mainly with charge degrees of freedom, leaving the spinon band almost unaffected.

For $g = 1.2$, the original triangular feature in the PES is completely collapsed to a flat structure. Also, if one looks at Fig. 5.3 for $k = 0$ and $k = k_F$ for the same value of $g$, the height of the first spectral peak is dramatically increased with respect to the case of $g = 1.0$. This indicates that one is entered in the strong el-ph coupling regime where the main band is followed by many side-bands coming from both holon and spinon bands. This description, as one can see in Fig. 5.4, is even more evident for $g = 1.5$, where the PES is broken in spectral lines whose weight decreases from the first structure to the following and extends beyond the Fermi momentum $k_F$. Besides, the separation between the holon and the spinon peak is not discernible anymore, suggesting that the system is going towards a state that can be described in terms of a spinless polaronic liquid where the spins are completely uncorrelated. Indeed, for $g = 2.0$, the physics of phonon
side-bands is dominating the PES, and several spectral structures have a smaller width (compared to $g = 1.5$ results), and larger height, while the first spectral structure has less weight than the second one.

At strong el-ph coupling, the ZFA approach provides $\tilde{f} = 0.675$ for $g = 1.5$ and $\tilde{f} = 0.975$ for $g = 2.0$. In these cases, the PES calculated within the ZFA approach gives the same number of phonon side bands with widths and heights of the same order of magnitude as the tDMRG results. Strikingly, the ZFA approach is giving qualitatively the same non-zero spectral weight distribution at momenta larger than $k_F$, confirming that, in this case, the system can be described as a polaron liquid.

In order to investigate further this behavior, we have studied the ground state momentum distribution function $n_k = (1/L) \sum_{i,j} e^{-ik(i-j)} \langle c_i^\dagger c_j \rangle$ and the spin-spin correlation function in real space, $\langle S_z(L/2)S_z(L/2+i) \rangle$ from the center of the chain. As expected for correlated 1D systems, the momentum distribution function shown in Fig.5.5 presents a smooth
decrease at the Fermi momentum $k_F$ for all el-ph coupling values. We point out that the el-ph coupling reduces the decrease at $k_F$ and, globally, it broadens the momentum distribution function. Eventually, for $g = 2.0$, one gets an almost flat profile with $n_{k=0} \simeq 0.45$ and $n_{k=\pi} \simeq 0.325$. In the inset of Fig.5.5, the Luttinger parameter $K$ extracted from the density-density correlation function slope at small momentum[150] is plotted as a function of the el-ph interaction. According to Luttinger liquid theory[151], in the weak el-ph coupling regime one has $K = 1/2$ as in the $U \to \infty$ limit without phonons. As one can observe in Fig.5.5, by increasing the el-ph interaction, $K$ remains constant and equal to 1/2 up to $g = 1.2$, and then increases because the el-ph coupling reduces the effective el-el interaction ($\tilde{U} = U - 2g^2\omega_0$).

In Fig.5.6, the spin-spin correlations as a function of the distance from the center of the chain are shown both in logarithmic (panel (a)) and in linear scale (panel (b)). In the first case, it decreases linearly and its slope is decreasing as a function of the el-ph interaction (see inset of panel (a)). Up to $g = 1.6$, spin-spin correlations decay approximately with the same behavior. For $g > 1.6$, one observes a smooth crossover towards a polaronic regime where spin degrees of freedom are completely uncorrelated. It is important to note that tDMRG results automatically contain information about the shift in the chemical potential mentioned in the previous section. The optimal shift given by the ZFA approach is in total agreement with the chemical potential calculated with static DMRG in the entire range of el-ph couplings.

5.2.2 tDMRG results for intermediate el-ph coupling

In this section, we extend the analysis by discussing the tDMRG results for intermediate el-ph coupling $g = 1.0$, as a function of the phonon frequency $\omega_0$. The results are shown in Fig.5.7. For $\omega_0 = 0.5$, we observe a behavior different from that discussed in the previous section. For instance, at $k = 0$, a dip structure at the left side of the spinon peak is shifted by a quantity equal to $\omega_0 = 0.5$, reproducing qualitatively the results discussed in Ref.[125]. In this reference, the PES is constructed by a superposition of a set of holon
dispersions forming a cosine band with width $4t$ in the absence of el-ph interaction. Moreover, each holon dispersion is characterized by one spinon momentum. In the presence of el-ph interaction, due to spin-charge separation each holon couples with phonons independently and the PES is interpreted as a spectrum of spinless electron dressed by Einstein phonons. This generates a split of the holon dispersion that is shifted from the top of the spectrum by an energy interval equal to $\omega_0$, and a transfer of spectral weight to high energy giving a characteristic peak-dip-hump structure. Our results are consistent with this picture, confirming that spin-charge separation is robust in this regime. In contrast to what discussed in the previous section for $\omega_0 = 2.0$, where polaronic effects dominate and the phonon frequency is smaller than the hopping $t$, the el-ph coupling effect gives rise to a dip in between the holon and spinon peak. Moreover, this dip structure in the spectrum shifts by an energy proportional to $\omega_0$ (see panel (b) of Fig.5.7 for $\omega_0 = 1.0$ and $k = 0$). In this case, our data shows also a shoulder on the left side of the holon peak, in contrast to what found in Ref.[125]. In our calculation, this feature can be interpreted as the onset of phonon side-bands. Increasing the phonon frequency to $\omega_0 = 2.0$, several sidebands in the PES are found as discussed in the previous section. Interestingly, at $k = k_F$, instead of a dip we find a peak separated from the spinon band by an energy difference equal to $\omega_0$. Eventually, at the Fermi momentum and for larger frequencies, these features become part of the first and the higher side-bands.

We can now briefly discuss the results described above making contact with the experiments described in Ref.[123]. In this paper, the authors measure the RIXS spectra of a family of quasi 1D cuprates $Ca_{2+5x}Y_{2-5x}Cu_5O_{10}$, an insulating system that can be doped over a wide range of hole concentrations. The experiment reveals a phonon with energy equal to 70 meV (a quantity larger than the typical transfer hopping $t$ along the chains in quasi 1-D cuprates) strongly coupled to the electronic state at different hole dopings. It is found that the spectral weight of phonon excitations in the RIXS spectrum is directly dependent on the el-ph coupling strength and doping, producing multiple peaks in the spectrum with an energy separation corresponding to the energy of the quanta of the lattice vibrations, in a fashion similar to what was obtained here[152]. We believe
that, even in ARPES spectra of these materials, phonon side-band structures could be experimentally observable in the PES.

5.3 Conclusions

In this chapter, we studied the spectral function of the 1D HH model using the tDMRG method, in the limit of large Coulomb repulsion, and away from electronic half-filling. The entire range of the el-ph coupling has been studied. Our results indicate that from weak to intermediate $g$ spin-charge separation is robust against el-ph coupling: the phonons couple mainly with the charge degrees of freedom, leaving the spinon band almost unaffected. For sufficiently strong el-ph interaction, the PES weight is redistributed in phonon side-bands, and the spinon and holon spectral features are not discernible anymore. In this regime, we support the numerical tDMRG results with an analytical calculation, determining variationally the amount of spectral redistribution and approximating the wave-function as a convolution of charge, spin and phonon parts. In this case, a very good qualitative
and quantitative agreement is obtained, and the system can be described as a polaronic liquid, with non-zero spectral weight at momenta larger than the Fermi momentum.
Chapter 6

Conclusions

In this work we have focused on the properties of one-dimensional models for strongly interacting electrons. In particular, we focused on the phenomenon of spin-charge separation, which is ubiquitous in these systems. We described this phenomenon within the formalism of Bethe Ansatz, using the Ogata-Shiba’s factorized wave-function. We have unambiguously shown, using variational and numerical techniques, that certain families of one-dimensional systems present spin-incoherent behavior in the ground-state. Two examples of such systems studied here are a $t-J$ ladder consisting of two antiferromagnetically coupled $t-J$ chains, and a $t-J-Kondo$ chain with strongly interacting conduction electrons coupled to localized spins. These spin-incoherent states can be accurately written as a factorized wave-function, with a spin wave-function that can be described within a valence bond formalism as it was generalized for our ladder problems. This enabled us to calculate exact expressions for the momentum distribution function and the entanglement entropy. We argued that this theory is quite universal and may describe a family of problems that could be considered spin incoherent.

In chapter 4, we showed a numerical approach to calculate the spectral function at zero and finite temperature. We used the tDMRG technique to calculate the dynamical contributions of the spin, to reconstruct the single-particle spectral function of the electrons for a strongly interacting Hubbard chain (with $U \to \infty$) at finite temperatures. We saw
a crossover to a spin-incoherent regime when the temperature is very small relative to the Fermi energy, but larger than the characteristic spin energy scale. The crossover is characterized by a redistribution of spectral weight both in frequency and momentum, with an apparent shift by $k_F$ of the minimum of the dispersion. This crossover can be understood by means of Ogata and Shiba’s factorized wave-function, where charge and spin are totally decoupled, and assuming that the charge remains in the ground state, while the spin is thermally excited and at an effective “spin temperature”.

Finally, we investigated the spectral properties by introducing the phonons into the problem. We calculated the spectral function of the 1D Hubbard-Holstein model using the tDMRG, focusing on the regime of large local Coulomb repulsion, and away from electronic half-filling. We have shown that from weak to intermediate electron-phonon coupling, phonons interact only with the electronic charge, and not with the spin degrees of freedom. For strong electron-phonon interaction, spinon and holon bands are not discernible anymore and the system is well described by a spinless polaronic liquid. In this regime, we observed multiple peaks in the spectrum with an energy separation corresponding to the energy of the lattice vibrations. We supported the numerical results by introducing a well controlled analytical approach based on Ogata-Shiba’s factorized wave-function, showing that the spectrum can be understood as a convolution of three contributions, originating from charge, spin, and lattice sectors. We recognized and interpreted these signatures in the spectral properties and discussed the experimental implications.

It would be desirable to follow up on these works by introducing hopping between chains to see how it affects the spin behavior. In addition, we have seen that the $t - J$-Kondo chain displays a mixture of Fermi-liquid-like behavior combined with Luttinger Liquid behavior. It would be useful to study larger systems to understand to what extent this behavior can be explained by finite-size effects.

A natural extension of these projects is to study the effects of second neighbor hopping along a single chain [153, 154, 155], in the $J \to 0$ limit. A second neighbor coupling would
introduce an effective ring exchange in the spin part of the factorized wave-function, and may lead to some exotic physics beyond the Luttinger liquid paradigm.

Another follow-up project would consist of studying electronic transport through a $t - J$ ladder (governed by the Hamiltonian described previously) by connecting the ladder to non-interacting leads, and applying a bias. The transport dynamics can be studied using the time-dependent DMRG. There is no hopping between the chains and since spins on both chains get entangled, it would be interesting to see how this entanglement effects the transport. This problem could be relevant to experiments in quantum point contacts, and the observed 0.7 anomaly (which has been attributed to SILL behavior) [31, 156, 157, 158, 159]. In this context, it would also be interesting to investigate the effect of a magnetic field, which is known to destroy this anomaly, since it introduces a new energy scale in the problem, making the spins point in the direction of the field.
Bibliography


Appendix A

Effective theory for the Hubbard model in the strong coupling limit: the $t - J$ Hamiltonian

In this appendix we will show how to carry out the mapping of a Hubbard Hamiltonian in the limits of $U \to \infty$ to a $t - J$ Hamiltonian, where we will be dealing with a reduced Hilbert space and a more feasible model for practical purposes. For more details one can refer to Ref. [160] and for a more complete derivation Appendix A. of Stephen W. Haas’s Ph.D. dissertation, 1995 is a great resource.

The Hubbard Hamiltonian in 1D is

$$H = -t \sum_{i,\sigma} \left( c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \quad (A.1)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (destroys) an electron of spin $\sigma$ on the $i^{th}$ site along a chain of length $L$, and $n_{i,\sigma}$ is the particle number operator.
We will consider the case of less than half feeling, as the half-filling case becomes a trivial problem and translates into the Heisenberg Hamiltonian that we discussed in Chapter 1. Electron-hole symmetry makes it equivalent to the case where the filling is more than one half. We define a new Hilbert space where all the states allowing double occupancy are excluded. Now our goal is to define an effective Hamiltonian acting on this reduced Hilbert space, dealing with a smaller number of configurations (the ones with no double occupancy) and a more practical model. In order to get this effective Hamiltonian one can use the unitary Schrieffer-Wolff transformation which will enable us to obtain effective low energy physics. \(^\dagger\)

We define the operator a projection operator \(P\) that projects the states it acts on onto the new reduced Hilbert space with no double occupancy. This operator satisfies the relation \(P^2 = P\), and as a consequence the operator \(Q = 1 - P\) projects the states onto a different Hilbert space of configurations with double occupancy.

Applying this unitary transformation on our Hamiltonian from Eq.(A.1) results in

\[
\tilde{H} = PHP - \frac{1}{U}PHQHP.
\]

The second term of Eq. (A.2) acts on doubly occupied states, otherwise it will return zero. The cost for the system of having this doubly occupied site is \(U\) and that’s equivalent to the increase in energy by \(U\) in this case. The \(P\) and \(Q\) definitions can be satisfied by

\(^\dagger\)One of the applications of Schrieffer-Wolff method is the derivation of the Kondo model from single impurity Anderson model, as first noticed by J.R. Schrieffer and P.A. Wolff.
\begin{align*}
PHP &= -t \sum_{i,\sigma} (c_{i\sigma}^\dagger (1 - n_{i, \bar{\sigma}}) c_{i+1\sigma} (1 - n_{i+1, \bar{\sigma}}) + h.c.), \\
QHP &= -t \sum_{i,\sigma} n_{i,\bar{\sigma}} c_{i\sigma}^\dagger c_{i+1\sigma} (1 - n_{i+1,\bar{\sigma}}), \\
PHQ &= -t \sum_{i,\sigma} (1 - n_{i,\bar{\sigma}}) c_{i\sigma}^\dagger c_{i+1\sigma} n_{i+1,\bar{\sigma}}. \tag{A.3}
\end{align*}

Using these transformations the transformed Hamiltonian becomes

\begin{align*}
\hat{H} &= -t \sum_{i,\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{i+1\sigma} + h.c.) + \frac{4t^2}{U} \sum_i (S_i S_{i+1} - \hat{n}_i \hat{n}_{i+1} - \frac{3}{4}) \\
&\quad - \frac{t^2}{U} \sum_{i\sigma} (\hat{c}_{i-1\sigma}^\dagger \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \hat{c}_{i+1\sigma} - \hat{c}_{i-1\sigma}^\dagger \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \hat{c}_{i+1\sigma} + h.c.). \tag{A.4}
\end{align*}

In this equation operator $\hat{c}_{i\sigma}^\dagger$ ($\hat{c}_{i\sigma}$) creates (annihilates) an electron with spin $\sigma$ at site $i$ in the reduced Hilbert space, where this creation (annihilation) is allowed only if there is no other electron (even with opposite spin) sitting on that site

\begin{align*}
\hat{c}_{i\sigma}^\dagger &= c_{i\sigma}^\dagger (1 - n_{i\bar{\sigma}}), \\
\hat{c}_{i\sigma} &= c_{i\sigma} (1 - n_{i\bar{\sigma}}), \\
\hat{n}_{i\sigma} &= c_{i\sigma}^\dagger c_{i\sigma}. \tag{A.5}
\end{align*}

These new projected operators do not satisfy the canonical anti-commutation relations. The spin operator $S_i$ is defined as

\begin{equation}
S_i = \frac{1}{2} \sum_{\alpha\beta} \sigma_{\alpha\beta} \hat{c}^\dagger_{i\alpha} \hat{c}_{i\beta}. \tag{A.6}
\end{equation}
In $\tilde{H}$, the three site term is leads to indirect hopping between nearest neighbors and could only exist for systems away from half filling. Comparing the magnitude of this hopping with the direct one, it’s in the order of $t/U$ of the direct hopping. In many low doping concentration cases this term is dropped and still we get a precise picture of the problem especially in the limit of large $U$ this term will play a negligible rule in the Hamiltonian.

In this case, our Hubbard Hamiltonian (Eq. A.1) becomes the $t - J$ Hamiltonian

$$H_{t-J} = -t \sum_{i,\sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{i+1\sigma} + h.c.) + J \sum_i (S_i S_{i+1} - \hat{n}_i \hat{n}_{i+1}/4),$$

(A.7)

In the limit of half filling, $H_{t-J}$ is the Hamiltonian of a Heisenberg antiferromagnet.
Appendix B

Entanglement entropy and correlations by variational tools

In this appendix we show the calculation of the entanglement entropy between the conduction electrons in one chain, and the bath. In the $t-J$ ladder, the bath is modeled by a second chain, while in the $t-J-$Kondo model, by localized impurities. As illustrated in Figures 3.2 and 3.5, we squeeze the chain by removing all the unoccupied sites, reducing the configuration space to a spin problem with no charge. In these cartoons, the black dots and white dots will be referred to as A and B sub-lattices. Each sub-lattice will have $N$ sites, instead of $L$ since we have removed the empty sites, where $N$ is the number of electrons in the chain.

We start by considering the $t-J$ ladder, in which both sub-lattices have the same number of sites, and the ground-state is represented by all possible VB coverings connecting the two. Instead of using the overcomplete VB basis for the calculation, we will work in the space of spin configurations. In this basis, the states can be classified by the number $N_\uparrow$ of down spins in sub-lattice A. Since the total spins projection $S^z$ is conserved, this
also fixes the number of down spins on sub-lattice B. The coefficient in front of each configuration is then given by

\[ g(N, N_\downarrow) = N_\downarrow!(N - N_\downarrow)! \times (-1)^{N_\downarrow}, \quad (B.1) \]

which counts the number of times each of them is repeated in the ground-state, times a sign arising from the singlets (we have ignored the normalization for the time being).

The Von Neumann entanglement entropy \( S \) is defined as

\[ S_A = -\text{Tr} \left( \rho_A \log \rho_A \right), \quad (B.2) \]

where \( \rho_A \) is the reduced density matrix for sub-lattice A, obtained by tracing over the states on sub-lattice B. It is easy to see that \( \rho_A \) can be separated into blocks, each labeled by \( N_\downarrow \), since it can assume values \( N_\downarrow = 0, \cdots, N \), the number of such blocks is \( N + 1 \).

The linear dimension for each block is given by the number of possible arrangements of \( N_\downarrow \) spins in \( N \) sites:

\[ d(N, N_\downarrow) = \frac{N!}{N_\downarrow!(N - N_\downarrow)!}. \]

It is easy to see that, since all configurations with fixed \( N_\downarrow \) will appear with the same coefficient, each block will have all matrix elements equal to \( \rho_A(N, N_\downarrow)_{i,j} = d(N, N_\downarrow)g^2(N, N_\downarrow) \):

\[ \rho_A(N, N_\downarrow) = d(N, N_\downarrow)g^2(N, N_\downarrow) \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \quad (B.3) \]

This matrix has only a single non-zero eigenvalue \( w(N, N_\downarrow) = d^2(N, N_\downarrow)g^2(N, N_\downarrow) = (N!)^2 \), the same for all blocks. Finally, the full matrix has to be normalized such that
\( \text{Tr}(\rho_A) = 1 \). Therefore, we obtain \( N + 1 \) blocks, each with a single non-zero eigenvalue \( w = 1/(N + 1) \). Hence, the entanglement entropy (B.2) is given by:

\[
S_A = \log (N + 1),
\]

which is our final result.

This expression is equivalent to two spins \( S = N/2 \) in a maximally entangled state, where each spin is obtained by the addition of the \( N \) spins 1/2 of each sub-lattice. This analogy can be made rigorous by observing that the spin wave-function is the ground-state of the Hamiltonian:

\[
H_{AB} = \sum_{i,j} \vec{s}_{i,A} \cdot \vec{s}_{j,B} = \vec{S}_A \cdot \vec{S}_B,
\]

with \( \vec{S}_A = \sum_i \vec{s}_{i,A} \), and a similar expression for sub-lattice B. The ground state is a singlet of two spins \( S = N/2 \), a maximally entangled state. Notice that this is not the actual spin Hamiltonian for the coupled \( t - J \) chains, since the spectra are different. Now we can make use of this solution to calculate the spin-spin correlations. The Hamiltonian can be re-written as:

\[
H_{AB} = \frac{1}{2} \left[ (\vec{S}_A + \vec{S}_B)^2 - \vec{S}_A^2 - \vec{S}_B^2 \right].
\]

From this expression, we obtain the ground-state energy:

\[
\langle H_{AB} \rangle = \sum_{i,j} \langle \vec{s}_{i,A} \cdot \vec{s}_{j,B} \rangle = -\frac{N}{2} \left( \frac{N}{2} + 1 \right).
\]

Since all the correlators should be equal, we find:

\[
\langle \vec{s}_{i,A} \cdot \vec{s}_{j,B} \rangle = \frac{1}{N^2} \langle H_{AB} \rangle = -\frac{1}{4} - \frac{1}{2N},
\]

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In order to calculate the correlations in the actual $t - J$ ladder we need to include the charge contribution:

$$\langle \vec{s}_{i,1} \cdot \vec{s}_{j,2} \rangle = (-\frac{1}{4} - \frac{1}{2N}) \langle n_{i,1} n_{j,2} \rangle = (-\frac{1}{4} - \frac{1}{2N}) \left( \frac{N}{L} \right)^2,$$

which indicates that the correlations saturate in the thermodynamic limit.

The calculation for the $t - J$–Kondo lattice follows identical steps, except that since the B sub-lattice has $L$ sites, the degeneracy for each sector acquires a slightly more elaborate form:

$$g(L, N, N_i) = \frac{(N - N_i)! (L - N + N_i)!}{(L - N)!} \times (-1)^{N_i}$$

In this case, the single non-zero eigenvalues for each sector are given by:

$$w(L, N, N_i) = d(L, N, N_i) g^2(L, N, N_i) d_B(L, N, N_i),$$

where

$$d_B(L, N, N_i) = \frac{L!}{(L - N + N_i)! (N - N_i)!}$$

is the number of configurations in the B sub-lattice, for each configuration of the A sub-lattice. Since the eigenvalues are different for each sector, the normalization and the entropy are obtained by adding numerically over the $N + 1$ blocks.
Appendix C

Independent Boson model

This appendix focuses on studying the single particle Green’s function of an electron placed in a tight-binding lattice and locally interacting with a bosonic bath. We will start with the simple example of one electron sitting on a single lattice site which was discussed in Mahan’s Many-particle physics, and will expand our treatment to the case of two and $n$ lattice sites.

C.1 One electron on a single lattice site

The Hamiltonian of one single localized electron with energy $\epsilon_c$ sitting on a lattice site interacting with a set of phonons with frequencies $\omega_q$ is given by

$$H = c^+ c [\epsilon_c + \sum_q (a_q + a_q^+) M_q] + \sum_q \omega_q a_q^+ a_q.$$  \hfill (C.1)
In this basis, electron and phonon operators are entangled which makes the Hamiltonian difficult to solve. A change of basis can be done by applying a standard unitary transformation to the Hamiltonian (C.1) and as a result one can separate electronic and phononic systems solving exactly the problem. The unitary transformation reads

$$\bar{H} = e^s He^{-s}. \quad (C.2)$$

where $s$ is an anti-Hermitian operator ($s^+ = -s$) given by

$$s = c^+ c \sum_q \frac{M_q}{\omega_q} (a_q - a_q^+). \quad (C.3)$$

By using the following identities

$$(ABC\ldots Z) = AB\tilde{C}\ldots \tilde{Z},$$

$$f(A) = f(\tilde{A}),$$

$$\tilde{A} = e^s Ae^{-s} = A + [s, A] + \frac{1}{2} [s, [s, A]] + \ldots,$$

$$[AB, C] = A\{B, C\} - \{A, C\}B,$$

and defining $\chi = e^{-\sum \frac{M_q}{\omega_q} (a_q - a_q^+)}$, our new electronic and phononic operators read

$$\tilde{c} = c \chi, \quad \tilde{c}^+ = c^+ \chi^+, \quad \tilde{a}_q = a_q - \frac{M_q}{\omega_q} c^+ c \quad \& \quad \tilde{a}_q^+ = a_q^+ - \frac{M_q}{\omega_q} c^+ c, \quad (C.4)$$

and the transformed Hamiltonian becomes

$$\bar{H} = \tilde{c}^+ \tilde{c} (\epsilon_c - \Delta) + \sum_q \omega_q \tilde{a}_q^+ \tilde{a}_q. \quad (C.5)$$
where $\Delta \equiv \sum_q \frac{M_q^2}{\omega_q}$. Note that $\bar{c}$ and $\bar{c}^+$ do not commute with $\bar{a}$ and $\bar{a}^+$ anymore. Even with this complication, it is important to point out that in the transformed Hilbert space the electrons and phonons decouple completely. In the next section we will briefly show how the calculation of the single particle Green’s function in this case becomes trivial and allows us to obtain the full interacting Green’s function in the original Hilbert space.

### C.1.1 Electronic Green’s function

At zero temperature the time ordered single particle electronic Green’s function is defined as

$$G(t) = -i \langle T_t \ c(t)c^+(0) \rangle. \quad (C.6)$$

For $t > 0$ one can obtain straightforwardly the retarded Green’s function

$$G(t) = -i e^{\beta \Omega} \ Tr[e^{-\beta H}(e^{iHt}c e^{-iHt}c^+ e^{-\beta}e^s)], \quad (C.7)$$

where we have introduced a temperature $T = 1/\beta$ for the phononic bath. Using the cyclic property and adding $e^{-s} e^s = 1$, one can transform the above expression back to the initial Hilbert space

$$G(t) = -i e^{\beta \Omega} \ Tr[e^{-\beta H} e^{i\bar{H}t}c e^{-i\bar{H}t}c^+], \quad (C.8)$$

where replacing $\bar{c}$ and $\bar{c}^+$ with their transformed counterparts yields to

$$G(t) = -i e^{\beta \Omega} \ Tr[e^{-\beta H} e^{i\bar{H}t}c \chi e^{-i\bar{H}t}c^+ \chi^+]. \quad (C.9)$$
We notice here that by the substitution $e^{iBt}c\chi e^{-iBt} = e^{-it(\epsilon_c-\Delta)}c\chi(t)$ where $\chi(t) = -\sum_q \frac{M_q}{\omega_q} (a_q^+ e^{i\omega_q t} - a_q e^{-i\omega_q t})$ one gets

$$G(t) = -i e^{\beta \Omega} \text{Tr}(e^{-\beta \bar{\epsilon}_c c^+ c}) e^{-it\bar{\epsilon}_c} \text{Tr}(e^{-\beta H_p} \chi(t) \chi^+(0)),$$

(C.10)

where $\bar{\epsilon}_c = \epsilon_c - \Delta$ and $H_p = \sum_q \omega_q a_q^+ a_q$.

Summarizing, the electronic part of the Green’s function can be calculated exactly giving

$$G_e(t) = -i(1 - n_F(\bar{\epsilon}_c)) e^{-it\bar{\epsilon}_c},$$

(C.11)

where we have used $e^{\beta \Omega} \text{Tr}(e^{-\beta \bar{\epsilon}_c c^+ c}) = 1 - n_F(\bar{\epsilon}_c)$. We can now obtain the phonon part by taking advantage of Feynman’s method of disentangling of operators. This approach is not trivial, and we carry it out exactly in the next section.

C.1.1.1 Feynman Disentangling of operators

For convenience, it is useful to rewrite the phononic part of the electronic Green’s function

$$F(t) = e^{\beta \Omega_{ph}} \text{Tr}[e^{-\beta \sum_q \omega_q n_q} \chi(t) \chi^+(0)],$$

(C.12)

which can be written as a multiplication of terms with different wave numbers

$$F(t) = \prod_q f_q(t),$$

(C.13)

where $f_q = e^{\beta \Omega_q} \sum_{n_q=0}^{\infty} e^{-\beta n_q \omega_q} \langle n_q | e^{-\lambda_q B_q(t)} e^{\lambda_q B_q(0)} | n_q \rangle$, and we have defined $\lambda_q = \frac{M_q}{\omega_q}$ and $B_q(t) = a_q^+ e^{i\omega_q t} - a_q e^{-i\omega_q t}$.  

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Using $e^{\beta \Omega_q} = \left( \sum_{n_q=0}^{\infty} e^{-\beta n_q \omega_q} \right)^{-1} = 1 - e^{-\beta \omega_q}$ and dropping $q$ for simplicity one gets

$$f(t) = (1 - e^{-\beta \omega}) \sum_{n=0}^{\infty} e^{-\beta n \omega} \langle n | e^{-\lambda (a^+ \omega t - a \omega t)} e^{\lambda (a - a^+)} | n \rangle,$$  \hspace{1cm} (C.14)

where $|n\rangle = \frac{(a^+)^n}{\sqrt{n!}} |0\rangle$.

We now will separate the exponents of the term in the trace by using Feynman’s theorem on the disentangling of operators

If $[A, [A, B]] = [B, [A, B]] = 0$ then $e^{A+B} = e^A e^B e^{-1/2 [A, B]}$.

Using this theorem we get

$$e^{-\lambda (a^+ \omega t - a \omega t)} e^{\lambda (a^+ - a)} = e^{-\lambda^2 (1 - e^{-i \omega t})} e^{\lambda a^+ (1 - e^{i \omega t})} e^{-\lambda a (1 - e^{-i \omega t})}$$

which gives

$$f(t) = (1 - e^{-\beta \omega}) e^{-\lambda^2 (1 - e^{-i \omega t})} \sum_{n=0}^{\infty} e^{-\beta n \omega} \langle n | e^{\lambda a^+ (1 - e^{i \omega t})} e^{-\lambda a (1 - e^{-i \omega t})} | n \rangle,$$  \hspace{1cm} (C.15)

But $(1 - e^{-\beta \omega}) \sum_{n=0}^{\infty} e^{-\beta n \omega} \langle n | e^{\omega^* a^+ - a \omega} | n \rangle = e^{-|\omega|^2} N$, where $N = \frac{1}{e^{\pi \omega^2} - 1}$ and $u = \lambda (1 - e^{-i \omega t})$, so

$$f(t) = e^{-\phi(t)},$$  \hspace{1cm} (C.16)

where $\phi(t) = \lambda^2 [(1 - e^{-i \omega t}) + N |1 - e^{i \omega t}|^2] = \lambda^2 [(N + 1)(1 - e^{-i \omega t}) + N (1 - e^{i \omega t})]$. Now we can write the phononic Green’s function, $F(t)$, as

$$F(t) = \prod_q f_q(t) = e^{\sum_q \phi_q(t)} = e^{-\Phi(t)},$$  \hspace{1cm} (C.17)

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where \( \Phi(t) = \sum_q (\frac{M_q}{\omega_q})^2 [N_q (1 - e^{i\omega_q t}) + (N_q + 1)(1 - e^{-i\omega_q t})]. \) \( (N_q = \frac{1}{e^{\beta \omega_q} - 1}) \)

We summarize the complete \( G \) as

\[
for \ t > 0 \quad G(t) = -ie^{-it(\epsilon_c - \Delta)} (1 - n_F) e^{-\Phi(t)}.
\] (C.18)

This is an exact equation. In the next section, we will apply the above method to the case where all the frequencies of the phononic bath are assumed equal to each other (Einstein model).

### C.1.2 Einstein model

Now let’s examine this model for a simple example where all the phonons have the same energy at zero temperature, \( T = 0 \)

\[ \omega_q = \omega_0, \quad T = 0 \Rightarrow N_q = N_0 = 0. \]

Since the phonon occupation factors are 0, we end up with a constant coupling

\[ g = \sum_q \frac{M_q^2}{\omega_0} \text{ (constant)}. \]

which results in \( \Delta = g \omega_0 \) and

\[ \Phi(t) = g(1 - e^{-i\omega_0 t}). \] (C.19)

The Green’s function will be evaluated for the case of a single particle so we set \( n_F = 0 \)

\[ G(t) = -i \theta(t) \exp[-i t \epsilon_c - g(1 - i\omega_0 t - e^{-i\omega_0 t})]. \] (C.20)
The same result is obtained for the retarded function, here $\theta(t)$ is a step function on time. The spectral function $A(\omega)$ is then the imaginary part of the retarded Green’s function of the frequency

$$A(\omega) = -2 \text{Im}\{ -i \int_{0}^{\infty} dt \ e^{i\omega t} \exp[-i t \epsilon_c - g(1 - i\omega_0 t - e^{-i\omega_0 t})]\}$$

$$= 2 \text{Re}\{ \int_{0}^{\infty} dt \ e^{i\omega t} \exp[-i t \epsilon_c - g(1 - i\omega_0 t - e^{-i\omega_0 t})]\}. \quad (C.21)$$

Using

$$\exp(g e^{-i\omega_0 t}) = \sum_{l} \frac{g^l}{l!} e^{-i\omega_0 tl},$$

$$\int_{0}^{\infty} dt \ \exp[i t(\omega - \epsilon_c + \Delta - \omega_0 l)] = \frac{i}{\omega + \Delta - \epsilon_c - \omega_0 l + i\delta},$$

and the integral

$$\delta \to 0 : \int_{0}^{\infty} dt \ \exp[i t(\omega - \epsilon_c + \Delta - \omega_0 l)] = P\frac{i}{\omega + \Delta - \epsilon_c - \omega_0 l} + \pi\delta(\omega + \Delta - \epsilon_c - \omega_0 l),$$

we get for the spectral function

$$A(\omega) = 2 \pi e^{-g} \sum_{l=0}^{\infty} \frac{g^l}{l!} \delta(\omega + \Delta - \epsilon_c - \omega_0 l). \quad (C.22)$$

Which is the probability of having a particle with frequency $\omega$. We see the distribution of peak heights follow a poisson distribution. The spectral function is shown in Figure C.1 for two values of $g = 0.5$ and $g = 5.5$.

For the case of no interaction, $g = 0$, energy of the electron is $\epsilon_c$ and there would be only a single delta peak at $\omega = \epsilon_c$. 

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For $g \neq 0 \Rightarrow \omega_l \equiv \epsilon_c - \Delta + l\omega_0$.

Testing the sum rule

Since there is only one electron we expect the sum over the spectral weight to be one

$$1 = \int_{\infty}^{\infty} \frac{d\omega}{2\pi} A(\omega) = e^{-g} \sum_{l} \int_{\infty}^{\infty} d\omega \delta(\omega - \omega_l) = e^{-g} \sum_{l} \frac{\omega_l}{\pi} = 1.$$ 

So the distribution of energy has to add up to the total energy of one electron which is $\epsilon_c$

$$\epsilon_c = \int_{\infty}^{\infty} \frac{d\omega}{2\pi} \omega A(\omega) = \langle \omega \rangle = \sum_{l} \frac{\omega_l}{\pi} (\epsilon_c - \Delta + \omega_0 l) = \epsilon_c - \Delta + g \omega_0 = \epsilon_c$$
C.2 One electron on two or more lattice sites

In this section we consider the case where a single electron is hopping on a two-lattice-site Hamiltonian

\[ H = \epsilon_1 c_1^+ c_1 + \epsilon_2 c_2^+ c_2 - t(c_1^+ c_2 + h.c.) \]  \hspace{1cm} (C.23)

\[ + \omega_1 (a_1^+ a_1 + \frac{1}{2}) + \omega_2 (a_2^+ a_2 + \frac{1}{2}) \]

\[ + M_1 c_1^+ c_1 (a_1 + a_1^+) + M_2 c_2^+ c_2 (a_2 + a_2^+). \]

We point out that all the calculations performed for the two sites lattice can be extended straightforwardly to the case of an \( n \) sites lattice Hamiltonian as explained below. Without loss of generality for our purposes we can simplify the Hamiltonian (C.23) by taking these values for the parameters

\[
\begin{align*}
\epsilon_1 &= \epsilon_2 = 0 \\
\omega_1 &= \omega_2 = \omega_0 \\
M_1 &= M_2 = M = g\omega_0.
\end{align*}
\]

The new Hamiltonian becomes

\[ H = -t(c_1^+ c_2 + h.c.) + \omega_0(a_1^+ a_1 + a_2^+ a_2 + 1) \]

\[ + g\omega_0 [c_1^+ c_1 (a_1 + a_1^+) + c_2^+ c_2 (a_2 + a_2^+)]. \] \hspace{1cm} (C.24)

Applying the transformation (\( \tilde{H} = e^s H e^{-s} \), which is a simple generalization of the transformation introduced in the single site lattice case) with \( s = s_1 + s_2 \) where \( s_i = \lambda c_i^+ (a_i^+ - a_i) \) for \( i = 1, 2 \) gives new operators
\[ \left\{ \begin{array}{ll}
\bar{c}_i = c_i \chi_i, & \bar{c}_i^+ = c_i^+ \chi_i^+ \\
\bar{a}_i = a_i - g c_i^+ c_i, & \bar{a}_i^+ = a_i^+ - g c_i^+ c_i,
\end{array} \right. \]

where \( \chi_i = e^{-g(a_i^+-a_i)} \), and the new transformed Hamiltonian \( \bar{H} \) becomes

\[ \bar{H} = -t(c_1^+ \chi_1^+ c_2 + h.c.) + \omega_0(a_1^+ a_1 + a_2^+ a_2 + 1) - g^2 \omega_0(c_1^+ c_1 + c_2^+ c_2). \tag{C.25} \]

Now we split the Hamiltonian (C.25) into two non-interacting \( (H_0) \) and interacting \( (V) \) parts. In the following we will also drop the bar coming from the transformation

\[ H = H_0 + V, \tag{C.26} \]

where

\[ H_0 \equiv H_{ph} + H_{eff}, \]

\[ V \equiv H - H_0, \]

where \( H_{ph} \) is defined as

\[ H_{ph} \equiv \omega_0(a_1^+ a_1 + a_2^+ a_2 + 1), \]

and \( H_{eff} \) includes the electronic terms in the Hamiltonian with no interaction but effected by the phonons

\[ H_{eff} \equiv \langle O_{ph}|H|O_{ph}\rangle. \]
Here \( |O_{ph,1} \rangle \times |O_{ph,2} \rangle \) is the phonon vacuum. Applying the phonon vacuum on \( H \) we get

\[
H_{\text{eff}} = -t(c_1^+ c_2 \langle \chi_1^+ \chi_2 \rangle + \text{h.c.}) - g^2 \omega_0(c_1^+ c_1 + c_2^+ c_2),
\]

having \( \langle \chi_1^+ \rangle = e^{-g^2/2} \) and \( \langle \chi_1^+ \chi_2 \rangle = \langle \chi_1^+ \rangle \langle \chi_2 \rangle = e^{-g^2} \) gives

\[
H_{\text{eff}} = -te^{-g^2} (c_1^+ c_2 + \text{h.c.}) - g^2 \omega_0(c_1^+ c_1 + c_2^+ c_2),
\]

(C.27)

Repeating this for \( H_0 \) and \( V \) results in

\[
H_0 = -te^{-g^2} (c_1^+ c_2 + \text{h.c.}) - g^2 \omega_0(c_1^+ c_1 + c_2^+ c_2) + \omega_0(a_1^+ a_1 + a_2^+ a_2 + 1),
\]

(C.28)

\[
V = -t[c_1^+(\chi_1^+ \chi_2 - e^{-g^2})c_2 + \text{h.c.}].
\]

(C.29)

In \( V \) the phonon and electron operators are not decoupled. In the following, we will neglect the effect of the perturbation \( V \) for calculating the electronic Green’s functions.

One can prove that this is justified if the phononic energy \( \omega_0 \) is much larger than the hopping parameter \( t \). This represents the particular regime studied analytically in this dissertation. As discussed in the dissertation the inclusion of \( V \) is left as future work.

The calculation of the retarded Green’s function is then straightforward (and can be then generalized trivially to the \( n \) site lattice case)

\[
G_{ij}^R(t) = -i\langle c_i(t) c_j^+(0) \rangle = -i\langle c_i(t) \chi_i(t) \chi_j^+(0) c_j^+(0) \rangle
\]

(C.30)

\[
\simeq -i\langle c_i(t) \chi_i(t) \chi_j^+(0) c_j^+(0) \rangle_{H_0}
\]

\[
= -i\langle c_i(t) c_j^+(0) \rangle_{H_0} \langle \chi_i(t) \chi_j^+(0) \rangle_{H_0},
\]

and one can factorize again electronic and phononic operator as done in the single lattice site case. Furthermore, by defining \( p_{ij}(t) \equiv \langle \chi_i(t) \chi_j^+(0) \rangle_{H_0} \) and \( g_{ij}^R(t) \equiv -i\langle c_i(t) c_j^+(0) \rangle_{H_0} \)
one can write the Green’s function in the frequency space as

\[
G_{ij}^R(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} g_{ij}^R(t) p_{ij}(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{\sqrt{2\pi}} g_{ij}^R(\omega - \epsilon) P_{ij}(\omega). \tag{C.31}
\]

It is important to point out that in frequency space \( p_{ij} \) is independent of the choice of the lattice sites and is just given by \( p_{ij}(\omega) = e^{-g^2} \). Once we have \( G_{ij}^R(\omega) \), \( A_{ij}(\omega) \) can be calculated by

\[
A_{ij}(\omega) = -2 \text{Im}[G_{ij}^R(\omega)]. \tag{C.32}
\]

In the next section we will discuss the calculation for \( g_{ij}^R(t) \) of the two and \( n \) lattice site Hamiltonian.

### C.2.1 Equation of motion technique for solving Green’s function

In this section we will solve the electronic part of the Green’s function with an alternative method known as the equation of motion technique. As explained in the following, this approach is particularly useful for calculating the Green’s function in a chain with many lattice sites.

Let’s first start with the electronic part. The Hamiltonian for a two-site lattice is

\[
H_0 = -t(c_1^\dagger c_2 + h.c.) + \epsilon(c_1^\dagger c_1 + c_2^\dagger c_2).
\]

By definition, the retarded Green’s function \( g_{ij}^R(t) \) is given by

\[
g_{ij}^R(t) = -i\theta(t)\langle \psi_0 | c_i(t) c_j^\dagger(0) | \psi_0 \rangle, \tag{C.33}
\]
which is a $2 \times 2$ matrix
\[
g^R(t) = \begin{pmatrix} g^R_{11}(t) & g^R_{12}(t) \\ g^R_{21}(t) & g^R_{22}(t) \end{pmatrix}.
\] (C.34)

Having $\frac{\partial}{\partial t} \theta(t) = \delta(t)$ and $i \frac{\partial}{\partial t} \epsilon = [c, H_0]$ one can derive the equation of motion for the Green’s function
\[
i \frac{\partial}{\partial t} G^R_{11}(t) = \delta(t) + \epsilon [-i \theta(t)\langle c_1(t), c_1^+(0) \rangle] - t [-i \theta(t)\langle c_2(t), c_1^+(0) \rangle]
= \delta(t) + \epsilon g^R_{11} - tg^R_{21}(t).
\] (C.35)

One can now Fourier transform with respect to the time variable obtaining
\[
\begin{pmatrix} \omega - \epsilon & -t \\ -t & \omega - \epsilon \end{pmatrix} g^R(\omega) = 1,
\] (C.37)

where $1$ represents the identity matrix. The Green’s function $G^R(\omega)$ is now easily obtained by matrix inversion.

$n$ sites

One can easily generalize the above equation to the case of a tight-binding chain of $n$ lattice sites with open boundary conditions. It is easy to show that the single particle
Green’s function (in the transformed space) is given by the following equation

\[
g^R(\omega) = \begin{pmatrix} \omega - \epsilon & t & 0 & \cdots & 0 \\ t & \omega - \epsilon & t & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega - \epsilon & t \end{pmatrix}^{-1}
\]  

\[\text{(C.38)}\]
Vita

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Articles


- **M. Soltanieh-ha**, and A. E. Feiguin, *Phys. Rev. B* 90, 165145 (2014), *Spectral function of the $U \to \infty$ one-dimensional Hubbard model at finite temperature and the crossover to the spin-incoherent regime.*


Selected Conferences and Presentations

- **M. Soltanieh-ha, and A. E. Feiguin** (Oral presentation)
  APS March Meeting, San Antonio, TX  
  **MAR 2015**
  *Magnetic phase diagram of the spatially anisotropic spin-1/2 zigzag ladder.*

- **M. Soltanieh-ha, A. Nocera, C.A. Perroni, V. Cataudella, and A. E. Feiguin**
  Conference on Computational Physics (Poster presentation)
  Boston University, Boston, MA  
  **AUG 2014**
  *Interplay of charge, spin and lattice degrees of freedom on the spectral properties of the one-dimensional Hubbard-Holstein model.*

- **M. Soltanieh-ha,** Preliminary Research Seminar
  Northeastern University, Boston, MA  
  **MAY 2014**
  *Interplay between charge, spin, and phonons in low dimensional strongly interacting systems.*

- **M. Soltanieh-ha, A. Nocera, and A. E. Feiguin** (Oral presentation)
  APS March Meeting, Denver, CO  
  **MAR 2014**
  *Understanding the interplay between charge, spin and phonons in the spectral properties of the 1D Hubbard-Holstein model.*

- **M. Soltanieh-ha,** Physics Department Journal Club Seminar
  Northeastern University, Boston, MA  
  **JAN 2014**
  *Spin-charge separation in one-dimensional electronic systems.*

- **M. Soltanieh-ha, and A. E. Feiguin** (Oral presentation)
  APS March Meeting Conference, Baltimore, MD  
  **MAR 2013**
  *Toward a unified description of spin-incoherent behavior at zero and finite temperatures.*