Temperature-driven spectral weight transfer in doped magnetic insulators

by

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Abstract

In this thesis we study the effects of finite temperature ($T$) on the single-electron spectral function of doped magnetic insulators.

First, we derive the low-temperature correction to the self-energy of a charge carrier injected with parallel spin into a ferromagnetic background which is modeled with both Heisenberg and Ising Hamiltonians so that differences due to gapless versus gapped magnons can be understood. Beside the expected thermal broadening of the $T = 0$ quasiparticle peak which becomes a resonance inside a continuum, we find that spectral weight is transferred to regions lying outside this continuum, because the carrier and a thermal magnon can bind into a spin-polaron. This work is valid in dimensions $d \geq 2$, because it does not include the role of magnetic domains which are important in $1d$.

We then consider the role of these magnetic domains in $1d$ systems, for models where spin-polaron formation is impossible. We present Monte Carlo simulations for the spectral function of three related models of a charge carrier that is injected into an Ising chain. Both ferromagnetic and antiferromagnetic coupling between the Ising spins are considered. The interaction between the carrier and the Ising spins is also of Ising type. In two of the models the charge carrier is hosted by a different band, while in the third model it is hosted by the same band as the Ising spins. We find that the carrier’s spectral function exhibits a distinctive fine structure due to its temporary entrapping inside small magnetic domains, and use these results to construct an accurate (quasi)analytic approximation for low and medium $T$. While at $T = 0$, for ferromagnetic order all three models have identical, low-energy quasiparticles, at finite $T$ the low-energy behavior of the first two models remains equivalent, but that of the third model is controlled by rare events due to thermal fluctuations, which transfer spectral weight below the $T = 0$ quasiparticle peak, generating a pseudogaplike phenomenology. Taken together, our results show that the temperature evolution of the spectral weight of weakly doped magnetic insulators can be very complex.
Preface

- A version of the work discussed in Chapter 2 is published as *M. Möller and M. Berciu, Physical Review B 88, 195111 (2013)*. It is an extension of the work on spin-polarons by Shastry and Mattis [95] and makes use of the formalism developed by Berciu and Sawatzky in Ref. [7].

- A version of the work discussed in Chapter 3 is published as *M. Möller and M. Berciu, Physical Review B 90, 075145 (2014)*.

- A version of the work discussed in Chapter 4 is published as *M. Möller and M. Berciu, Physical Review B 92, 214422 (2015)*. It makes use of the formalism that was developed in the publication above.

- During the final two years of my PhD I also worked on polarons in models for which the electron-phonon coupling modulates the hopping integrals. A part of this work was published as *M. M. Möller and M. Berciu Physical Review B 93, 035130 (2016)*, while another manuscript is currently in preparation. I chose not to discuss this work in the thesis, because the topic is rather different from my previous work.

I carried out all the analytical and numerical work for these publications and wrote the first draft of the manuscripts. The preparation of the final drafts was assisted by M. Berciu. I also benefited from discussions with G. A. Sawatzky, especially for the work on electron-phonon coupling.
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Chapter 1

Introduction

Magnetic materials and their fascinating properties have been studied for centuries. Their applications range from the use as compass needles and refrigerator magnets to the use in hard drives and magnetoresistive random-access-memory (MRAM) in computers [106]. While some of the properties of magnetic materials can be explained with classical electrodynamics, it is now well understood that the theory of magnetism is inherently a quantum mechanical theory. The exchange interactions which lead to the formation and interaction of magnetic moments are linked to the indistinguishability of particles and the antisymmetry of fermionic many-body wavefunctions under particle exchange.

In many cases the magnetic moments which collectively give a magnet its properties are constituted by the partially filled 3d or 4f shells of transition metal (TM) or rare earth (RE) ions, respectively. These orbitals have a very small radial extent which causes strong Coulomb repulsion among the electrons which fill them. In order to minimize the Coulomb energy these electrons tend to align their spins, a rule known in atomic physics as Hund’s first rule [32,41]. By maximizing the total spin it is ensured that the spatial part of the many-electron wavefunction is antisymmetric and the Coulomb repulsion is minimized.

When TM or RE ions are incorporated into crystals the 3d or 4f shells only hybridize weakly with the surrounding atoms. Compared to the ionic case the Coulomb repulsion of these orbitals may be screened substantially, but it is generally still much larger than the hybridization with the surrounding atoms. As a consequence the electrons in the 3d and 4f shells often remain localized in the solid and give rise to local magnetic moments. It is also possible that the 3d/4f orbitals form a narrow conduction band in which case one speaks of itinerant moment magnetism, but this scenario is not the focus of this thesis.

The interactions between local magnetic moments give rise to magnetic order. There are many possibilities, including antiferromagnetic (AFM) order which is observed for example in the parent cuprates [88] and ferromagnetic (FM) order, for instance in FM chalcogenides like EuO and EuS.
More complicated types of magnetic order include zig-zag order in iridates \[16, 61, 99\] and FM layers that are stacked antiferromagnetically in manganite perovskites \[81, 87\] and KCuF\(_3\) \[50, 54\]. For the latter two materials the magnetic order is furthermore inseparably linked to orbital order resulting in a highly complicated ground state.

When conduction electrons (or holes) are present, their interaction with the local magnetic moments can also affect the magnetic order. This is especially true in dilute magnetic semiconductors such as Ga\(_{1-x}\)Mn\(_x\)As \[22, 83\] where the interaction between magnetic moments is mediated by the conduction electrons. In heavy fermion materials like CeSi\(_x\) \[58, 81\], the conduction electrons have a tendency to screen the local magnetic moments, and in the manganite perovskites a rich, doping dependent phase diagram exists \[38\].

Likewise, the presence of magnetic order can hinder the motion of charge carriers in a conduction band and lead to effective interactions between them. When the interactions are strong enough they renormalize the effective mass and other properties of the charge carriers and it becomes convenient to use a quasiparticle (QP) picture, where QP refers to a charge carrier that is “dressed” by local excitations of the magnetic environment. The extent to which this happens depends on the type of magnetic order (generally FM order is preferred over AFM order by itinerant charge carriers) and on whether the mobile charge carriers are hosted by a separate band or the same band which hosts the magnetic moments. Another important factor are finite temperature effects which lead to the formation of magnetic defects and domain walls off which the carriers are scattered. In certain cases the interaction with magnons can lead to the formation of spin-polarons which are QP states in which the carrier continuously absorbs and reemits a magnon. To discuss all these interesting properties one needs a model that incorporates the charge carrier degrees of freedom, the spin degrees of freedom and the interactions between the two subsystems. Such a model and its zero temperature properties are presented below. However, before discussing them we first present a brief review of experimental and theoretical work on the cuprates which motivates some of the work in this thesis.
1.1 Anomalous temperature-dependence in the parent cuprates

A class of materials with unusual $T$-dependence of the spectral weight are the cuprates. While the models studied in this thesis are simpler than those needed to study the complex many-body physics of the cuprates, this class of materials serves as a motivation for our work. Even the simpler models studied in this thesis show a variety of interesting and non-trivial properties which could help understand some of the puzzling behavior observed in the cuprates.

Upon doping the cuprates become high-temperature superconductors which is why, over the past decades, they have been studied in great detail, one of the tools of choice is angle resolved photoemission spectroscopy (ARPES) (see Ref. [19] for a review). It is widely believed that the electronic properties of the cuprates are captured by CuO$_2$ layers. The Cu is in a 3d$^9$ configuration corresponding to a single spin 1/2 hole per Cu atom. In the undoped, parent compounds these holes tend to align antiferromagnetically due to a superexchange interaction mediated by the oxygens. Doping of these materials introduces holes which tend to occupy the oxygens. The low-energy state of the hole-doped compound is believed to be the famous Zhang-Rice singlet [114] in which a doped hole which is hosted by the four oxygens surrounding a Cu atom forms a singlet with the Cu-spin at the center. Even though its validity is still being debated [26, 27, 56], theoretical studies of these materials are often carried out within the $t - J$-model where it is assumed that the Zhang-Rice singlets form effective holes in an otherwise AFM ordered background. Often longer range hopping is included to match the experimental dispersion, in that case one speaks of the $t - t' - t'' - J$-model.

Instead of a sharp QP peak, the low-energy part of the ARPES spectra of the parent cuprates has a very broad feature which has the $d_{x^2-y^2}$-symmetry of the Zhang-Rice singlet, and is often referred to as the QP peak [51]. As will be discussed below this terminology is actually not quite correct and therefore we will refer to this feature simply as the lower Hubbard band (LHB) [98]. What is puzzling about the LHB, are both its width which is much larger than what one would expect for a coherent QP peak and its strong $T$-dependence. ARPES data acquired by Kim et al. [51] shows that both the width and the center of the LHB change with $T$ and that the energy scale of this change is incompatible with conventional electron-phonon coupling or a mere broadening of the Fermi-Dirac distribution. Fur-
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Furthermore it was found that the broadening of the LHB is linear in $T$ for $200K < T < 400K$ and then levels off $[98]$ and that the $T$-dependence is much weaker for doped materials $[51]$.

To explain the anomalous $T$-dependence Kim et al. propose a heuristic model in which an ARPES measurement of initial states which are close in energy leads to final states which are further apart in energy. When $T$ is increased the distribution of initial states changes which can lead to the transfer of spectral weight to different final states which are energetically well-separated from the final states that are observed at low $T$. This idea is very similar to the ideas which lead to spectral weight transfer in the models investigated in this thesis.

The heuristic model proposed by Kim et al. has the potential to explain the anomalous $T$-dependence of the LHB, but it does not explain the broadness of this feature at low-$T$. Here a breakthrough was achieved by Shen et al. $[97]$ who showed that for the parent cuprates the QP peak has vanishingly small spectral weight and is therefore not seen in ARPES measurements. Instead one observes the various “shakeup” peaks that occur when an electron is removed and since these are very close to each other in energy the observed feature appears as a broad Gaussian peak. This effect is similar to the Franck-Condon principle from molecular spectroscopy (see also Refs $[92]$ and $[19]$), but the excitations leading to the Gaussian-like feature need not be vibrational in nature.

Finite $T$ calculations for a single hole in the $t – t' – t'' – J$-model were carried out by van den Brink and Sushkov with the Self Consistent Born Approximation $[105]$. They find a broadening of the QP peak, but not sufficient to explain the broadening observed in ARPES spectra. Furthermore they find a uniform, momentum-independent shift of the QP peak to lower energy as $T$ increases. They attribute this to the fact that at finite $T$ the magnetic background no longer has long range order making it easier for the hole to propagate. The shift of the QP peak could be related to the anomalous $T$-dependence observed in optical measurements by Choi et al. $[17]$. Their data shows a large redshift of a peak in the optical conductivity which they associate with an excitonic process creating an electron in a Cu 3d and a hole in an O 2p orbital. They argue that the hole on the O 2p orbital will be in a state corresponding to the QP peak in the $t – t' – t'' – J$-model and that the energy shift of this peak predicted by van den Brink and Sushkov is consistent with the observed redshift.

Other theoretical studies of the $T$-dependence of the LHB have focused on the effects of electron phonon coupling which are not included in the calculation by van den Brink and Sushkov. Mishchenko and Nagaosa used
1.1. Anomalous temperature-dependence in the parent cuprates

Diagrammatic Monte Carlo to study the spectral function of the $t - J$-model at $T = 0$ [67]. They found that interactions with the spin-background lead to an effective enhancement of the electron-phonon coupling and argued that the parent cuprates are in the strong-coupling regime where the formation of a small polaron occurs. Their calculated spectra at strong electron-phonon coupling show a broad peak corresponding to the Franck-Condon peak and a QP peak with vanishing spectral weight, in agreement with the experimental ARPES data. The broad peak follows the dispersion of the regular $t - J$-model without electron-phonon coupling. An explanation for this behavior was given by Rösch et al. based on an adiabatic approximation [89, 90] which also allows them to include coupling to different phonon branches.

An extension of the results by Mishchenko and Nagaosa was carried out by Cataudella et al for the $t - J$-model [14] and $t - t' - t'' - J$-model [15]. They use a method combining the Momentum Average approximation [8] for electron-phonon coupling and the Self Consistent Born Approximation for electron-magnon coupling. Their results for the thermal broadening of the LHB are in qualitative agreement with ARPES data and show the linear $T$ behavior mentioned above.

Experimental data supporting strong electron-phonon coupling in the cuprates was provided by Shen et al. who studied the $T$-dependence of $\pi$-bonding O 2p$\pi$ bands and the Ca 3p bands in Ca$_2$CuO$_2$Cl$_2$ [98]. These bands do not couple to the spin-background and therefore can be used as a “benchmark” for the effect of electron-phonon coupling. Indeed Shen et al. find a substantial $T$-dependence of these bands, but not as large as that of the LHB. This suggests that electron-phonon coupling does indeed play an important role, but that magnons (or other excitations) also contribute to the $T$-dependence of the LHB. This is supported by the findings of Lau et al. who carried out exact diagonalization for a CuO$_2$ layer [56]. In contrast to the $t - J$-like model they explicitly include the $\sigma$-bonding O 2p orbitals and find that besides the Zhang-Rice-like states a low-energy spin-polaron with spin 3/2 exists. This spin-polaron is invisible to ARPES at $T = 0$, but could be thermally activated, suggesting a $T$-dependent broadening mechanism with the same energy scale as the phononic mechanism discussed above.

In summary, while a lot of progress in understanding the $T$-dependence of ARPES spectra of the parent cuprates has been made in recent years, the microscopic mechanism behind it is not yet fully understood. From experimental data and theory it is clear that phonons play an important role and that the electron-phonon coupling is increased by the presence of the magnetic background. However, there is evidence which suggests that apart from this indirect role magnons also play a more direct role. It is there-
fore desirable to obtain a better understanding of the $T$-dependence caused by electron-magnon interactions. To achieve this one must first study simpler models without the added complexity of coupling to both magnons and phonons. The $T$-dependent spectral weight transfer of such models is investigated in this thesis. In the following sections we discuss the Hamiltonian needed to model these simpler problems and the origin of its various terms.

### 1.2 Exchange interactions

The exchange interactions which lead to all the interesting behavior mentioned above were first discovered by Heisenberg [37] and Dirac [23] and have the form

$$H_{\text{exc}} = \sum_{i,j} J_{i,j} S_i S_j,$$

where $S_i$ is the local magnetic moment at site $R_i$. Often the sum is restricted to nearest neighbors. In the initial formulation of this model the coupling constant $J_{i,j}$ was given by exchange integrals of the Coulomb energy

$$J_{i,j} = \int \text{d}r \int \text{d}r' \frac{\phi_i^*(r)\phi_j^*(r')e^2}{|r-r'|} \phi_i(r')\phi_j(r),$$

where $\phi_i$ and $\phi_j$ are wavefunctions centered at site $R_i$ and $R_j$, respectively. In most cases these direct exchange integrals between neighboring atoms are not large enough to explain the magnetic order observed in many materials. Instead, the underlying physics which governs the sign and size of the coupling $J$ is often intricately related to the crystal structure and orbital structure of the material under study and can be deduced with the so called Goodenough-Kanamori-Anderson rules (for a review see Refs [50] and [49]).

In the following we sketch a few examples of exchange mechanisms that lead to either AFM or FM coupling. These sketches are not intended as rigorous treatments, but instead are supposed to give a qualitative idea of the physics behind these mechanisms.

#### 1.2.1 Hund’s coupling

Hund’s coupling is an intraatomic coupling and given by the case where $\phi_i$ and $\phi_j$ in Eq. (1.2) belong to different orbitals centered on the same atom. This coupling is responsible for Hund’s first rule (originally formulated by Hund in 1925 [41], see also Refs [50] and [32]) from atomic physics...
1.2. Exchange interactions

which states that when occupying orbitals of a given subshell the electrons maximize the total spin. The underlying physics is that when the spin is maximized the spatial part of the wavefunction must be antisymmetric and therefore minimizes the Coulomb repulsion. This is especially important for the highly localized 3d and 4f orbitals. Consequently Hund’s coupling is responsible for the existence of magnetic moments. For example in the Eu chalcogenides the magnetic moments are constituted by the half filled 4f orbitals.

However, since it is mainly an intraatomic effect, Hund’s coupling is not directly responsible for the interaction of adjacent magnetic moments. Note that Hund’s coupling also exists for orbitals of different subshells, but still on the same atom. In the Eu chalcogenides this leads to the coupling of conduction electrons, partially hosted by the Eu 5d orbitals, to the local magnetic moments which are constituted by the half filled Eu 4f orbitals.

1.2.2 Kinetic exchange and super exchange:

The simplest model that leads to kinetic exchange is the single-band Hubbard model at half filling. The Hamiltonian is given by

\[ \hat{H}_U = -t \sum_{\langle i,j \rangle} \sum_\sigma c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \]  

The operator \( c^\dagger_{i,\sigma} \) \( (c_{i,\sigma}) \) creates (annihilates) an electron with spin \( \sigma \) at site \( i \) and \( n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma} \) is the occupation operator for site \( i \).

We start from a configuration where every site is occupied by one electron, minimizing the Hubbard repulsion \( U \). When neighboring electrons have antiparallel spins they can tunnel into states with double occupancy and back. To second order in perturbation theory this results in an energy gain \( \Delta E_{\uparrow\downarrow} = -t^2/U \) (see Fig. 1.1(a)). Due to the Pauli exclusion principle this process is forbidden for neighboring electrons with parallel spins. When one projects onto the subspace with single occupancy this situation is captured by an effective Heisenberg Hamiltonian with AFM coupling \( |J| = 4t^2/U \).

A simple example that leads to FM kinetic exchange is given by a two-orbital Hubbard model at half filling. We assume that the two orbital types are degenerate, but hopping is only possible between nearest neighbor orbitals of the same type. The possible spin configurations for two electrons are depicted in Fig. 1.1. Note that in this case an FM configuration is favored because of the intraatomic Hund’s coupling \( J_H \). The superexchange
1.2. Exchange interactions

\[ \Delta E_{\uparrow \downarrow} = -\frac{t^2}{U} \]

\[ \Delta E_{\uparrow \uparrow} = 0 \]

\[ \Delta E_{\downarrow \downarrow} = -\frac{t^2}{(U-JH)} \]

Figure 1.1: Superexchange in a two-orbital Hubbard model. After Ref. \[49\].
Note that panel (a) and (c) also show the electron configurations that lead to AFM superexchange in a one-orbital Hubbard model.

coupling is proportional to the energy difference between the AFM configuration and the FM configuration. Assuming \( J_H \ll U \) this gives \( |J| = \frac{4t^2 J_H}{U} \).
This type of exchange interaction is also called kinetic exchange.

These ideas can be generalized to more complex models where the local magnetic moments are hosted by TM or RE ions that do not hybridize directly, but through their ligands, often oxygens \[2, 3, 52\]. In this case the exchange interaction is referred to as superexchange. Hopping from one TM ion to another is a second order process and \( J \) is therefore obtained by fourth order perturbation theory. Furthermore one needs to consider not just the Coulomb repulsion \( U_{dd} \) on the TM ions, but also the energy difference \( \Delta_{pd} \) between the ligand orbitals and the TM orbitals. In addition more than one orbital per TM ion can be involved in the exchange mechanism and the bond-angles may also play a role. This complexity can lead to both AFM and FM coupling constants and has been studied extensively by Goodenough and Kanamori who developed a set of rules to determine the type (FM or AFM) and strength of the coupling \[33–35, 43–45\]. An excellent review of these rules can be found in Ref. \[50\]. Note that in most cases superexchange leads to AFM order, very specific conditions are needed for FM order \[49, 50\].

Note that higher order terms in perturbation theory can also be considered and lead to interactions which are for example proportional to \( (S_1 S_2)^2 \) and can even involve more than two spin operators \[31, 102, 110\].
1.2. Exchange interactions

1.2.3 Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction

Localized magnetic moments in a metal can interact with each other by polarizing the conduction electrons. This type of interactions leads to a coupling constant that oscillates as a function of the distance $r$ between the local magnetic moments. To leading order one obtains

$$J \sim \frac{\cos(2k_F r)}{r^3}.$$  \hspace{1cm} (1.4)

This interaction was first derived by Ruderman and Kittel to explain the interaction of nuclear spins via conduction electrons [91]. The extension to materials with magnetic moments due to localized d or f electrons was carried out by Yosida [109] and Kasuya [47, 47].

Since we are restricting ourselves to models with a single conduction electron, the RKKY interaction as described above is not relevant for the physics described in this thesis. However a variant of it, sometimes referred to as the Bloembergen-Rowland-mechanism [10], is responsible for the magnetic ordering in the Eu chalcogenides. In these materials virtual excitations of electrons across the semiconducting gap lead to an effective coupling between neighboring 4f electrons. For instance it is possible that an f electron tunnels into the conduction band composed primarily of Eu 5d orbitals. Hund’s rule exchange with the neighboring Eu 4f orbitals can then lead to a FM coupling. On the other hand, if two 4f electrons tunnel into the conduction band the Pauli exclusion principle favors a singlet, leading to AFM exchange. In both cases the existence of the energy gap leads to an exponential decay of the exchange interaction with the distance between local magnetic moments [10, 49, 62]. The competition between AFM and FM coupling leads to the different types of magnetic order observed in the Eu chalcogenide series [48, 49, 57, 64]. EuO and EuS are ferromagnets with Curie temperatures of 70 K and 17 K, respectively. EuSe has a complicated magnetic structure and EuTe is an antiferromagnet with a Néel temperature of 10 K [82].

1.2.4 Double exchange

This type of exchange interaction also requires a finite concentration of charge carriers. It arises in doped perovskite manganites [49, 50, 111, 112]. In these materials the crystal field due to the oxygen ligands causes the Mn 3d orbitals to split into two $e_g$ and three $t_{2g}$ orbitals. The conduction electrons which are hosted by Mn $e_g$ orbitals experience a strong Hund’s coupling with the localized magnetic moments, constituted by the half filled...
1.2. Exchange interactions

\[ \varepsilon_f + U \]

\[ E_F \]

Figure 1.2: An energy level diagram of the Anderson-impurity model with the impurity level singly occupied. The shaded area is occupied by the conduction electrons.

Mn \( t_{2g} \) orbitals. This Hund’s coupling is of the same order as the conduction band width which makes the RKKY theory inapplicable \[50\]. In this situation, even when the superexchange between neighboring local magnetic moments is AFM, a finite concentration of conduction electrons can lead to FM order. The reason is that an AFM magnetic background suppresses the hopping of the conduction electrons since hopping to an adjacent site would cost an energy of the order of the Hund’s coupling. It can therefore be energetically preferable for the system to be in a FM state, or at least a canted FM state \[20\], which allows the conduction electrons to lower their kinetic energy by delocalizing.

A somewhat similar situation occurs in the half-filled, single band Hubbard model for \( U \to \infty \). In this case the AFM superexchange coupling goes to zero. If one now dopes holes into the system their motion reshuffles the spins of the magnetic background breaking AFM bonds. This hinders the motion of the hole and in the limit \( U \to \infty \) the ground state of the doped system is FM. This was first described and proved rigorously by Nagaoka \[72\] for the case of a single hole. An extension and short, yet rigorous proof can be found in Ref. \[104\]. The situation for more than one hole is significantly more complicated \[24, 30, 96\].

1.2.5 Coupling of conduction electrons to a magnetic impurity

The coupling of conduction electrons to magnetic impurities is important for dilute magnetic semiconductors. For simplicity we consider a single spin 1/2 impurity, but the ideas presented here can be generalized to multiple impurities and larger spin values. The coupling between the conduction
1.2. Exchange interactions

The exchange interaction between the conduction electrons and the impurity is described by the Anderson-impurity model

\[
\hat{H}_{A-I} = \sum_{\mathbf{k}, \sigma} \epsilon(\mathbf{k}) c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + \sum_{\sigma} \epsilon_f f_{\sigma}^\dagger f_{\sigma} + U f_{\uparrow}^\dagger f_{\uparrow} f_{\downarrow}^\dagger f_{\downarrow} + \sum_{\mathbf{k}, \sigma} \left[ V_{\mathbf{k}} f_{\sigma}^\dagger c_{\mathbf{k}, \sigma} + V_{\mathbf{k}}^* c_{\mathbf{k}, \sigma}^\dagger f_{\sigma} \right]
\]

Here \(\epsilon(\mathbf{k})\) is the dispersion of the conduction electrons and \(c_{\mathbf{k}, \sigma}^\dagger, c_{\mathbf{k}, \sigma}\) are their creation and annihilation operators, respectively, while \(\mathbf{k}\) denotes the momentum and \(\sigma = \pm 1/2\) is the spin. The impurity with creation operator \(f_{\sigma}^\dagger\) is assumed to be located at the origin and has an on-site energy \(\epsilon_f\). It interacts with the conduction electrons via a hybridization \(V_{\mathbf{k}}\). Double occupation of the impurity orbital costs an additional energy \(U\) due to Coulomb repulsion.

We are interested in the situation where the Fermi energy, \(E_F\), lies between \(\epsilon_f\) and \(\epsilon_f + U\). In that case the impurity level is on average singly occupied, as shown in Fig. 1.2, and acts as a local magnetic moment. States with the impurity level unoccupied or doubly occupied are energetically unfavorable, yet, as we will see, they are still important for the interaction with the conduction electrons. One can derive an effective, low-energy Hamiltonian by projecting on the states where the impurity is singly occupied. Starting from this subspace, first order processes in \(V_{\mathbf{k}}\) lead to either a doubly occupied or an unoccupied impurity level. The first correction is therefore
1.2. Exchange interactions

\[ \Delta E = \varepsilon_f + U - \varepsilon(k') \]

Figure 1.4: The same as Fig. [1.3] but for the second channel.

of second order in \( V_k \). The derivation of the effective Hamiltonian can be carried out by using projection operators as described in Ref. [40] or by using a canonical transformation as was first shown by Schrieffer and Wolff [94]. The result is an exchange interaction between the conduction electrons and the impurity and a scattering term which is not of interest to us. The exchange coupling is given by [40]

\[ J_{k,k'} = 2V^*_k V_{k'} \left[ \frac{1}{\epsilon(k) - \epsilon_f} + \frac{1}{\epsilon_f + U - \epsilon(k')} \right]. \tag{1.6} \]

It is instructive to qualitatively discuss the origin of this exchange interaction. There are two channels corresponding to the first and second term in Eq. (1.6). All processes which contribute to the channels start and end with a singly occupied impurity level. The first channel corresponds to processes where the electron that occupies the impurity level “jumps” into the conduction band (see Fig. [1.3]). The energy difference between this intermediate state and the original state is \( \epsilon(k) - \epsilon_f \). The empty impurity level is then occupied by another conduction electron. Since this electron does not necessarily have the same spin as the electron which previously occupied the impurity, this process can result in a flip of the impurity spin.

The processes belonging to the second channel are sketched in Fig. [1.4]. Here a conduction electron first “jumps” into the impurity level which is then doubly occupied. The energy difference between the intermediate state and the original state is therefore given by \( \epsilon_f + U - \epsilon(k') \). Note that this process is only possible for a conduction electron whose spin is antiparallel to that of the singly occupied impurity. In the second step one of the electrons hosted
1.3 Model Hamiltonian for magnetic semiconductors

A minimal model for magnetic semiconductors must consist of three parts: (i) A part describing the conduction electrons which are assumed to be hosted by a broad band; (ii) a part describing the local magnetic moments and their tendency to order and (iii) a part describing the interaction between the local magnetic moments and the conduction electrons. This is accomplished by the Kondo-lattice model which in the context of magnetic semiconductors is often referred to as the s-f model. This terminology originates with the Eu chalcogenides, where the conduction electrons are hosted by the Eu 5d and 6s orbitals while the local magnetic moments are hosted by the half-filled Eu 4f orbitals [64, 82]. In the case of materials with transition metal ions such as the manganites this model is also referred to as the s-d model [49, 111-113].

We consider the limit where the conduction band hosts a single spin-\(1/2\) charge carrier. This charge carrier propagates on a hypercubic lattice with periodic boundary conditions after \(N_i\) sites in the direction \(i = 1, d\); the total number of sites is \(N = \prod_{i=1}^{d} N_i\). In Chapter 2 we present results for \(d = 2\) and \(d = 3\), while in Chapters 3 and 4 we present results for a simplified version of this model for \(d = 1\). Of course, long-range FM order at finite \(T\) only exists in \(d = 3\). However, we also consider anisotropic layered compounds, like the manganites, which have \(2d\) FM layers whose finite-\(T\)
long-range order is stabilized by weak interlayer coupling, but where one can assume that at very low $T$ the intralayer carrier dynamics determine its properties. In principle, similar arguments can be employed to study $d = 1$ chains with FM order at finite $T$ maintained by their immersion in $3d$ lattices or by other mechanisms. For instance, the existence of FM edge states in graphene nanoribbons is a current topic of investigations [13, 46]. An important point to be aware of is that in contrast to higher dimensions, in $1d$ the energy cost of magnetic domains does not necessarily scale with their size. Consequently approximations which work well in $2d$ and $3d$ may perform very poorly in $1d$. This is part of the reason why in Chapter 2 we only present results for $d > 1$.

The carrier is an electron in an otherwise empty band or a hole in an otherwise full band, described by a tight binding model with nearest neighbor (nn) hopping:

$$\hat{T} = \sum_{\mathbf{k}, \sigma} \epsilon(\mathbf{k}) c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma},$$  \hspace{1cm} (1.7)

with $\epsilon(\mathbf{k}) = -2t \sum_{i=1}^{d} \cos k_i$ for lattice constant $a = 1$. $c_{\mathbf{k}, \sigma}^\dagger$ creates a carrier with momentum $\mathbf{k}$ and spin $\sigma$.

The local magnetic moments are described by either a Heisenberg [37] interaction:

$$\hat{H}_S = -J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - S^2),$$  \hspace{1cm} (1.8)

or an Ising interaction [42, 60]:

$$\hat{H}_I = -J \sum_{\langle i,j \rangle} (S^z_i S^z_j - S^2),$$  \hspace{1cm} (1.9)

where $\mathbf{S}_i$ is the spin-$S$ moment located at site $\mathbf{R}_i$ and only nn exchange is included in both models.

When $J$ is FM (i.e. $J > 0$ in Eqs (1.8) and (1.9)) the undoped ground state for both $\hat{H}_S$ and $\hat{H}_I$ is $|\text{FM}\rangle = |S, S, \ldots \rangle$ and has zero energy. The simplest excited states of interest are the single magnon states:

$$|\Phi(\mathbf{q})\rangle = \frac{S_q}{\sqrt{2S}} |\text{FM}\rangle = \sum_j e^{i\mathbf{q}\mathbf{R}_j} S^+_j |\text{FM}\rangle.$$  \hspace{1cm} (1.10)

Here $S^\pm_i = S^x_i \pm iS^y_i$ are the raising (+) and lowering (−) operators. The key difference between the Heisenberg and Ising interactions is the dispersion of the single magnon states. For the Heisenberg model this is
1.3. Model Hamiltonian for magnetic semiconductors

\[ \Omega_q = 4JS \sum_{i=1}^{d} \sin^2(q_i/2), \]  whereas for the Ising model the magnons are dispersionless, \( \Omega_q = \Omega = 2dJS . \) Thus, studying both models allows us to evaluate the relevance of having gapped or gapless magnons.

The case of AFM coupling, \( J < 0 \) is significantly more difficult to treat. For the Ising spins the GS is the Néel state in which nearest neighbor spins point into opposite directions. For the Heisenberg case, on the other hand the true AFM GS is only known for \( d = 1 \) and \( S = 1/2 \), and even with those restrictions its form is rather complicated [110]. Consequently AFM coupling will only be treated in Chapters 3 and 4 for simplified versions of the s-f(d) model.

The interaction between the carrier and the local moments is also a Heisenberg exchange:

\[
\hat{H}_{\text{exc}} = J_0 \sum_j \mathbf{s}_j \cdot \mathbf{S}_j,
\] (1.11)

where \( \mathbf{s}_i = \sum_{\alpha,\beta} c_{i,\alpha}^\dagger \sigma_{\alpha,\beta} c_{i,\beta} \) is the carrier spin operator and \( \sigma \) are the Pauli matrices. The coupling \( J_0 \) can be either FM or AFM; we will consider both cases. As mentioned above the FM case occurs for example when the conduction electrons experience Hund’s coupling with local magnetic moments. This is the case for the Eu chalcogenides. AFM coupling can occur when a hybridization between the conduction electrons and the orbitals hosting the local magnetic moments is present and the local magnetic moments have maximum spin. In that case only conduction electrons with opposite spin can make use of the hybridization term to reduce their energy. In this case one can use a Schrieffer-Wolff transformation [94] to rewrite the hybridization term as an exchange interaction.

It is convenient to split \( \hat{H}_{\text{exc}} = \hat{H}_{\text{exc}}^z + \hat{H}_{\text{exc}}^{x,y} \), where

\[
\hat{H}_{\text{exc}}^z = \frac{J_0}{2} \sum_j \left( c_{j,\uparrow}^\dagger c_{j,\uparrow} - c_{j,\downarrow}^\dagger c_{j,\downarrow} \right) S_j^z
\] (1.12)
\[
\hat{H}_{\text{exc}}^{x,y} = \frac{J_0}{2} \sum_j \left( c_{j,\uparrow}^\dagger c_{j,\downarrow} S_j^- + c_{j,\downarrow}^\dagger c_{j,\uparrow} S_j^+ \right).
\] (1.13)

The first term causes an energy shift \( \pm J_0 S/2 \). The second term is responsible for spin-flip processes, where the carrier flips its spin by absorbing or emitting a magnon.

The total Hamiltonian is:

\[
\hat{H} = \hat{T} + \hat{H}_{S/L} + \hat{H}_{\text{exc}}.
\] (1.14)
Due to translational invariance, the total momentum is conserved. Furthermore, the $z$-component $S_{\text{tot}}^z$ of the total spin (the sum of the carrier spin and lattice spins), is also conserved. Therefore, eigenstates $\hat{H} |\psi_{\alpha}^{(m)}(k)\rangle = E_{\alpha}^{(m)}(k) |\psi_{\alpha}^{(m)}(k)\rangle$ are indexed by the total momentum of the system, $k$, by the number $m$ of magnons when the carrier has spin-up so that $S_{\text{tot}}^z = NS + \frac{1}{2} - m$, and by $\alpha$ which comprises all the other quantum numbers.

The s-f model poses a difficult many-body problem and can only be solved in limiting cases. One of them is the zero bandwidth limit \cite{76}, while the other cases are that of a single carrier injected into completely ordered FM background at $T = 0$ \cite{95} and that of two carriers with opposite spin \cite{68,69} at $T = 0$. In the single carrier case the solution depends dramatically on the spin orientation of the carrier. If the carrier has its spin aligned with the magnetic background (spin up) the system is in the $NS + 1/2$ subspace and no spin-flip processes are possible. The solution is therefore trivial. If on the other hand the carrier is injected with its spin opposite to the magnetic moments, the system is in the $NS - 1/2$ subspace and for sufficiently strong AFM $J_0$ a bound state consisting of a magnon and the carrier, a so-called spin-polaron can form. We will review this solution below, after introducing the formalism of single particle Green’s functions.

### 1.4 Single particle Green’s functions

**1.4.1 Zero temperature**

The single particle GF is a powerful tool in condensed matter physics. As we show below it gives us access to the eigenenergies and QP weights, properties which can be measured in photoemission experiments \cite{19}. In this thesis we are restricting ourselves to models of a single fermion which interacts with the degrees of freedom of a lattice of local magnetic moments. Consequently only the single particle, retarded GF is of interest to us. At $T = 0$ it is defined as \cite{28,63,115}

$$G_{\alpha,\alpha'}(k,\tau) = -i\Theta(\tau)\langle 0|c_{k,\alpha}(\tau)c_{k,\alpha'}^\dagger(0)|0\rangle$$

(1.15)

Here $c_{k,\alpha}(\tau) = e^{i\hat{H} \tau} c_{k,\alpha}(0)e^{-i\hat{H} \tau}$ is a fermionic annihilation operator in the Heisenberg picture (we set $\hbar = 1$). The index $k$ is the momentum and $\alpha$ is to be considered a place holder for spin and band indices. The state $|0\rangle$ is the ground state of the local magnetic moment part of $\hat{H}$ whose energy $E_0^{-S/1}$ we choose to be zero. Finally the Heaviside function, $\Theta(\tau)$, is defined
1.4. Single particle Green’s functions

as

$$\Theta(\tau) = \begin{cases} 
1 & \tau > 0 \\
0 & \tau < 0 
\end{cases}$$  \hspace{1cm} (1.16)

Physically $G_{\alpha,\alpha'}(k, \tau)$ corresponds to the probability amplitude that a fermion which is injected into the system in state $(k, \alpha')$ will be in state $(k, \alpha)$ after a time $\tau$ while the rest of the system remains unchanged. Note that we are restricting ourselves to systems where the total momentum is conserved and consequently $k$ cannot change during such a process. If, as is usually the case, the state $|0\rangle$ has total momentum zero, then $k$ is the total momentum of the system.

In many cases it is convenient to work in the frequency domain rather than the time domain. This is achieved by Fourier transforming

$$G_{\alpha,\alpha'}(k, \omega) = \int_{-\infty}^{\infty} d\tau \ e^{i\omega \tau} G_{\alpha,\alpha'}(k, \tau).$$  \hspace{1cm} (1.17)

To carry out the integral we first insert the identity operator in the form $1 = \sum_n |n\rangle \langle n|$, where $|n\rangle$ are the eigenvectors of $\hat{H}$ with eigenvalues $E_n$. This yields

$$G_{\alpha,\alpha'}(k, \omega) = -i \sum_n \int_{-\infty}^{\infty} d\tau \ e^{i(\omega + E_0^{S/I} - E_n) \tau} \Theta(\tau) \langle 0 | c_{k,\alpha} | n\rangle \langle n | c_{k,\alpha'}^{\dagger} | 0 \rangle$$  \hspace{1cm} (1.18)

Note that since the GS energy of the local magnetic moments $E_0^{S/I} = 0$ the energy difference $E_0^{S/I} - E_n$ simplifies to $-E_n$. However, we will see that for finite temperatures the appearance of energy differences in the exponential is unavoidable and has physical consequences.

We proceed by using the following integral representation for the Heaviside function \[115\]

$$\Theta(\tau) = \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} \frac{dx}{2\pi i} \frac{e^{-ix\tau}}{x + i\eta}.$$  \hspace{1cm} (1.19)

Inserting this into Eq. (1.18) we first perform the integration over $x$ as a contour integral and subsequently the integration over $\tau$ to obtain

$$G_{\alpha,\alpha'}(k, \omega) = \lim_{\eta \to 0^+} \sum_n \frac{\langle 0 | c_{k,\alpha} | n\rangle \langle n | c_{k,\alpha'}^{\dagger} | 0 \rangle}{\omega - E_n + i\eta}.$$  \hspace{1cm} (1.20)
1.4. Single particle Green’s functions

This representation of the GF is known as the Lehmann representation. In this form it becomes clear that \( G_{\alpha,\alpha'}(k, \omega) \) has poles at the eigenenergies \( E_n \) of \( \hat{H} \), and that their weights correspond to the overlap of the free carrier states \( c_{k,\alpha}^{\dagger}|0\rangle \) with the eigenstates \( |n\rangle \) of \( \hat{H} \). When \( \alpha = \alpha' \) these weights are referred to as the QP weights \( Z_n^\alpha(k) = |\langle n|c_{k,\alpha}|0\rangle|^2 \).

The easiest way to extract the eigenenergies and QP weights from the GF is to calculate the spectral function \( A_{\alpha,\alpha}(k, \omega) = -\frac{1}{\pi} \text{Im} \, G_{\alpha,\alpha}(k, \omega) \). Using the well-known identity \( \lim_{\eta \to 0^+} \frac{1}{x + i\eta} = P \frac{1}{x} + i\pi \delta(x) \), where \( P \) denotes the Cauchy principal value [28], this becomes

\[
A_{\alpha,\alpha}(k, \omega) = -\frac{1}{\pi} \text{Im} \, G_{\alpha,\alpha}(k, \omega) = \sum_n Z_n^\alpha(\omega - E_n). \tag{1.21}
\]

When carrying out numerical calculations we will usually use a small, but finite value for \( \eta \). This results in a broadening of the delta-peaks from Eq. (1.21) into Lorentzians. By reverse Fourier transforming Eq. (1.20) one can show that choosing a finite value for \( \eta \) introduces a finite lifetime \( \sim 1/\eta \) for the free carrier.

From Eq. (1.21) it is clear that the spectral function obeys the sum rule

\[
\int_{-\infty}^{\infty} d\omega \, A(k, \omega) = \sum_n Z_n^\alpha = 1, \tag{1.22}
\]

where we used the completeness relation \( \sum_n |n\rangle\langle n| = 1 \). Furthermore the density of states (DOS) \( \rho(\omega) \) is related to \( A(k, \omega) \) via

\[
\rho(\omega) = \frac{1}{N} \sum_q A(q, \omega). \tag{1.23}
\]

Eq. (1.20) can be recast in the form of the expectation value of an operator by introducing the resolvent of \( \hat{H} \)

\[
\hat{G}(\omega) = \frac{1}{\omega - \hat{H} + i\eta}. \tag{1.24}
\]

The GF is then given by

\[
G_{\alpha,\alpha'}(k, \omega) = \langle 0|c_{k,\alpha}\hat{G}(\omega)c_{k,\alpha'}^{\dagger}|0\rangle. \tag{1.25}
\]

The advantage of working with the resolvent \( \hat{G}(\omega) \) is that it obeys Dyson’s identity. If we write the Hamiltonian as the sum of two parts \( \hat{H}_0 \) and \( \hat{V} \) it is easy to verify that

\[
\hat{G}(\omega) = \hat{G}_0(\omega) + \hat{G}(\omega)\hat{V}\hat{G}_0(\omega) \tag{1.26}
\]
1.4. Single particle Green’s functions

This holds independent of the choice of $\hat{H}_0$ and $\hat{V}$, but generally one chooses $\hat{H}_0$ in such a way that it is easy to calculate the expectation values of $\hat{G}_0$. By repeatedly using Dyson’s identity, one can construct a hierarchy of equations of motion (EOM) of the GF. In the subsequent Chapters we will make use of this approach to calculate the GFs for various Hamiltonians.

1.4.2 Finite temperature

The finite temperature GF is usually defined in the grand canonical ensemble \[28, 63, 115\]. However, for the models investigated in this thesis there is always exactly one fermion in the system and only the number of bosonic excitations varies. We therefore need to formulate the finite temperature theory in the canonical ensemble. The natural extension of Eq. (1.15) to finite temperatures is then

$$G_{\alpha,\alpha'}(k, \tau) = -\frac{i}{2} \Theta(\tau) \frac{Z}{Z} \text{Tr} \left[ e^{-\beta \hat{H}_S/\gamma} c_{k,\alpha}(\tau) c_{k,\alpha'}(0) \right],$$

(1.27)

where $\beta = T^{-1}$ is the inverse temperature (we set the Boltzmann constant $k_B = 1$). The trace runs over all the eigenstates of the lattice part, $\hat{H}_{S/I}$, of $\hat{H}$, i.e. all possible configurations of the system before injection of the charge carrier. As usual the partition function $Z$ is given by

$$Z = \text{Tr} \left[ e^{-\beta \hat{H}_{S/I}} \right]$$

(1.28)

We can use the same procedure as for the zero temperature GF to transform to the frequency domain. In doing so we obtain

$$G_{\alpha,\alpha'}(k, \omega) = \sum_n \frac{e^{-\beta E_n^{S/I}}}{Z} \langle S/I, n | c_{k,\alpha} \hat{G}(\omega + E_n^{S/I}) c_{k,\alpha}' | S/I, n \rangle.$$  

(1.29)

Here $|S/I, n \rangle$ are the eigenstates of $\hat{H}_{S/I}$ with eigenenergies $E_n^{S/I}$. It is crucial to realize that $\omega$ is shifted by $E_n^{S/I}$. This shift comes about because

$$\langle S/I, n | e^{i \hat{H} \tau} c_{k,\alpha} \cdots \rangle = e^{i E_n^{S/I} \tau} \langle S/I, n | c_{k,\alpha} \cdots \rangle$$

(1.30)

Physically it means that all energies are measured with respect to the energy of the system before injection of the charge carrier. For the zero temperature GF this is also true, but when the carrier is injected the lattice is in its ground state, which we assume to have zero energy.
Before concluding this section, we emphasize that all the calculations in this thesis are in a canonical ensemble. The chemical potential is not fixed at $\omega = 0$, as customary in grand canonical formulations, instead it can be calculated as $\mu = \left(\frac{\partial F}{\partial N}\right)_{T \to \min} \alpha,\beta [E_{N+1,\alpha} - E_{N,\beta}]$ as $T \to 0$, where $F$ is the free energy and $N$ is the particle number. As pointed out above, here $\omega = 0$ marks the energy of the undoped system.

### 1.5 The spin-polaron

In this section we apply the formalism of zero temperature GFs to the Hamiltonian of Eq. (1.14) to study the spin-polaron. This problem was first solved by Shastry and Mattis [95] and later generalized to complex lattices by Berciu and Sawatzky [7]. An approach that does not rely on GFs, but yields all the eigenfunctions was presented by Henning et al. [39] and Nakano et al. [73].

To distinguish the $T = 0$ GFs we denote them by $G_\uparrow(0)(k, \omega)$ for a carrier injected with spin up ($m = 0$ sector) and $G_\downarrow(0)(k, \omega)$ for a carrier injected with spin down ($m = 1$ sector). Let us start with the solution in the $m = 0$ sector, where the total magnetization is $S_{\text{tot}} = NS + 1/2$. In that case no spin flips are possible and the eigenenergies are simply given by $E_\uparrow(k) = \epsilon(k) + J_0S/2$. The spectral function $A_\uparrow(0)(k)$ consists of a single $\delta$-peak at $E_\uparrow(k)$ and $G_\uparrow(0)(k, \omega) = [\omega - E_\uparrow(k) + i\eta]^{-1}$ is just the free particle propagator up to a shift $J_0S/2$.

For the $m = 1$ sector we need to work a little harder. The GF is defined as

$$G_\downarrow(0)(k, \omega) = \langle FM|c_{k,\downarrow}\hat{G}(\omega)c_{k,\uparrow}|FM\rangle. \quad (1.31)$$

Splitting $\hat{H}$ into $\hat{H}_0 = \hat{T} + \hat{H}_S/2$ and $\hat{V} = \hat{H}_{\text{exc}}$ and using Dyson’s identity we obtain

$$G_\downarrow(0)(k, \omega) = \left[1 + J_0\sqrt{\frac{S}{2N}} \sum_q F(0)(k, q, \omega)\right] G_\uparrow(0)(k, \omega + J_0S), \quad (1.32)$$

where we defined $F(0)(k, q, \omega) = \langle FM|c_{k,\downarrow}\hat{G}(\omega)c_{k-q,\uparrow}\sqrt{\frac{S}{2N}}|FM\rangle$.

We proceed by using Dyson’s identity again to obtain the EOM for
1.5. The spin-polaron

\[ F^{(0)}(k, q, \omega). \] This yields

\[ F^{(0)}(k, q, \omega) = \left[ \frac{J_0 \sqrt{S}}{\sqrt{2N}} G_\uparrow^{(0)}(k, \omega) - \frac{J_0}{2N} \sum_Q F^{(0)}(k, Q, \omega) \right] G_\uparrow^{(0)}(k - q, \omega - \Omega_q) \] \hspace{1cm} (1.33)

Note that on the right hand side of both EOM \( F^{(0)}(k, q, \omega) \) only appears as a sum. We therefore define \( f^{(0)}(k, \omega) \) as:

\[ f^{(0)}(k, \omega) = \frac{J_0 \sqrt{S} G(k, \omega) g^{(0)}(k, \omega)}{1 + \frac{J_0}{2} g^{(0)}(k, \omega)} \] \hspace{1cm} (1.34)

where \( g^{(0)}(k, \omega) = N^{-1} \sum_q G_\uparrow^{(0)}(k - q, \omega - \Omega_q) \) can be calculated since \( G_\uparrow^{(0)}(k, \omega) \) is known. This can be done numerically or by bringing it into the form of an elliptical integral for which a variety of methods of calculation exist \[9, 70]. Note that \( g^{(0)}(k, \omega) \) depends on the magnon dispersion \( \Omega_q \) and thus is different for \( \hat{H}_S \) and \( \hat{H}_I \).

Finally, we can plug \( f^{(0)}(k, \omega) \) into Eq. (1.32) to obtain

\[ G_\downarrow^{(0)}(k, \omega) = \left[ \omega - \epsilon(k) + \frac{J_0 S}{2} \right]^{-1} \] \hspace{1cm} (1.35)

As pointed out above the difference between the Ising and Heisenberg magnetic background is contained completely in \( g^{(0)}(k, \omega) \). Note furthermore that the last term on the right corresponds to the self-energy, up to a constant shift \( J_0 S/2 \).

We can now investigate the spectral function \( A_\downarrow^{(0)}(k, \omega) \). Our main focus will be to understand when a spin-polaron state forms in the \( m = 1 \) sector, but we will also verify the presence of the continuum at the expected location. We assume that \( |J_0| \) is the largest energy scale, experimentally this is true for example in the manganite perovskites. While realistically one expects \( J \ll t \), we will set \( J/t = 0.5 \) so that its role can be discerned easily. We furthermore specialize to the case \( S = 1/2 \) since it is to be expected that effects of the quantum nature of the spins will be the most pronounced in this limit.

Figure 1.5 shows \( E_\uparrow(k_x, k_y = 0) \) (thick full green line) and the spectral weight \( A^{(0)}_\downarrow(k_x, k_y = 0, \omega) \) (contour map) for the 2d s-f(d) model, for AFM
1.5. The spin-polaron

Figure 1.5: Energy $E_\uparrow(k)$ (thick full green line) and spectral weight $A_\downarrow^{(0)}(k,\omega)$ (contour map) vs. $k_x$ at $k_y = 0$, for the Heisenberg model (left) and the Ising model (right) in 2$d$, for AFM coupling $J_0/t = 3$. The dashed red lines mark the expected continuum boundaries in the $m = 1$ subspace. Other parameters are $J/t = 0.5$, $S = 0.5$, $\eta/t = 0.01$.

coupling $J_0 = 3$ and Heisenberg and Ising local magnetic moments. The spectrum of the $m = 1$ sector consists of a discrete state at low energies, the spin-polaron, and the up-carrier + magnon (c+m) continuum at higher energies.

We start by discussing the origin of the c+m continuum. Since it is injected with spin-down the carrier can flip its spin and emit a magnon. In doing so it transfers a momentum $q$ to the magnon. Consequently the carrier momentum after the emission of a magnon is $k - q$. Furthermore since the carrier has flipped its spin it experiences an energy shift $+J_0S/2$. The c+m continuum is caused by states where the carrier and the emitted magnon are far apart. One also refers to this type of states as scattering states. Since any momentum $q$ can be transferred to the magnon, the c+m continuum spans the energy range $\{E_\uparrow(k - q) + \omega_q\}$. 

Let us now discuss the spin-polaron. Because we will encounter a different spin-polaron later on, we will refer to this spin polaron as “sp1”. While in the c+m continuum the carrier and the magnon are far apart, in the sp1 state the carrier continuously emits and reabsorbs a magnon in a coherent fashion. To get a better understanding of this we can use perturbation theory \[7\]. In the absence of $\hat{T}$ and $\hat{H}_{S/I}$ the singlet-like state $\sqrt{2S+1} \sum_j e^{ikR_j} \left[ \sqrt{2S}c_{j,\uparrow} + c_{j,\downarrow} \right] |FM\rangle$ is an eigenstates of $\hat{H}_{exc}$ with eigenenergy $-J_0(S + 1)/2$. The first order corrections to its energy
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Figure 1.6: Left: $A_{k}^{(0)}(0,\omega)$ for FM $J_{0}/t = -2$ in 2$d$. The lower c+m continuum edge is marked with dashed red lines. The Ising model has a discrete state (sp2) below the continuum, but the Heisenberg model does not. Right: Spectral weight $A_{k}^{(0)}(\omega)$ for the Ising model in 2$d$ for $k_{y} = 0, k_{x} < 0.3\pi$. The dashed red line marks the lower c+m continuum edge. The sp2 state appears for small $k$ and then merges into the continuum. Other parameters are $J/t = 0.5, S = 0.5, \eta/t = 0.01$.

are

$$E_{sp1}(k) \approx -\frac{J_{0}}{2}(S+1) + \frac{2S}{2S+1}\varepsilon(k) + \frac{2dJ}{2S+1}$$  \hspace{1cm} (1.36)

For $J_{0} \gg t, J$ this approximation is indeed very accurate [7, 69] (not shown). Note that to first order the effective mass of the sp1 state is a factor of $(2S+1)/2S$ larger than the bare carrier mass. The reason for this is that the carrier needs to move the magnon along with it, when it propagates on the lattice. For AFM $J_{0} > 0$ sp1 is the ground state since states in the continuum have the carrier with spin up and cost $\sim J_{0}S/2$ in exchange energy. This suggests that for FM coupling $J_{0} < 0$, the sp1 polaron should be located above the c+m continuum. This expectation is confirmed below. Perturbation theory also suggests that the symmetry of the sp1 state is singlet-like.

Comparing the two panels of Fig. 1.5 we see that the sp1 dispersion is very similar for the two models. This is expected because this is a coherent state where the magnon is locked into a singlet with the carrier, and this process is controlled by $J_{0} \gg J$. Whether the magnon is localized (Ising) or has a finite speed $\sim J$ (Heisenberg) is irrelevant. A difference appears in the shape of the c+m continuum, however. As mentioned, this must span energies $\{E_{\uparrow}(k-q) + \Omega_{q}\}$ since it consists of up-carrier and magnon
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scattering states. The dashed red lines show the boundaries of this range, in agreement with the data (this is more difficult to see for the upper edge, on this scale, due to the reduced spectral weight at high energies). Since Ising magnons are dispersionless the continuum boundaries do not change with \( k \). In contrast, the continuum boundaries for the Heisenberg model vary with \( k \), the continuum being wider at the center of the Brillouin zone than near its edges.

This difference has consequences for a FM coupling \( J_0 < 0 \). As mentioned, in this case the c+m continuum is expected to be the low-energy feature in the \( m = 1 \) spectrum, with the sp1 state appearing above it. This is indeed the case for the Heisenberg model, however in the Ising model, for a sufficiently large \( J \), a second discrete state emerges below the c+m continuum. We will refer to this state as “sp2” to distinguish it from sp1. The left panels of Fig. 1.6 show its presence (absence) for the Ising (Heisenberg) model at \( k = 0 \). The right panel shows that even for the Ising model, the sp2 only exists for small \( k \), at least for these parameters.

The origin of the sp2 state is suggested by the findings of Henning et al. who showed that for \( J = 0 \), polaron-like states exist inside the c+m

Figure 1.7: Ground-state energy of the Ising sp2 polaron as a function of \( J_0/t \) for \( J/t = 0.5 \) (top) and as a function of \( J/t \) for \( J_0/t = -2 \) (bottom), for \( S = 0.5 \).
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Figure 1.8: Spectral weight $A^{(0)}(k, \omega)$ vs $k_x$ for the 2d Heisenberg model at $k_y = 0$ (left) and $k_y = \pi$ (right) and FM $J_0/t = -2$. Sp1 appears above the continuum only near the Brillouin zone edge. No sp2 peak is seen below the continuum. The dashed red lines mark the c+m continuum boundaries and the green line marks $E_{\uparrow}(k)$. Other parameters are $J/t = 0.5, S = 0.5, \eta/t = 0.01$.

We believe that the addition of $\hat{H}_1$ pushes one of them below the continuum. This is possible because for an Ising coupling, the lower continuum edge moves up by $\Omega = 2dJS$, whereas the polaron-like states experience a smaller energy shift since they include a component with the carrier having spin-down. For the Heisenberg model, on the other hand, inclusion of $\hat{H}_S$ does not change the location of the lower continuum edge at $k = 0$ since $\Omega_{q=0} = 0$, so the polaron-like state remains a resonance inside the continuum.

The ground-state energy of the sp2 polaron is explored in Fig. 1.7. The top panel shows its dependence on $J_0/t$. The sp2 state has weight on both the down-carrier and on the up-carrier+magnon components. For $J_0 = 0$ the weight of the latter component must vanish since no spin-flips are possible and the sp2 state is the same as a free down-carrier, whose energy $-J_0S/2 - 4t$ is also indicated (dashed blue line). These results suggest that as $|J_0|/t$ increases, the sp2 state shifts weight from the down-carrier component to the up-carrier+magnon component until it essentially becomes a continuum-like state.

The bottom panel in Fig. 1.7 shows the sp2 ground-state energy vs. $J/t$ for fixed $J_0/t = -2$. This value of $J_0/t$ was chosen because here the polaronic character of sp2 is especially strong because if we neglect $H_{\text{exc}}^{x,y}$, the energy of the down-carrier component is equal to that of the up-carrier+magnon component. The distance between sp2 and the continuum increases with...
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$J/t$, as expected from our previous discussion.

While we have only seen the $sp2$ polaron for the Ising model, we cannot rule out the possibility that for a very narrow range of momenta and carefully chosen parameters, an $sp2$ state might also appear in the Heisenberg model. Another important point is that the $sp1$ state is not guaranteed to exist for all $k$, either. In Fig. 1.8 we show $A^{(0)}_1(k, \omega)$ for the 2$d$ Heisenberg model. No $sp2$ state appears below the continuum, and $sp1$ separates above the continuum only near the Brillouin zone edge. This is not a surprise given the rather small value of $|J_0|$ which controls the separation between $sp1$ and the continuum. For sufficiently large $|J_0|$, the $sp1$ polaron splits off the continuum in the entire Brillouin zone [95].

To summarize, the spectrum in the $m=1$ (one-magnon) subspace contains the expected c+m continuum. For AFM $J_0$ the low-energy feature is the $sp1$ polaron for both the Heisenberg and the Ising models. For FM $J_0$, $sp1$ becomes the high energy feature and may only appear in a small region of the Brillouin zone if $|J_0|$ is small. For the Ising model and FM $J_0$, an $sp2$ polaron is also found to appear below the c+m continuum, in a central region of the Brillouin zone that increases with increasing $J$. For the Heisenberg model and FM $J_0$ we cannot entirely rule out the existence of $sp2$, although we provided arguments which suggest that this is unlikely.

We focused here more on the $sp2$ polaron because, to our knowledge, this solution had not been discussed before, while the $sp1$ state has been analyzed in great detail [7, 39, 73, 95]. We also note that while we presented only (computationally less costly to generate) 2$d$ results, we find qualitatively similar results in 3$d$. This will become clear from the finite-$T$ results shown in Chapter [2].

1.6 Markov-chain Monte Carlo simulations

Monte Carlo simulations can be used to calculate finite-$T$ expectation values of the type given in Eq. 1.29. We will use this technique in Chapters 3 and 4 for simplified versions of the s-f(d) model. This section gives a short review of the technique.

Many textbooks have been written on the subject of Markov-chain Monte Carlo simulations. The ideas presented here are loosely based on the textbook by Landau and Binder [55] and a set of lecture notes by N. Prokof’ev [86]. Markov-chain Monte Carlo simulations are a powerful technique to
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calculate expectation values of the form

\[
\langle A \rangle = \sum_i \rho(s_i) A(s_i).
\]  

(1.37)

Here \( A \) is some physical quantity of interest, e.g. the magnetization of a lattice of local magnetic moments, and the sum runs over all the microstates \( \{s_1, s_2, \ldots \} \) of the many body system under study. The probability \( \rho(s_i) \) for a given microstate is given by \( \rho(s_i) = Z^{-1} e^{-\beta E(s_i)} \), where \( E(s_i) \) is the energy of microstate \( s_i \) and \( \beta \) is the inverse temperature (we set \( k_B = 1 \)).

In many cases the sum in Eq. (1.37) cannot be calculated exactly because of the sheer number of microstates that exist. For instance for an Ising chain with \( L \) spins the number of microstates is \( 2^L \). The simplest approach would therefore be to use a Monte Carlo algorithm which randomly generates \( N \) microstates, \( r_1, r_2, \ldots, r_N \) from a uniform distribution and approximate \( \langle A \rangle \) by

\[
\langle A \rangle \approx \bar{A}(N) = \sum_{i=1}^{N} \rho(r_i) A(r_i)
\]  

(1.38)

When \( N \to \infty \) the estimate \( \bar{A}(N) \) converges to the exact result \([55]\).

The problem with the above approach is that one is likely to generate microstates which have small weights \( \rho(r_i) \). Consequently their contribution to the sum is small and the convergence is slow. This can be avoided if instead of generating microstates from a uniform distribution one generates them from the distribution \( \rho(s_i) \) itself.

To do this we start from a microstate of the system and simulate the evolution of the system. If at the beginning of the Monte Carlo simulation the system is in state \( x_0 \) it will be in state \( x_n \) after \( n \) steps of the simulation. The number \( n \) of Monte Carlo steps therefore plays the role of time. For this approach to work it is crucial that the system is \emph{ergodic}, i.e. that any state \( s_j \) of the system can be reached from any state \( s_i \). Furthermore we require that the evolution of the system can be described by a \emph{Markov process}.

A Markov process is defined as follows. Let \( P(x_{n+1} = s_{i_{n+1}} | x_n = s_{i_n}, x_{n-1} = s_{i_{n-1}}, \ldots) \) denote the conditional probability that the system is in state \( s_{i_{n+1}} \) after \( n + 1 \) Monte Carlo steps if it was in state \( s_{i_n} \) after \( n \) steps and in state \( s_{i_{n-1}} \) after \( n - 1 \) steps and so on. Processes which satisfy \( P(x_{n+1} = s_{i_{n+1}} | x_n = s_{i_n}, x_{n-1} = s_{i_{n-1}}, \ldots) = P(x_{n+1} = s_{i_{n+1}} | x_n = s_{i_n}) \), i.e. the evolution of the system only depends on its current state and not on its history, are called Markov processes.
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The conditional probability \( P(x_{n+1} = s_j | x_n = s_i) \) is also called the transition probability from state \( s_i \) to state \( s_j \). For notational convenience we will refer to it as \( w_{i \rightarrow j} \). Our goal is to find a simple expression for \( w_{i \rightarrow j} \) which allows us to generate states from the probability distribution \( \rho(s_i) \). To achieve this we make use of the master equation governing the probability \( P(x_n = s_j) \) that the system is in state \( s_j \) at "time" \( n \).

\[
\frac{\partial P(x_n = s_j)}{\partial n} = -\sum_{i \neq j} w_{j \rightarrow i} P(x_{n-1} = s_j) + \sum_{i \neq j} w_{i \rightarrow j} P(x_{n-1} = s_i) \tag{1.39}
\]

The master equation can be thought of as a flow equation. The first term on the left hand side describes the probability flow out of the state \( s_j \) while the second term describes the flow into the state \( s_j \). In equilibrium \( P(x_n = s_j) \) must be independent of \( n \) and identical to \( \rho(s_j) \). Therefore we have

\[
\sum_{i \neq j} w_{j \rightarrow i} \rho(s_j) = \sum_{i \neq j} w_{i \rightarrow j} \rho(s_i) \tag{1.40}
\]

A common way to satisfy Eq. (1.40) is to require that

\[
\frac{w_{i \rightarrow j}}{w_{j \rightarrow i}} = \frac{\rho(s_j)}{\rho(s_i)} = e^{-\beta(E(s_j) - E(s_i))}, \tag{1.41}
\]

a condition which is referred to as detailed balance. Physically, detailed balance implies that every change in the state of the system is reversible. In other words if the system can change from state \( s_i \) to state \( s_j \) the reverse process, changing from state \( s_j \) to state \( s_i \), must also be allowed if detailed balance is to be satisfied.

When performing a Monte Carlo simulation we split the transition probability into two separate parts: \( w_{i \rightarrow j} = P_u(s_i, s_j)P_{\text{acc}}(s_i, s_j) \). The first part, \( P_u(s_i, s_j) \) is the probability that when the system is in state \( s_i \) an update to state \( s_j \) is suggested. The second part \( P_{\text{acc}}(s_i, s_j) \) is the probability that the update to state \( s_j \) is accepted. If we choose \( P_u(s_i, s_j) \) in such a way that \( P_u(s_i, s_j) = P_u(s_j, s_i) \), then it drops out from the detailed balance condition. We are therefore left with the task of choosing \( P_{\text{acc}}(s_i, s_j) \) in a way which satisfies the detailed balance condition. In 1953 Metropolis et al. proposed \( P_{\text{acc}}(s_i, s_j) = \min(1, e^{-\beta(E(s_j) - E(s_i))}) \) \[36 \] \[65 \]. It is easy to verify that this choice does indeed obey detailed balance. Furthermore it has the advantage that states with a lower energy are automatically accepted.

Note that the probability \( P_{\text{acc}}(s_i, s_j) \) does not necessarily need to be normalized. The normalization is added when calculating the desired expectation value, as shown below. Because it is likely that consecutive states
1.6. Markov-chain Monte Carlo simulations

$x_n$ and $x_{n+1}$ are correlated, one often uses only every $m$th state in the calculation of the expectation value. Furthermore one usually discards the first $N_{th}$ states to ensure that the states are thermalized. The desired expectation value is then given by

$$\bar{A}(N) = \frac{1}{N} \sum_{n=1}^{N} A(x_{mn+N_{th}}),$$  \hspace{1cm} (1.42)

where the states $\{x_1, x_2, \ldots, x_{mN+N_{th}}\}$ were generated with the Monte Carlo simulation and the factor $1/N$ ensures normalization.

The simplest Metropolis Monte Carlo scheme for calculating the magnetization of an Ising model consists of the following steps (cf. [55]):

1. Initialize the system in any state
2. Randomly choose a spin (corresponds to $P_u$).
3. Calculate the energy change $\Delta E$ which would result if the spin was flipped.
4. If $\Delta E < 0$ accept the spin flip. Otherwise generate a random number $0 < r < 1$ and accept the spin flip if $r < e^{-\beta \Delta E}$ (Corresponds to $P_{acc}$).
5. Calculate the magnetization and store its value.
6. Go to step 2.

Generally one refers to the sequence 2-4 as one Monte Carlo step, while step 5 is referred to as a Monte Carlo measurement. Note that in this simple scheme a measurement is performed after every step which will lead to correlations between the measurements. It is important that the magnetization is also calculated when the spin flip in the preceding step was not accepted. Once the simulation has ended, the average magnetization and its standard error can be calculated. A more sophisticated implementation which circumvents the problem of correlations is discussed in Appendix C.

1.6.1 The effect of correlations

There are multiple sources of errors which need to be considered when working with Monte Carlo simulations. In this section we discuss statistical errors which arise due to a finite sample size and correlations between Monte Carlo measurements. There are also other sources of error which are not discussed in this section, for instance finite size effects.
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Let us assume that during a Monte Carlo simulation we made \( N \) ordered measurements \( A_1, \ldots, A_N \). By ordered we mean that measurement \( A_{n+1} \) was made immediately after measurement \( A_n \), but it is possible that a fixed number of states was discarded in between the two measurements to reduce their correlation. The measurement index \( n \) can then be interpreted as a discrete time variable with stepsize \( \delta t \) which is directly proportional to the number of states discarded in between measurements.

The mean value is given by \( \bar{A} = \frac{1}{N} \sum_{i=1}^{N} A_i \) and a measure of its uncertainty is given by its variance. The variance of the \( i \)th measurement is defined as \( \text{Var}(A_i) = \langle (A_i - \langle A \rangle)^2 \rangle \). Since all the \( A_i \) were drawn from the same distribution \( \text{Var}(A_i) = \text{Var}(A) \) is independent of \( i \). It is also useful to define the covariance \( \text{Cov}(A_i, A_j) = \langle (A_i - \langle A \rangle)(A_j - \langle A \rangle) \rangle \) which is a measure of the correlation between \( A_i \) and \( A_j \). Note from its definition it follows that \( \text{Cov}(A_i, A_j) = \text{Cov}(A_j, A_i) \) and since all the \( A_i \) were drawn from the same distribution and the system is assumed to be in equilibrium \( \text{Cov}(A_i, A_j) = \text{Cov}(A_1, A_{1+j-i}) \). The variance of the mean is given by:

\[
\text{Var}(\bar{A}) = \frac{1}{N^2} \left[ \sum_{i=1}^{N} \text{Var}(A_i) + \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \text{Cov}(A_i, A_j) \right]
\]  

(1.43)

Using the shorthands \( \text{Var}(A) = \sigma_A^2 \) and \( \text{Cov}(A_i, A_j) = \sigma_A^2 C_{j-i}^A \), this can be brought into the following form

\[
\sigma_{\bar{A}}^2 = \frac{\sigma_A^2}{N} \left[ 1 + 2 \sum_{t=1}^{N-1} (1 - \frac{t}{N}) C_t^A \right]
\]  

(1.44)

The function \( C_t^A \) is known as the autocorrelation function of \( A \). From its definition it is clear that \( C_0^A = 1 \). Furthermore one expects \( C_t^A \to 0 \) for large \( t \) since \( A_t \) and \( A_{i+t} \) are not correlated in that case. If we assume that \( C_t^A \) is already negligibly small for \( t \ll N \) the second term in the equation above can be approximated as \( \sum_{t=0}^{\infty} C_t^A \approx \frac{1}{\delta t} \int_0^{\infty} \text{d}t \text{C}_t^A =: \tau_A/\delta t \) [7]. The quantity \( \tau_A \) is known as the autocorrelation time of \( A \). Reinserting this we obtain the following expression for the variance \( \sigma_{\bar{A}}^2 \) of the mean \( \bar{A} \)

\[
\sigma_{\bar{A}}^2 = \frac{\sigma_A^2}{N} \left[ 1 + 2 \frac{\tau_A}{\delta t} \right].
\]  

(1.45)

Equation (1.45) confirms the well known result that the variance of the mean scales as \( 1/N \). The simplest way to improve the accuracy of the simulation is therefore to increase the sample size. However, often calculating
the observable $A$ for a given state is expensive. In that case the accuracy of the simulation can be increased by keeping the sample size fixed but increasing the time step $\delta t$ which corresponds to discarding more states between measurements, \textit{i.e.} waiting longer between measurements.

### 1.6.2 The blocking method

There are various methods to assess the effect of correlations on the outcome of a Monte Carlo simulation. The simplest one is to calculate the autocorrelation function. Another useful method is the so-called blocking method. To implement the blocking method we combine $M$ measurements into a block average $B_n$

$$B_n = \frac{1}{M} \sum_{i=1}^{M} A_{i+nM} \quad (1.46)$$

Let’s assume that we can form $N_b$ of such blocks and that $N_b$ is a power of two. This will prove useful later on.

In terms of the block averages the mean $\bar{A}$ is given by

$$\bar{A} = \frac{1}{N_b} \sum_{n=1}^{N_b} B_n. \quad (1.47)$$

Since all of the blocks comprise an equal number $M$ of measurements we assume that they also have the same variance. To estimate it we calculate.

$$(\sigma_B^{(0)})^2 = \frac{1}{N_b} \sum_{n=1}^{N_b} (B_n - \bar{A})^2. \quad (1.48)$$

In a next step we combine adjacent blocks $B_n^{(1)} = (B_{2n-1} + B_{2n})/2$. This is possible since $N_b$ is a power of two. Note also that the choice of combining adjacent blocks is merely a choice of convenience, more sophisticated methods where randomly chosen pairs of blocks are combined are also possible.
The variance of the superblocks $B_{n}^{(1)}$ is estimated as

$$
(\sigma_B^{(1)})^2 = \frac{2}{N_b} \sum_{n=1}^{N_b/2} (B_n^{(1)} - \bar{A})^2
= \frac{1}{2N_b} \sum_{n=1}^{N_b} (B_n - \bar{A})^2 + \frac{1}{N_b} \sum_{n=1}^{N_b/2} (B_{2n-1} - \bar{A})(B_{2n} - \bar{A})
= \frac{(\sigma_B^{(0)})^2}{2} + \frac{1}{N_b} \sum_{n=1}^{N_b/2} (B_{2n-1} - \bar{A})(B_{2n} - \bar{A})
$$

The last term in the equation above has the form of a covariance and is a measure of the correlation between adjacent blocks. If $B_{2n-1}$ and $B_{2n}$ are correlated we expect this term to always be larger than zero and contribute to $\sigma_B^{(1)}$. If, on the other hand, $B_{2n-1}$ and $B_{2n}$ are uncorrelated the sign of $(B_{2n-1} - \bar{A})(B_{2n} - \bar{A})$ will oscillate and the term will be zero on average. Note that when there are no correlations we have $(\sigma_B^{(1)})^2 = (\sigma_B^{(0)})^2 / 2$, whereas correlated blocks lead to $(\sigma_B^{(1)})^2 > (\sigma_B^{(0)})^2 / 2$.

Since we chose $N_b$ to be a power of two the process of combining adjacent blocks can be continued and in the absence of correlations we have $(\sigma_B^{(m)})^2 = (\sigma_B^{(m-1)})^2 / 2 = \cdots = (\sigma_B^{(0)})^2 / 2^m$. Furthermore we know from the preceding section that in the absence of correlations the variance of the mean is given by

$$
(\sigma_A^{(m)})^2 = \frac{(\sigma_B^{(m)})^2}{N_b/2^m} = \frac{(\sigma_A^{(0)})^2}{N_b}.
$$

This means that in the absence of correlations $(\sigma_A^{(m)})^2$ is independent of $m$. When correlations are present, on the other hand, we have shown above that $(\sigma_B^{(m)})^2 > (\sigma_B^{(m-1)})^2 / 2$ and consequently $(\sigma_A^{(m)})^2 > (\sigma_A^{(m-1)})^2$.

The effect of correlations can therefore be estimated by plotting $\sigma_A^{(m)}$ against the number of blocks $N_b^{(m)} = N_b / 2^m$. At large values of $N_b^{(m)}$ the blocks will be small and likely to be correlated. Consequently $\sigma_A^{(m)}$ will be underestimated in this regime. As we move towards smaller values of $N_b^{(m)}$ correlations should play less of a role and the size of $\sigma_A^{(m)}$ should increase until it becomes roughly constant or at least tapers off to a finite value which constitutes a good estimate for the standard error of the mean.
1.7 Outline of this thesis

At zero $T$ the spectral function of a spin-up carrier injected into a FM with all spins up is strikingly different from that of a spin-down carrier. The reason for this is that the spin-up carrier spectrum belongs to the $S_{z \text{tot}} = NS + 1/2$ subspace where spin-flips are impossible while the spin-down carrier spectrum belongs to the $S_{z \text{tot}} = NS - 1/2$ subspace. This naturally leads to the question what happens to the spin-up spectrum at finite $T$. In that case the carrier is injected into a magnetic background where thermal magnons may already be present and consequently the different subspace of $S_{z \text{tot}}$ mix. Therefore one expects that spectral weight will be transferred from the $T = 0$ $\delta$-peak to the spin-polaron states leading to an interesting $T$ dependence of the spin-up spectrum.

How this transfer of spectral weight occurs is the topic of Chapter 2, where we develop a low-$T$ expansion for the spin-up GF. The expansion becomes exact in the limit $T \to 0$. In contrast to previous work we use a canonical ensemble which ensures that exactly one carrier is present in the system at all times. The small parameter in which we expand is the Boltzmann factor $e^{-\beta \Omega q}$. Essentially the idea for this expansion is that at low $T$ only states with few magnons contribute to the temperature average and consequently the trace over the states of the magnetic background can be truncated. The advantage of this method and the restriction to a single carrier is that it allows us to treat the carrier-magnon interaction exactly rather than using a mean field approach. It furthermore allows us to compare Ising and Heisenberg magnetic backgrounds just as we did for the $T = 0$ spin-polaron above. This work applies for $d \geq 2$. In $d = 1$, a single domain with opposite FM order costs the same energy as a magnon and restriction to a single magnon is not a good approximation.

To understand the role played by these domains in 1d, we introduce, in Chapter 3, a simplified model where all the exchange interactions are of Ising type. This simplification makes it possible to obtain exact, numerical results with a Metropolis algorithm and for any temperature to study both FM and AFM chains on equal footing. We find that for both AFM and FM magnetic backgrounds the carrier spectrum shows a distinctive structure of small resonances. These resonances can be attributed to small magnetic domains which entrap the carrier. A similar phenomenon occurs in binary alloys of the type $A_xB_{1-x}$ where charge carriers can become localized in domains of like-atoms. However, there are also some key differences between our model and binary alloys. In binary alloys one uses a disorder average that keeps the concentration of atoms constant and generally there are no
correlations. In this cases the carrier can become truly localized. In our model, on the other hand, we use a temperature average which includes correlations. Furthermore the carrier never becomes truly localized because the magnetic background is not static.

The numerical results allow us to identify the type of magnetic domains which contribute most to the entrapment of the carrier. This information is then used to construct an analytical approximation that works well at low to medium $T$ and reproduces most of the resonances found in the exact spectrum.

In Chapter 4 we study the differences between multi-band and single-band models. In single-band models the carrier is hosted by the same band that gives rise to the magnetic moments, while in multi-band models it is hosted in a separate band. Specifically we compare three different models (one of them being the model from Chapter 3) that for FM order and $T = 0$ have identical QPs. The models can be mapped onto each other in a fashion that resembles the famous Zhang-Rice mapping from the three band Emery model to the $t-J$ model in the cuprates [114]. Surprisingly we find that even though the mapping between our models works at $T = 0$, it does not work at any finite $T$. The reason for this is again linked to the local environment into which the carrier is injected. For a single-band model the carrier effectively removes one of the magnetic moments when it is injected. If this leads to the removal of a magnetic moment which was previously misaligned with its neighbors the energy of the system is lowered. In two-band models on the other hand such a process is impossible because the carrier is hosted by a separate band and therefore does not remove magnetic moments upon its injection. At $T = 0$ for FM coupling all the magnetic moments are aligned and these processes do not play any role. However, at any finite $T$ they cause the low-energy states of the single-band to be qualitatively different from the multi-band models. The ramifications of this effect and its generalization to more complicated models are discussed in detail in Chapter 4.

Chapter 5 contains a summary and discussion of the work presented in this thesis and suggestions for further work and extensions.
Chapter 2

Signatures of spin-polaron states at low temperatures

2.1 Introduction

In the previous chapter we derived the zero temperature spectrum for a single carrier injected into a FM ordered magnetic background. At finite temperature, an exact solution is no longer possible since one needs to consider states with arbitrary numbers of magnons when performing the temperature average. A natural approach for low $T$ is to consider states with a small number of magnons; this is what we do here. As a result, the solution we propose becomes asymptotically exact in the limit of very low temperatures, where “low” means well-below the Curie critical temperature $T_C$ of the FM background.

As mentioned, a spin-up carrier has a very simple spectrum at $T = 0$, mirroring that of the free carrier, with a single eigenstate for a given momentum. At $T \neq 0$ thermally activated magnons are present in the system and the carrier can now flip its spin by absorbing one of them. Interaction with even one such magnon takes the problem in the Hilbert subspace appropriate for the $T = 0$ spin-down carrier, which has a very different spectrum. As a result, we expect that spectral weight is transferred from the spin-up QP peak to energies in the spectrum of the spin-polaron, as $T$ increases. How exactly does this occur at very low $T$, and what happens to the infinitely-lived discrete state that was the only feature in the spectrum at $T = 0$, is the topic of this chapter.

Furthermore, we consider two types of exchange between the local moments, namely Heisenberg exchange and Ising exchange (in both cases, the characteristic energy scale is $J$). For the latter the magnon spectrum is gapped, whereas for the former the magnon spectrum is gapless. This allows us to contrast the two cases to understand the relevance of the magnon’s spectrum on the evolution with $T$ of the up carrier’s spectral function.

Finite temperature studies in the single carrier limit have been previously...
carried out by Nolting *et al.* [81], Kubo [53] and Auslender *et al.* [5]. In the following paragraphs we summarize their approaches and comment on the differences to our method.

Nolting *et al.* account for the kinetic energy of the carrier with a tight-binding model with an energy scale $t$, and for the exchange between the local moments and the carrier with a Heisenberg exchange with a coupling $J_0$. Unlike the models we consider, Nolting *et. al.* do not include the exchange $J$ between local moments; this is one key difference between our work and theirs. The second is the approach employed. While, as mentioned, we use a low-$T$ expansion to calculate the propagator, Nolting *et al.* proposed an ansatz for the self-energy chosen so as to reproduce asymptotic limits where an exact solution is available, specifically the $T = 0$ solution mentioned above and the case of finite $T$ but zero bandwidth, $t = 0$ [76] (This approach was later generalized to finite carrier concentrations as well [80]). Their ansatz for the self-energy contains several free parameters which are fixed by fitting them to a finite number of exactly calculated spectral moments. A similar approach for the spectral weight was previously used by Nolting and Oleś in Refs [77–79]. The temperature dependence is contained implicitly in the magnetization which enters the self-energy as an external parameter. In the limit of very low $T$ we consider here, the average local moment is essentially unchanged from its $T = 0$ value, so the effects we uncover are basically absent in the ansatz of Nolting *et al.*. In other words, besides studying different Hamiltonians by very different means, our studies also focus on very different regimes: very low $T$, in our work, vs. medium and high $T$ in Ref. [81]. Needless to say, in the absence of an exact solution it is likely that a collection of approximations valid in different regimes will be needed in order to fully understand this problem.

Kubo [53] used the coherent potential approximation (CPA) to calculate the carrier LDOS at finite $T$ (see also [103]). The CPA is an approximation that was introduced by Soven [100] as a means to deal with the disorder average in binary alloys through the introduction of an effective medium. In Ref. [53] Kubo extends this procedure to the s-f(d) model by neglecting spin-spin correlations. Instead the spin part $H_S$ of the Hamiltonian is treated in the molecular field approximation which is essentially a mean field approximation. The approximation is expected to fail at low temperatures, where spin-spin correlations are important, and is therefore not applicable in our case. The advantage of the CPA is that it can be extended to models for dilute magnetic semiconductors where the local magnetic moments are disordered [101].

Auszlender *et al.* [5] derived an expression for the single particle GF of
2.2 The low-temperature expansion

the s-f(d) model at temperatures much lower than the Curie temperature $T_C$. Their result is also obtained by using an EOM approach, but they use a Dyson-Maleev transformation to represent the local spins $S_i$ with bosonic operators. This type of transformation generally works best when $S$ is large while our low-$T$ approximation does not impose any requirements on $S$ and also allows us to study the limiting case $S = 1/2$. Furthermore Auslender et al. neglect spin-spin interactions which are taken into account in our work. Nevertheless the self energy derived by Auslender et al. is remarkably close to our result. However, in their analysis they focus on the effect that finite temperature has on the $T = 0$ QP peak and not on the transfer of spectral weight to spin-polaron states.

2.2 The low-temperature expansion

To calculate the low-$T$ expression of the GF for a spin-up carrier, $G^\uparrow(k, \omega)$ we start from Eq. (1.29)

$$G^\uparrow(k, \omega) = \sum_n \frac{e^{-\beta E_n^{S/I}}}{Z} \langle S/I, n|c_{k, \uparrow} \hat{G}(\omega + E_n^{S/I})c_{k, \uparrow}^\dagger|S/I, n\rangle. \quad (2.1)$$

Remember that we are in a canonical (not grand-canonical) ensemble, assuming that the carrier is injected in the otherwise undoped FM which is in thermal equilibrium. As a result, the trace is over the eigenstates $|S/I, n\rangle$ of $\hat{H}_{S/I}$ (in the absence of carriers, $\hat{H} \equiv \hat{H}_{S/I}$).

At $T = 0$, the trace reduces to a trivial expectation value over $|FM\rangle$, and we recover the result from Chapter 1.5

$$G^{0\uparrow}(k, \omega) = \langle FM|c_{k, \uparrow} \hat{G}(\omega)c_{k, \uparrow}^\dagger|FM\rangle = \frac{1}{\omega - E^{\uparrow}(k) + i\eta}. \quad (2.2)$$

The eigenenergy is $E^{\uparrow}(k) = \epsilon(k) + J_0 \frac{S}{2}$ for both the Heisenberg and Ising models. As discussed, this shows that at $T = 0$ a spin-up carrier propagates freely and acquires an energy shift from $\hat{H}^{z}_{\text{exc}}$.

At finite temperature, we expect to find:

$$G(k, \omega) = \frac{1}{\omega - E^{\uparrow}(k) - \Sigma(k, \omega) + i\eta}$$

$$= G^{0\uparrow}(k, \omega) + G^{0\uparrow}(k, \omega)\Sigma(k, \omega)G^{0\uparrow}(k, \omega) + \ldots \quad (2.3)$$

Strictly speaking, the energy shift $J_0 \frac{S}{2}$ is part of the self-energy, however it is convenient to separate it as we do here so that $\Sigma(k, \omega)$ contains only the finite-$T$ terms.
2.2. The low-temperature expansion

Since we are interested in the lowest-$T$ contribution to $\Sigma(k, \omega)$, we consider only the first two terms of Eq. (1.15), i.e. the completely FM ordered state and states with one magnon. In doing so we find

$$G_\uparrow(k, \omega) = \frac{G_\uparrow(0)(k, \omega) + \sum_\mathbf{q} e^{-\beta \Omega_\mathbf{q}} G_\uparrow(1)(k, \mathbf{q}, \mathbf{q}, \omega) + \ldots}{1 + \sum_\mathbf{q} e^{-\beta \Omega_\mathbf{q}} + \ldots},$$

(2.4)

where we define the new propagators

$$G_\uparrow(1)(k, \mathbf{q}, \mathbf{q}', \omega) = \langle \Phi(\mathbf{q}') | c_{k\uparrow} \hat{G}(\omega + \Omega_\mathbf{q}') c_{k+\mathbf{q}'-\mathbf{q}\uparrow} | \Phi(\mathbf{q}) \rangle.$$

(2.5)

Note that the argument of the resolvent is shifted by the magnon energy, meaning that the carrier’s energy is measured with respect to that of the state in which the carrier is injected. Furthermore only diagonal $\mathbf{q}' = \mathbf{q}$ terms contribute to the trace. Following calculations detailed in Appendix [A], we find:

$$\sum_\mathbf{q} e^{-\beta \Omega_\mathbf{q}} G_\uparrow(1)(k, \mathbf{q}, \mathbf{q}, \omega) = \sum_\mathbf{q} e^{-\beta \Omega_\mathbf{q}} \left\{ G_\uparrow(0)(k, \omega) - \frac{J_0}{2N} \left[ G_\uparrow(0)(k, \omega) \right]^2 \right\},$$

(2.6)

where

$$g(k, \mathbf{q}, \omega) = \frac{1}{N} \sum_\mathbf{Q} G_\uparrow(0)(k + \mathbf{q} - \mathbf{Q}, \omega + \Omega_\mathbf{q} - \Omega_\mathbf{Q})$$

(2.7)

is a known function. When this expression is used in Eq. (2.4), we obtain

$$G_\uparrow(k, \omega) = \frac{G_\uparrow(0)(k, \omega)(1 + \sum_\mathbf{q} e^{-\beta \Omega_\mathbf{q}} + \ldots) + [G_\uparrow(0)(k, \omega)]^2 \Sigma(k, \omega)(1 + \ldots) + \ldots}{1 + \sum_\mathbf{q} e^{-\beta \Omega_\mathbf{q}} + \ldots},$$

(2.8)

$$= G_\uparrow(0)(k, \omega) + [G_\uparrow(0)(k, \omega)]^2 \Sigma(k, \omega) + \ldots,$$

(2.9)

since the terms in the brackets are the expansion of $Z$ (to the order considered here; higher order contributions will come from including many-magnon processes) and cancel with the denominator. This has the expected form of Eq. (2.3), so we can identify the lowest-$T$ correction to the self-energy:

$$\Sigma(k, \omega) = -\frac{J_0}{2N} \sum_\mathbf{q} e^{-\beta \Omega_\mathbf{q}} \left[ 1 + J_0 S G_\uparrow(0)(k + \mathbf{q}, \omega + \Omega_\mathbf{q}) + \frac{J_0}{2} g(k, \mathbf{q}, \omega) \right] + \ldots$$

(2.10)
2.2. The low-temperature expansion

It is important to mention that although we only considered states with zero or one magnon in our derivation, we will see some higher-order effects in our results when using $G_\uparrow(k, \omega) = [\omega - E_\uparrow(k) - \Sigma(k, \omega) + i\eta]^{-1}$, i.e. when the self-energy is placed in the denominator. These are from states where multiple magnons are present in the system but the carrier interacts only with one of them while the rest are “inert” spectators.

Equation (2.10) is the main result of this chapter. The only difference between Heisenberg and Ising backgrounds is the expression for the magnon energy $\Omega_q$. For the Ising case, this energy is independent of momentum, resulting in a self-energy $\Sigma(\omega)$ independent of $k$.

Before presenting results, let us consider what the spectral weight given by $A_\uparrow(k, \omega) = -\frac{1}{\pi} \text{Im} G_\uparrow(k, \omega)$ should be expected to reveal. The Lehmann representation of the propagator in its expanded form is (cf. Eq. (1.20))

$$G_\uparrow(k, \omega) = \frac{1}{Z} \left[ \frac{1}{\omega - E_\uparrow(k) + i\eta} + \sum_{\alpha, q} e^{-\beta \Omega_q} \frac{\langle \phi(q) \mid c_{k, \uparrow} \rangle \langle \Psi_\alpha(1)(k + q) \rangle^2}{\omega + \Omega_q - E_\alpha^{(1)}(k + q) + i\eta} + ... \right].$$

(2.11)

At $T = 0$ only the first term contributes, giving a single QP peak at $\omega = E_\uparrow(k)$. The second term has poles at $\omega = E_\alpha^{(1)}(k + q) - \Omega_q$. The $m = 1$ subspace also corresponds to a spin-down carrier injected in the FM at $T = 0$, thus we can find the energies $E_\alpha^{(1)}(k)$ from the spectral weight $A_\uparrow^{(0)}(k, \omega)$ which was discussed in Chapter 1.5.

As already mentioned and further detailed below, the spectrum $E_\alpha^{(1)}(k)$ certainly contains an up-carrier+magnon continuum spanning the energies $\{E_\uparrow(k - q') + \Omega_q\}_{q'}$; in the right circumstances, a coherent spin-polaron state with the magnon bound to the carrier may also appear, see below. Thus, for $T \neq 0$, $A_\uparrow(k, \omega)$ should have weight at all energies $\{E_\uparrow(k + q - q') + \Omega_{q'} - \Omega_q\}_{q, q'}$. In the Ising case the magnon energies cancel out so weight should be expected at all energies $\{E_\uparrow(q)\}_{q}$ in the spin-up carrier spectrum, not just at $E_\uparrow(k)$. This automatically implies that the $T = 0$ infinitely lived QP of energy $E_\uparrow(k)$ acquires a finite lifetime at $T \neq 0$. This remains true for the Heisenberg case, with the added complication that now, $\{E_\uparrow(k + q - q') + \Omega_{q'} - \Omega_q\}_{q, q'}$ will generally span a wider range of energies than $\{E_\uparrow(q)\}_{q}$.

If a spin-polaron appears in the $m = 1$ sector, additional weight is expected at energies in its band minus the magnon energy. Higher order terms will contribute similarly (remember that our solution for the propagator does include partial contributions from many-magnon states). To conclude, at finite $T$ one can no longer assume that energies for which the spectral weight $A_\uparrow(k, \omega)$ is non-zero are necessarily in the spectrum of the momentum-$k$
Hilbert subspace. This makes the interpretation of the spectral weight less straightforward than it is at $T = 0$.

## 2.3 Results

We now present and analyze low-$T$ results for the spectral weight of the spin-up carrier. Since the calculation of $G_\uparrow(k, \omega)$ becomes numerically very expensive in 3d, most of our analysis is in 2d. However, we will also show a selection of 3d spectra which prove that the 3d results are qualitatively similar to the 2d results. The low-$T$ expansion derived above is expected to fail in 1d where, at least for Ising coupling, the energy of magnetic domains is independent of their length. We therefore do not show any 1d results.

The spectral weight $A_\uparrow(k, \omega)$ and the self-energy $\Sigma(k, \omega)$ are shown for the Heisenberg and Ising models with AFM coupling $J_0/t = 10$ in Figs. 2.1 and 2.2 respectively. In both cases the top panel is for $k = (0, 0)$ and the bottom one is for $k = (\pi, \pi)$. However, for the Ising model the self-energy is independent of $k$ and therefore in Fig. 2.2 it is only shown beneath the $k = (0, 0)$ spectral weight. The value of $J_0/t$ was chosen so large in order to ensure that the different features in the spectrum are well separated, to simplify the analysis. Results for smaller values of $J_0$ will be shown below.

From the previous discussion of the $m = 1$ sector at $T = 0$ we know that for smaller $J_0$ the spin-polaron states change their nature as they become resonances in the c+m continuum. Similar behavior is expected to occur at finite $T$ and its signatures are discussed below.

$A_\uparrow(k, \omega)$, which at $T = 0$ is the peak $\delta(\omega - E_\uparrow(k))$ (indicated by the thick green line), broadens into a continuum at finite $T$. As discussed at the end of the previous section, this continuum has its origin in the c+m continuum of the $m = 1$ sector, thus we continue to call it the “c+m” continuum, and should span $\{E_\uparrow(k + q - q') + \Omega_{q'} - \Omega_q\}_{q, q'}$. The red dashed lines show the boundaries of this energy range, in excellent agreement with the broadening observed in $A_\uparrow(k, \omega)$. We note that most of the spectral weight is still located near $E_\uparrow(k)$.

This broadening confirms that at finite $T$ the QP acquires a finite lifetime (the peak at $E_\uparrow(k)$ is now a resonance inside a broad continuum, not a discrete state). Clearly, this is due to processes where the spin-up carrier absorbs a thermal magnon and then re-emits it with a different momentum, thus scattering out of its original state.

The finite lifetime of the carrier in the c+m continuum is also evident in the self-energy. The inset in Fig. 2.2 shows that for energies within the
2.3. Results

Figure 2.1: Spectral weight $A(k,\omega)$ and the real (solid line) and imaginary (dashed line) part of the self-energy $\Sigma(k,\omega)$ for the 2$d$ Heisenberg model with AFM $J_0/t = 10$ and $\beta t = 1$, at $k = (0,0)$ (top) and $k = (\pi,\pi)$ (bottom). The expected sp1 continuum boundaries are marked with dash-dotted blue lines and the expected c+m continuum boundaries with dashed red lines. The $E_\uparrow(k)$ energy of the $T = 0$ $\delta$-peak is marked with a thick green line. Other parameters are $J/t = 0.5, S = 0.5, \eta = 0.02$ (top) and $\eta = 0.05$ (bottom).
2.3. Results

Figure 2.2: Same as Fig. 2.1 but for the Ising model. All parameters are the same except $\beta t = 0.5$ and $\eta = 0.01$ in both panels. Note that for the Ising model $\Sigma(\omega)$ is independent of $k$. The inset shows a zoom on $\Sigma(\omega)$ at high energies.
2.3. Results

c+m continuum the imaginary part of the self-energy is finite. The same is true for the Heisenberg model (not shown).

While the broadening of the T=0 δ-peak may be thought of as quite trivial, Figs. 2.1 and 2.2 show that it is not the only effect of the finite T: spectral weight is also transferred to a new continuum located below the c+m continuum. We attribute this continuum to the sp1 state. Indeed, if we denote by $E_{sp1}(k)$ the energy of the sp1 polaron, we find that this continuum spans \{\[E_{sp1}(k + q) - \Omega_q\]q \} (the boundaries of this range are marked by the dashed-dotted blue lines). Its presence agrees with the Lehmann representation and reveals this spectral weight transfer to be due to processes where the spin-up carrier binds a thermal magnon and turns into an sp1 polaron.

The sp1 continuum is also where both the real and imaginary part of $\Sigma(k, \omega)$ take their largest values. Consequently the lifetime of these states is roughly two orders of magnitude smaller than that of the states within the c+m continuum. This is not surprising as the c+m continuum stems from a δ-peak with an infinite lifetime at T=0, whereas the sp1 continuum vanishes at T=0.

There is furthermore a qualitative difference between the real-part of $\Sigma(k, \omega)$ in the sp1 continuum and in the c+m continuum. For the latter the real part falls off relatively smoothly (cf. inset in Fig. 2.2), whereas for the sp1 continuum it is highly singular and almost discontinuous.

Note that there are no major differences between the Heisenberg and Ising models, except for the fact that the boundaries of these continua are momentum dependent for the former and momentum independent for the latter, due to their different magnon dispersions.

Figures 2.1 and 2.2 also show a very puzzling discrete state at low energies. Before we turn our attention to the analysis of this peak, we quickly discuss the case with FM coupling $J_0 < 0$. Ising and Heisenberg results are depicted in Fig. 2.3 for $J_0/t = -2$ and $J/t = 0.5$. From the discussion of the $T = 0$ spectrum in the $m = 1$ Hilbert space, we know that for these parameters the Ising model has an sp2 state below its c+m continuum and therefore expect to find its signature in the finite-T spectrum, as well. This is indeed the case, as seen more clearly in panel (b) which expands the low-energy part of the Ising spectrum shown in (a), revealing weight at energies spanning \{\[E_{sp2}(k + q) - \Omega_q\]q \} (its lower boundary is marked by dashed-dotted blue lines). Note that since the sp2 state merges with the c+m continuum (boundaries marked by red dashed lines), their corresponding continua also merge, but panel (b) reveals a clear discontinuity where they overlap. The high-energy sp1 continuum is also clearly observed in
2.3. Results

Figure 2.3: Spectral weight $A_\tau(0,0,\omega)$ for the 2d Ising model (panels (a) and (b)) and 2d Heisenberg model (panel (c)) for FM $J_0/t = -2$ at $\beta t = 0.5, \eta/t = 0.01$ (Ising) and $\beta t = 1, \eta/t = 0.02$ (Heisenberg). The expected location of various features are also indicated (see text for more details). Other parameters are $J/t = 0.5, S = 0.5$.

Panel (a), again merged with the c+m continuum since the sp1 state is not fully separated at such a small $|J_0|$, either.

The Heisenberg model (panel (c)) only shows the c+m and sp1 continua, since there is no sp2 polaron here. Again, agreement with the expected boundaries is excellent (the weight seen below the c+m lower edge is due to the finite $\eta$ and the fact that we zoomed in close to the axis to make it easier to see the sp1 continuum).

It is worth noting that since for small $|J_0|$ the various features merge, it would be easy to misinterpret the thermal broadening as being all of c+m origin, i.e. to entirely miss the role played by the spin-polaron solutions in the $m = 1$ subspace. This is also illustrated in Fig. 2.4, where we return to an AFM $J_0$ coupling and show how the $k = 0$ spectra change as $J_0$ is decreased. All features discussed previously can be easily identified for large $J_0$ but merge into one another as $J_0$ decreases, so that by the time $J_0/t = 3$ there is only one very broad feature, albeit with a non-trivial structure, left
2.3. Results

Figure 2.4: Spectral weight $A_\uparrow(0,0,\omega)$ for the 2d Ising (dashed lines) and Heisenberg (full lines) models for $J_0/t = 10, 5, 3$ in the top, middle and bottom panels, respectively. Other parameters are $J/t = 0.5, S = 0.5$ and $\beta t = 0.5, \eta/t = 0.01$ (Ising), and $\beta t = 1, \eta/t = 0.02$ (Heisenberg). The oscillations visible especially in the sp1 continuum are due to finite-size effects (we used $N = 100^2$ and $N = 500^2$ for Heisenberg and Ising models, respectively).

in the spectrum (apart from the low-energy discrete peak, which we will discuss later). If one assumed that this is all of $c+m$ origin, i.e. scattering of the carrier on individual thermal magnons, one would infer very wrong values of the parameters from the boundaries’ locations.

The results shown so far are for large temperatures $k_B T \sim t = 2J$ (for our parameters), where higher order corrections should certainly become quantitatively important. On the other hand, from the Lehmann decomposition we expect that the location of the various features does not depend on temperature; only how much spectral weight they carry can change with $T$. For a more thorough analysis we return to the case of AFM $J_0$, using a rather large value so that the various features are well separated, and plot in Fig. 2.5 the spectral weight in the sp1 continuum for several different temperatures, for both the Ising and Heisenberg models. This confirms that,
2.3. Results

Figure 2.5: Spectral weight $A_\tau(k = 0, \omega)$ for the 2d Heisenberg (left) and Ising (right) models with AFM $J_0/t = 7$, at different temperatures. Only the sp1 continuum is shown. Its edges are indicated with dot-dashed blue lines. Other parameters are $J/t = 0.5$, $S = 0.5$ and $\eta/t = 0.01$ and 0.02 for Ising and Heisenberg, respectively.
2.3. Results

Indeed, the weight in this continuum decreases fast as $T \to 0$ while its location is not affected (the location of the low-energy peak shifts with $T$, but as we argue below, we do not believe that this is a physical feature).

To quantify the spectral weight transferred, we calculate $\int_{c+m} d\omega A_\uparrow(k, \omega)$, i.e. how much is in the $c+m$ continuum. Since at $T = 0$ all the weight is in the $\delta$-peak at $E_\uparrow(k)$ located inside the $c+m$ continuum, this value starts at 1 and decreases with increasing $T$, as weight is transferred into the $sp1$ continuum; one can easily check that the spectral weight obeys the sum rule $\int_{-\infty}^\infty d\omega A_\uparrow(k, \omega) = 1$.

The results are shown in Fig. 2.6 for both models, both at the center and at the corner of the Brillouin zone. Note that because of the finite value of $\eta$, some spectral weight “leaks” outside the continuum’s boundaries. This problem is more severe at lower $T$ because $E_\uparrow(k)$ is located very close to an edge of the continuum; this explains why the value saturates below 1 as $\beta \to \infty$. This explanation is also consistent with the observation that the amount of “missing weight” as $T \to 0$ is of order $\eta$.

Two features are immediately apparent. First, there is a substantial difference in the amount of spectral weight transferred out of the $c+m$ continuum at $k = (0,0)$ vs. $k = (\pi, \pi)$. This is expected for the Heisenberg...
model where the location of all features changes with $k$, but may come as a surprise for the Ising model where their location is independent of $k$. However, for both models $E^\uparrow(k)$, where most of the weight is found, moves from the lower edge of the $c+m$ continuum when $k = 0$, to the upper edge for $k = (\pi, \pi)$. As a result, it is reasonable that weight is transferred into the low-energy sp1 continuum more efficiently at $k = (0, 0)$ than at $k = (\pi, \pi)$, since in the former case the “effective” energy difference between the two features is smaller.

The second observation is that spectral weight is transferred into the sp1 continuum more efficiently in the Heisenberg model than in the Ising model. This difference is also clearly visible in Fig. 2.5 where the weight in the sp1 continuum of the Heisenberg model is still respectable at $\beta t = 20$, while for the Ising model this weight is already negligible at $\beta t = 8$.

An explanation for this difference comes from assuming that the weight in the sp1 continuum is proportional to the average number of thermal magnons, since no sp1 polaron can appear in their absence. Because the Ising magnon spectrum is gapped, at low $T$ this number is proportional to the Boltzmann factor $e^{-\beta \Omega}$. This suggests an integrated weight in the $c+m$ spectrum of $a - be^{-\beta J S}$, where $a = 1 - O(\eta)$ is the limiting value as $T \to 0$. We fitted the data points for $\beta t > 5$ with this form and found a very good fit (solid lines), which moreover works well for a larger range of $\beta$ values than used in the fit.

Magnons of the Heisenberg model are gapless so their number increases much faster with $T$. A simple estimate for a 2$d$ unbounded parabolic dispersion suggests $\langle n \rangle \sim k_B T^{1/3}$. The lines shown for the Heisenberg model in Fig. 2.6 are fits to $a - b/\beta$ for the data points with $\beta t > 5$. The fit is again reasonable over a wider range, and much superior to other simple functional forms we tried, such as $a - b/\beta^n$, $n > 1$ or $a - be^{-\beta c J}$ (the former assuming that we misidentified the power law, the second to see if Ising-like fits might be more appropriate). Of course, one can find excellent fits for all data using more complicated functions with additional parameters, but they are much harder to justify physically than our simple hypothesis resulting in an effectively one parameter fit.

Let us now discuss the discrete peak appearing below the sp1 continuum for both models, for AFM $J_0$. After carefully investigating many of its properties, such as how its energy and the region in the Brillouin zone where

1The prefactor contains the Riemann number $\zeta(1) = \infty$. However, as mentioned in Section 1.3 we assume that long range magnetic order is stabilized by an external mechanism such as weak interlayer coupling. The same mechanism should remove the singularity.
2.3. Results

Figure 2.7: Spectral weight $A_{\mathbf{r}}(\mathbf{k} = 0, \omega)$ for the 3$d$ Heisenberg model at $\beta t = 1$ for FM $J_0/t = -3$ (top) and AFM $J_0/t = 10$ (bottom) couplings. The edges of the $c+m$ continuum (dashed red lines) and sp1/sp2 continuum (dot-dashed blue lines) are indicated, as is $E_\uparrow(0)$ (thick green line). Other parameters are $J/t = 0.5, S = 0.5, \eta = 0.1$.

If it exists depend on various parameters including $T$, we believe that this is an unphysical artefact of our approximation. Arguments for this are: (i) the temperature dependence of its location, clearly visible in Fig. 2.5 (note that for the Ising model, the peak only separates below the sp1 continuum at higher $T$. At $\beta t = 2$ one just starts to see weight piling up near the lower edge, in preparation for this). According to the Lehmann decomposition, the ranges where finite spectral weight is seen cannot vary with $T$; (ii) the fact that the problem is worse at higher $T$, where we know that higher order corrections ought to be included in the self-energy; these could easily remove an unphysical pole; (iii) the fact that this is a discrete peak, not a resonance inside a continuum (this can be easily verified by checking that its lifetime is set by $\eta$). According to the Lehmann decomposition, discrete peaks cannot appear in the $T \neq 0$ spectral weight. Even if the carrier binds all thermal magnons in a coherent QP, the finite-$T$ spectral weight would reveal only a continuum associated with it, as is the case for the sp1 and sp2 polarons. To summarize, we believe that this discrete peak is an artefact and that in
2.3. Results

Figure 2.8: Spectral weight $A_T(k = 0, \omega)$ for the 3d Ising model at $\beta t = 0.5$ for FM $J_0/t = -3$ (top) and AFM $J_0/t = 10$ (bottom) couplings. The edges of the c+m continuum (dashed red lines) and sp1/sp2 continuum (dot-dashed blue lines) are indicated, as is $E_\uparrow(0)$ (thick green line). Other parameters are $J/t = 0.5, S = 0.5, \eta = 0.01$.

reality, its weight is part of the sp1 continuum from which it came. Ideally, these arguments would be strengthened by a calculation of the next correction to the self-energy, to check its effects. We found the exact calculation of the two-magnon term to be daunting even for the Ising model. The difficulty is not so much in evaluating different terms, but in tracing over all possible contributions – so far we did not find a sufficiently efficient way to do this. One can use approximations to speed things up, but that defeats the purpose since it would not be clear if the end results are intrinsic or artefacts, as well. Given this, we cannot entirely rule out that the discrete peak is a (precursor pointing to a) real feature, but we believe that to be very unlikely.

So far we have done the whole analysis in 2d, simply because the calculation of $\Sigma(k, \omega)$, especially for the Heisenberg model, is numerically much faster [2]. However, we did investigate the 3d models and found essentially

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2 All calculations were performed on a personal computer. For 2d spectra the calculation
2.4 Conclusions

To summarize, we calculated analytically the lowest-$T$ correction to the self-energy of a spin-up carrier injected in a FM background. We used both Heisenberg and Ising couplings to describe the background, to understand the relevance of gapped vs. gapless magnons. These results show how the spectral weight evolves from a discrete peak at $T = 0$ to a collection of continua for $T \neq 0$ (these can merge, in the appropriate circumstances), and explain their origin and how their locations can be inferred.

We were aided in this task by the fact that this model conserves the $z$-component of the total spin, allowing us to consider the contribution to the spectral weight coming from Hilbert subspaces with different numbers $m$ of magnons when the carrier has spin up. Although we focused on the $m = 1$, lowest-$T$ contribution, based on the knowledge we acquired we can extrapolate with some confidence to higher $T$, as we discuss now.

One definite conclusion of this work is that knowledge of the $T = 0$ carrier spectrum (in the $m = 0$ sector) $E_\uparrow(k)$, and of the magnon dispersion, $\Omega_q$, is generally not sufficient to predict a priori all features of the finite-$T$ spectral weight, although a fair amount can be inferred from them. To see why, let us assume that magnons do not interact with one another. (This is not true for either model, for example due to their hard-core repulsion; we will return to possible consequences of their interactions below.) If magnons were non-interacting, then Lehmann decomposition of the higher-order contributions in Eq. (1.15) would predict finite-$T$ spectral weight for all intervals \( \{ E_\alpha^{(m)}(k + \sum_{i=1}^{m} q_i) - \sum_{i=1}^{m} \Omega_{q_i} \}_{q_1 + \cdots + q_m}, m = 0, 1, \ldots \). Since we move from the $m$ to the $m + 1$ subspace by adding a magnon, and given that total momentum is conserved, we know that the spectrum in subspace $m + 1$ necessarily includes the convolution between the spectrum

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Footnote:

time is on the order of hours, whereas for $3d$ spectra it is on the order of days.
of the subspace $m$ and the magnon dispersion, i.e. $\{E^{(m)}_\alpha(k - q) + \Omega_q\}_q$ is part of the spectrum $E^{(m+1)}_\alpha(k)$ (these are the scattering states between the extra magnon and any eigenstate in the $m$ spectrum).

This observation allows us to infer the location of some of the finite-$T$ spectral weight, by recurrence. $E^{(1)}_\alpha(k)$ must include all scattering states $\{E^{(1)}_\alpha(k - q) + \Omega_q\}_q$, so the $m = 1$ contribution to the spectrum must span $\{E^{(1)}_\alpha(k + q') - \Omega_{q'}\}_q' = \{E^{(1)}_\alpha(k - q + q') - \Omega_{q'} + \Omega_q\}_q,q'$. We called this the $c+m$ continuum and verified that it is indeed seen in the finite-$T$ spectral weight. Knowledge of this part of the $m = 1$ spectrum allows us to infer scattering states that are part of the $m = 2$ spectrum and therefore their Lehmann contribution, etc. The conclusion is that all intervals $\{E^{(1)}_\alpha(k + \sum_{i=1}^m q'_i - \sum_{i=1}^m q_i) - \sum_{i=1}^m \Omega_{q'_i} + \sum_{i=1}^m \Omega_{q_i}\}_q,\ldots,q'_m$ will contain some spectral weight at finite $T$. For the dispersionless Ising magnons this interval is the same for all $m$. For dispersive Heisenberg magnons this interval broadens with $m$. For very small $J$, the additional broadening as $m$ increases is very small and moreover one would expect little spectral weight in the high-$m$ sectors if $T$ is not too large. Thus, we expect weight to be visible in the $c+m$ continuum up to high(er) temperatures; its boundaries may also slowly expand with $T$, for a Heisenberg background, as higher $m$ subspaces become thermally activated.

Apart from these scattering states, $E^{(m+1)}_\alpha(k)$ might also contain bound states where the extra magnon is coherently bound to all the other particles. The existence and location of such coherent states cannot be predicted a priori, as they depend on the details of the model (however, they certainly cannot appear unless coherent states exist in the $m$ space). An example is the $E^{(1)}_\alpha(k)$ spectrum which indeed contains the scattering states discussed above, but also contains the sp1 and/or sp2 discrete polarons states. These give rise to their own continua of scattering states in higher $m$ subspaces, whose locations can be inferred by recurrence.

The question, then, is if it is likely to find such new, bound coherent states for all values of $m$, i.e. if the number of additional continua becomes arbitrarily large with increasing $T$. Generally, the answer must be “no”, since this requires bound states between arbitrarily large numbers of objects. For the problem at hand, we believe that it is quite unlikely that they appear even in the $m = 2$ subspace, since that would involve one carrier binding two magnons. This is a difficult task given the weak nearest-neighbour attraction of order $J$ between magnons (due to the breaking of fewer FM bonds), and the fact that the carrier can interact with only one magnon at a time. The exception is likely to be in 1$d$ systems where magnons can
2.4. Conclusions

coalesce into magnetic domains.

Let us now consider the role of magnon interactions. Because of them, many-magnon states are not eigenstates of the Heisenberg Hamiltonian so higher-order terms are not obtained by tracing over states with many independent magnons (in the Ising model this complication can be avoided by working in real space). If the attraction between magnons is too weak to bind them, this is not an issue since their spectra will still consist of scattering states spanning the same energies like for non-interacting magnons. As a result, the location of various features is not affected, but the distribution of the spectral weight inside them will be since the eigenfunctions are different. Magnon pairing is unlikely for $d > 1$ unless the exchange is strongly anisotropic. However, if it happens and if the spectrum of the magnon pairs is known, one could infer its effects on the carrier spectral weight just like above.

Based on these arguments, we expect the higher-$T$ spectral weight to show the same features we uncovered at low $T$ (the distribution of the weight between them might be quite different, though). These expectations could be verified with numerical simulations (conversely, our low-$T$ results can be used to test codes). Such simulations would also solve the issue of the discrete peak that we observed for AFM $J_0$, and which we argued to be an artefact of our low-$T$ approximation.

To conclude, although quantitatively our results are only valid at extremely low $T$, we believe that this study clarifies qualitatively how the spectral weight of a spin-up carrier evolves with $T$. Our arguments can be straightforwardly extended to predict what features appear in the spectral weight of a spin-down carrier, as well.

A general feature demonstrated by our work is that finite $T$ does not result in just a simple thermal broadening of the QP peak, as it becomes a resonance inside a continuum. Spectral weight can also be transferred to quite different energies if the QP can bind additional magnons into coherent polaron. When this happens, interpretation of experimentally measured and/or of computationally generated spectra could become difficult, unless one is aware of this possibility.
Chapter 3

Local environment effects on a charge carrier injected into an Ising chain

3.1 Introduction

In this Chapter we try to answer the question of what role, if any, is played by the local environment. Is there a class of configurations that contributes more than others? How does an AFM ordered environment compare to a FM ordered one, and are there any similarities between the two? Answering such questions is crucial for the development of a better understanding (and hopefully better approximations) for the finite-$T$ spectral weight of the carrier. In order to do this one must move away from mean-field like approximations such as the CPA \cite{53} and the method of Nolting et. al. \cite{81} (see Section 2.1 for a brief discussion of their approaches).

Our approach is to study a simplified model which allows us to obtain the first (to the best of our knowledge) finite-$T$, exact numerical results in the thermodynamic limit. These teach us valuable lessons about the physics of this simpler problem; some of these are relevant for more complex models, too. The simplification consists in neglecting all spin-flip processes, i.e. assuming that all interactions between the lattice spins, and between them and the carrier, are Ising-like. While, compared to the model discussed in the previous chapter, the $T = 0$ behavior of this model is trivial, we find that it produces rich physics at finite $T$, which needs to be understood before considering the additional complications introduced by allowing spin-flip processes.

Apart from making an exact solution possible, this simple model also allows us to consider both FM and AFM backgrounds on equal footing, which is not possible in general. Interestingly, we find considerable similarities between the results for the two cases, which we are able to explain as being due to similarities between the local background configurations that control the
(at least low and medium-$T$) carrier dynamics. We then use these insights to construct an analytical approximation which accurately reproduces the features of the exact solution in the range of low to medium temperatures.

By ignoring spin-flip processes, we create a situation that is in some ways similar to that of disorder binary alloys of the type $A_xB_{1-x}$. A carrier in the conduction band of such an alloy experiences a different on-site energy if it sits on an A or a B site. In our model the on-site carrier energy is $\pm J_0$, depending on whether the local spin at that site points up or down. Thus, any configurations of the alloy can be exactly mapped into a spin configuration of the magnetic background.

These binary alloys have been extensively studied. An exact numerical solution can be obtained for the disorder-averaged GFs, as pointed out by Schmidt[93] and Dyson[25]. It was used for numerical studies of the phonon DOS[21] and the DOS of carriers in the conduction band[1,28]. Many approximations have been proposed, the most well-known and used being the CPA[100]. Diagrammatic expansions of the self-energy have been developed by several authors, see for instance Refs.[12, 75, 108], but were shown to result in non-analytic behavior and thus unphysical GFs[74]. Later this problem was resolved by a careful consideration of which diagrams to sum[66].

This knowledge cannot be directly used in our problem, despite the similarities between the models, because for binary alloys one performs a disorder average whereas we use a thermal average. The disorder average keeps the concentration $x$ fixed; all configurations consistent with it are equally likely (one generally ignores correlations in the disorder), all the others are forbidden. In contrast, a thermal average includes all possible configurations but with a Boltzmann factor that controls the extent of spin-spin correlations. These correlations are key, as no magnetic order can exist in their absence. The problems also have different symmetry properties. Our problem is truly translationally invariant, whereas for binary alloys translational invariance is only restored by averaging over all possible disorder configurations. For example, while all eigenstates are localized in a $1d$ disordered alloy model, the eigenstates of our model remain extended at any $T$. Despite these differences, there are similarities between the resulting spectral weights which help us understand our results, as discussed below.
3.2 Simplified model of a 1d magnetic semiconductor

We consider a single spin-$\frac{1}{2}$ charge carrier which interacts with a chain of Ising spins, also of magnitude $\frac{1}{2}$. Note that the exact method that we use can be generalized straightforwardly to higher dimensions. The advantage of 1d chains (apart from speed of computations) is that a host of analytic results are available for the undoped case [42, 55, 84]. We therefore limit ourselves here to Ising chains with periodic boundary conditions after $N \to \infty$ sites. The $n^{th}$ site is located at $R_n = na$, and we set $a = 1$.

The exchange between lattice spins is Ising-like:

$$\hat{H}_I = -J \sum_i \hat{\sigma}_i \hat{\sigma}_{i+1} - h \sum_i \hat{\sigma}_i,$$  

(3.1)

and is FM ($J > 0$) or AFM ($J < 0$). The second term describes the effect of an external magnetic field $h$. The spin operator at site $i$ is $S_i^z = \frac{1}{2} \hat{\sigma}_i$, with the prefactors absorbed into the coupling constants. The eigenstates $\hat{H}_I|\{\sigma\}\rangle = E_{\{\sigma\}}^{I} |\{\sigma\}\rangle$ are described by the set $\{\sigma\} \equiv \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ of eigenvalues $\sigma_i = \pm 1$ of each spin, and $E_{\{\sigma\}}^{I} = -J \sum_i \sigma_i \sigma_{i+1} - h \sum_i \sigma_i$ is the eigenenergy.

The kinetic energy of the carrier is described by a tight-binding model

$$\hat{T} = -t \sum_{i,\sigma} \left( c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.} \right) = \sum_{k,\sigma} \epsilon(k) c_{k,\sigma}^\dagger c_{k,\sigma},$$  

(3.2)

where $c_{i,\sigma}$ is the creation operator of a spin-$\sigma$ carrier at site $i$. The creation operator in momentum-space is $c_{k,\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_n e^{ikR_n} c_{n,\sigma}^\dagger$, and $\epsilon(k) = -2t \cos(k)$.

The exchange between the carrier and the lattice spins is also of Ising type:

$$\hat{H}_{\text{exc}} = J_0 \sum_{i,\sigma} \sigma_i c_{i,\sigma}^\dagger c_{i,\sigma} \hat{\sigma}_i,$$  

(3.3)

where again a factor $1/4$ is absorbed into $J_0$. Since no spin-flips are allowed in this model, from now on we assume without loss of generality that the carrier has spin-up, $\sigma = \uparrow$, and do not write it explicitly. We also set $J_0 > 0$. Results for a spin-down carrier are obtained from these by switching $J_0 \to -J_0$. 

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3.3. Method

For the undoped Ising chain, an exact solution at finite $T$ is possible and reviewed in Appendix [B]. Note that a 1$d$ chain has long-range magnetic order only at $T = 0$. We can, however, mimic a finite-$T$, ordered state by turning on the magnetic field $h$. This leads to a finite, long-range spin-spin correlation.

3.3 Method

We want to calculate the finite-$T$, retarded single-particle GF, which in the frequency-domain and canonical ensemble is defined as (c.f. Eq. (1.29)):

$$G(k, \omega) = \sum_{\{\sigma\}} e^{-\beta E^I_{\{\sigma\}}} Z \langle \{\sigma\} | c_k \hat{G}(\omega + E^I_{\{\sigma\}}) c_k^\dagger | \{\sigma\} \rangle, \quad (3.4)$$

where $\hat{G}(\omega) = (\omega - \hat{H} + i\eta)^{-1}$ is the resolvent of $\hat{H}$. The small, real quantity $\eta > 0$ ensures retardation and sets a finite carrier lifetime $1/\eta$. Note that the argument of the resolvent in Eq. (3.4) is shifted by $\hat{H}_I$. This means that the energy is measured from that of the Ising chain at the time of injection. This becomes clear when using a Lehmann representation by projecting on the one-carrier eigenstates $\hat{H}|n\rangle = E^I_n |n\rangle$:

$$G(k, \omega) = \sum_n \sum_{\{\sigma\}} \frac{e^{-\beta E^I_{\{\sigma\}}} Z}{\omega} g_{0,n}(\omega, \{\sigma\}) |\langle n| c_k^\dagger |\{\sigma\} \rangle|^2, \quad (3.5)$$

$G(k, \omega)$ has poles at energies $\omega = E^I_n - E^I_{\{\sigma\}}$ that measure the change in total energy due to the carrier’s injection. The weights correspond to the overlap between the true eigenstates $|n\rangle$ and the free-carrier states $c_k^\dagger |\{\sigma\}\rangle$.

For any configuration $\{\sigma\}$, the contribution to the thermal average can be evaluated using continued fractions.[6] First, we need to shift to the real-space representation. Making use of the translational invariance we then obtain

$$G(k, \omega) = \sum_n e^{ikRn} \sum_{\{\sigma\}} \frac{e^{-\beta E^I_{\{\sigma\}}} Z}{g_{0,n}(\omega, \{\sigma\})}, \quad (3.6)$$

where we define:

$$g_{m,n}(\omega, \{\sigma\}) = \langle \{\sigma\} | c_m \hat{G}(\omega + E^I_{\{\sigma\}}) c_n^\dagger |\{\sigma\} \rangle. \quad (3.7)$$
Physically $g_{m,n}(\omega,\{\sigma\})$ is related to the probability that the carrier is injected at site $n$ and propagates to site $m$. For any state $\{\sigma\}$ (except the fully ordered ones) the translational invariance is broken, $g_{m,n}(\omega,\{\sigma\}) \neq g_{0,n-m}(\omega,\{\sigma\})$. This symmetry is only restored by the ensemble average, which then leads to Eq. (3.6).

To obtain the GF EOM we use Dyson’s identity $\hat{G}(\omega) = \hat{G}_0(\omega) + \hat{G}(\omega) \hat{V} \hat{G}_0(\omega)$ where $\hat{H} = \hat{H}_0 + \hat{V}$ and $\hat{G}_0(\omega)$ is the resolvent for $\hat{H}_0$. Choosing $\hat{H}_0 = \hat{H}_I + \hat{H}_{exc}$, we find:

$$g_{0,n}(\omega,\{\sigma\}) = G_0(\omega - J_0 \sigma_n)(\delta_{0,n} - tg_{0,n-1}(\omega,\{\sigma\}))$$

(3.8)

where $G_0(\omega) = (\omega + i\eta)^{-1}$. Since the EOM do not change the values of $\omega$ and $\{\sigma\}$, to shorten notation we do not write them explicitly in the following.

The EOM are solved with the ansatz \cite{6} $g_{0,n} = A_n g_{0,n-1}$ for $n > 0$ and $g_{0,n} = B_{-n} g_{0,n+1}$ for $n < 0$ ($N \to \infty$ is assumed and implemented as explained below). Then

$$A_n = \frac{-tG_0(\omega - J_0 \sigma_n)}{1 + tG_0(\omega - J_0 \sigma_n) A_{n+1}},$$

(3.9)

and similarly for $B_n$. We now introduce a cutoff $M_c \gg 1$ at which we truncate these relations by setting $A_{M_c+1} = B_{M_c+1} = 0$. The justification is provided by the finite lifetime $1/\eta$ of the carrier, which prevents it from propagating arbitrarily far from its injection site. As a result $g_{0,n}$, which measures the amplitude of probability that the carrier propagates between sites $n$ and 0, must vanish for sufficiently large $|n| \geq 6$.

It is then straightforward to calculate all $A_1, \ldots, A_{M_c}$ and $B_1, \ldots, B_{M_c}$ for the configuration $\{\sigma\}$ and a given $\omega$, to find:

$$g_{0,0} = \frac{1}{\omega - J_0 \sigma_0 + t(A_1 + B_1)}$$

(3.10)

$$g_{0,n} = A_{M_c} \ldots A_1 g_{0,0}, \text{ if } n > 0$$

(3.11)

$$g_{0,-n} = B_{M_c} \ldots B_1 g_{0,0}, \text{ if } n < 0$$

(3.12)

Let us now discuss the cutoff $M_c$ in more detail. In practice $M_c$ is increased until convergence is reached. Since $g_{0,0}$ for the fully ordered configuration is known analytically, it can be used to verify the convergence.

We need to have $M_c \ll N/2$, otherwise the carrier may travel between sites $n$ and 0 on both sides of the closed loop, which is at odds with the ansatz chosen above. This condition is automatically satisfied.
3.3. Method

if $N \to \infty$. To take this limit, we note that $g_{0,n}$ only depend on the spins $\sigma_{-M_c}, \sigma_{-M_c+1}, \ldots, \sigma_{M_c}$. We make use of this by splitting the full set $\{\sigma\}$ into the set $\{M_c\}$ containing just the aforementioned spins, and the complementary set $\{M_c\}^C$. The energy of the Ising chain is also split:

$$E^I_{\{M_c\}} = E^I_{\{M_c\}} + E^I_{\{M_c\}^C, \sigma_{-M_c}, \sigma_{M_c}};$$

where

$$E^I_{\{M_c\}} = -J \sum_{n=-M_c}^{M_c-1} \sigma_n \sigma_{n+1} - h \sum_{n=-M_c}^{M_c} \sigma_n$$

and $E^I_{\{M_c\}^C, \sigma_{-M_c}, \sigma_{M_c}}$ contains the energy of all other bonds and spins, including the “boundary” bonds $\sigma_{M_c}, \sigma_{M_c+1}$ and $\sigma_{-M_c-1}, \sigma_{-M_c}$. This is why it also depends on $\sigma_{\pm M_c}$, not just on the $\{M_c\}^C$ spins.

Eq. (3.6) can then be rewritten as:

$$G(k, \omega) = \sum_n e^{ikR_n} \sum_{\{M_c\}} \frac{e^{-\beta E^I_{\{M_c\}}}}{Z g_{0,n}(\omega, \{M_c\})} \times Z_{\text{bath}}(\beta, \sigma_{-M_c}, \sigma_{M_c}),$$

(3.14)

where

$$Z_{\text{bath}}(\beta, \sigma_{-M_c}, \sigma_{M_c}) = \sum_{\{M_c\}^C} e^{-\beta E^I_{\{M_c\}^C, \sigma_{-M_c}, \sigma_{M_c}}}.$$  

(3.15)

$Z_{\text{bath}}$ is the partition function of the complementary set of spins $\{M_c\}^C$, for set values of its “boundary” spins $\sigma_{-M_c}$ and $\sigma_{M_c}$. Using transfer matrices (see Appendix B and Ref. [84]), we find that:

$$Z_{\text{bath}}(\beta, \sigma_{M_c}, \sigma_{-M_c}) = (\mathcal{T}^{N-2M_c})_{\sigma_{M_c}, \sigma_{-M_c}}.$$  

(3.16)

Thus, $\lim_{N \to \infty} Z_{\text{bath}}(\beta, \sigma_{M_c}, \sigma_{-M_c})/Z$ is known analytically. The average in Eq. (3.14) now involves only the spins $\{M_c\}$ in the chain sector that can be explored by the carrier within its finite lifetime $1/\eta$. Effectively, the rest of the infinite chain is treated as a bath that is integrated out analytically. We use the Metropolis algorithm to estimate the sum over the $\{M_c\}$ set. The results are discussed next.

3The autocorrelation time ranges from 4 Monte Carlo (MC) steps ($\beta t = 1$) to 6630 MC steps ($\beta t = 5$). During one MC steps an attempt to flip each of the $2M_c + 1$ Ising spins is made exactly once. For most spectra 204800 MC measurements were used. The time waited between measurements is identical to the autocorrelation time. More details can be found in Appendix C.
3.4 Results

We begin by briefly reviewing the $T = 0$ solution which can be calculated exactly and serves as a useful reference.

For FM coupling $J > 0$, at $T = 0$ all Ising spins point either up or down, $m = \pm 1$. Then $\hat{H}_{\text{exc}}$ simply shifts the energy of the carrier by $J_0 m$: $E_{m}^{\text{FM}}(k) = \varepsilon_k + J_0 m$. As $T \rightarrow 0$ and for $h = 0$, an infinite chain will arbitrarily choose as its ground state one of these two possible FM configurations. One can control which configuration is chosen by cooling the system in a small magnetic field, which is then switched off. However, as long as the temperature is not exactly zero and if $h = 0$, then the presence of large domains with opposite order is possible, especially in $1d$. If the carrier is injected into one of these large domains it is unable to leave it within its finite lifetime $1/\eta$. Consequently as $T \rightarrow 0$ and for $h = 0$ we expect to see contributions from both subspaces $m < 0$ and $m > 0$, and the GF becomes:

$$G^{\text{FM}}(k, \omega) = \frac{1}{2} \left( \frac{1}{\omega - E_+^{\text{FM}} + i\eta} + \frac{1}{\omega - E_-^{\text{FM}} + i\eta} \right).$$

(3.17)

For AFM coupling there are also two possible ground states: either all spins of the even sublattice point up and all spins of the odd sublattice point down, or vice versa. The doubling of the unit cell results in the appearance of two bands in the reduced Brillouin zone $(-\pi/2, \pi/2]$, with energies $E_{\pm}^{\text{AFM}}(k) = \pm \sqrt{J_0^2 + \varepsilon_k^2}$. Averaging over both contributions for the reasons discussed above, the $T \rightarrow 0$, $h = 0$ GF is found to be:

$$G^{\text{AFM}}(k, \omega) = \frac{\omega + \varepsilon_k + i\eta}{(\omega - E_+^{\text{AFM}} + i\eta)(\omega - E_-^{\text{AFM}} + i\eta)}$$

(3.18)

for any $k \in (-\pi, \pi]$.

Contour plots of the spectral function $A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega)$ for these GFs are shown in Figs 3.1 and 3.2. As expected from applying the Lehmann representation, Eq. (3.5), to these GFs, the spectrum consists of two bands for both FM and AFM coupling. For FM coupling, the bands have bandwidths of $4t$, are centered at $\pm J_0$ and have equal weights for all $k$. For AFM coupling, the bands span $[-\sqrt{J_0^2 + 4t^2}, -J_0]$ and $[J_0, \sqrt{J_0^2 + 4t^2}]$, respectively. The eigenenergies show the $\pi$ periodicity expected for the two-site unit cell. Spectral weight is transferred from the lower to the upper band as $|k|$ increases, because the GF combines contributions from both sublattices with a $k$-dependent phase factor.

Note that for $J_0/t \leq 2$ the two FM bands overlap. In order to simplify future analysis, we set $J_0/t = 2.5$ from now on. We also set $|J|/t = 0.5$, 60
3.4. Results

Figure 3.1: Contour plot of the $T = 0$ spectral functions for FM coupling, $|J|/t = 0.5$. Other parameters are $J_0/t = 2.5$, $h = 0$, $\eta/t = 0.04$.

Figure 3.2: The same as in Fig. 3.1, but for AFM coupling.
3.4. Results

although we note that if $h = 0$, $J$ only appears in conjunction with $\beta$ so a choice for $J$ simply sets the temperature scale. We use a cutoff of $M_c = 400$, which for $\eta = 0.04$ is sufficient for convergence for the fully ordered FM chain (this is the most slowly converging case).

We now discuss the results of the Monte Carlo simulations. In Figs 3.3 and 3.4 we plot $k = 0$ spectral functions for different values of $\beta$ for FM and AFM couplings, respectively. In both cases the $\beta t = 5.0$ results are in very good agreement with those at $T = 0$, defining “low-temperatures” to mean $\beta t \geq 5$. As $\beta$ decreases ($T$ increases), the sharp peaks broaden considerably and new peaks appear. For FM coupling, the lowest energy state still lies at the bottom of the low-energy $T = 0$ band. For AFM coupling, however, new states appear below the $T = 0$ spectrum. This is expected since at finite-$T$, FM domains can form in the AFM background and the carrier lowers its energy when located in such domains. Of course, these energies are bounded from below by the lowest FM eigenenergy.

At first sight the appearance of these new peaks (in fact resonances, as discussed below) may seem to signal lack of convergence of the MC simulations, or finite-size issues related to a $M_c$ cutoff that is not big enough. However, the results are converged and do not change upon further $M_c$ increase; these features are real.
3.4. Results

Figure 3.4: The same as in Fig. 3.3 but for AFM coupling.

The appearance of similar features is a well documented phenomenon for the disordered binary alloys with which our problem has similarities, as discussed above. Studies of binary alloys have revealed that these peaks (which are truly discrete states, in that context) mark the appearance of bound states where the carrier is trapped by small clusters of atoms of the same type. [21, 28]. As we show now, the resonances we observe have similar origin. For instance, in the FM case they are due to the charge carrier being trapped into spin-down domains formed into an otherwise spin-up background, or vice versa.

The eigenenergies for trapping the carrier inside several such short domains embedded in an otherwise ordered FM or AFM background can be obtained by calculating the real-space GFs $g_{0,n}(\omega, \{\sigma\})$ where $\{\sigma\}$ corresponds to the state of the Ising-chain with said domain centered at site 0. The simplest case is that of a single flipped spin inside an otherwise FM ordered background. We denote the corresponding real-space GFs by $g_{FM,1}^{0,0}(\omega)$. Assuming that all the spins, except for the flipped spin at the origin, are up and suppressing the $\omega$-dependence the EOM are (cf. Eq. (3.8))

\begin{align}
  g_{FM,1}^{0,0}(\omega + i\eta + J_0) &= 1 - t g_{FM,1}^{0,1} - t g_{FM,1}^{0,-1} \quad (3.19) \\
  g_{FM,1}^{0,n}(\omega + i\eta - J_0) &= -t g_{FM,1}^{0,n+1} - t g_{FM,1}^{0,n-1} \quad n \neq 0 \quad (3.20)
\end{align}
3.4. Results

![Figure 3.5: Spectral functions $A(k, \omega)$ for $\beta t = 1$ and $k = 0, \pi/2, \pi$, for FM coupling. Solid vertical lines mark the trapping energies of the carrier in small domains. The corresponding numbers show the length of the domain (see Table 3.1). The dashed vertical lines mark the band-edges of the $T = 0$ low-energy band. Other parameters are $|J|/t = 0.5$, $J_0/t = 2.5$, $h = 0$, $\eta/t = 0.04$.]

Since the carrier has a finite lifetime $\sim 1/\eta$ we must have $g_{0,n}^{FM,1} \to 0$ for $|n| \to \infty$. Consequently, for $n > 0$, the EOM can be solved with the ansatz $g_{0,n}^{FM,1} = z_{FM}^{1} g_{0,n-1}^{FM,1}$, where $|z_{FM}| < 1$. A similar ansatz can be made for $n < 0$. Plugging this ansatz back into the EOM above, we obtain

$$g_{0,0}^{FM,1} = \frac{1}{\omega + i\eta - J_0 - 2t z_{FM}}, \quad (3.21)$$

$$z_{FM} = \frac{\omega + i\eta - J_0}{2t} \pm \sqrt{\left[\frac{\omega + i\eta - J_0}{2t}\right]^2 - 1}. \quad (3.22)$$

From this all the other GFs can be obtained with the relation $g_{0,n}^{FM,1} = z_{FM}^{n} g_{0,n-1}^{FM,1}$. The procedure can easily be generalized to longer domains. Once the expression for the real-space GFs $g_{0,n}^{FM,l}$ of a domain of length $l$ is known the eigenenergies of the trapped carrier states for this domain can be obtained by finding the poles of these GFs. This can be done by explic-
3.4. Results

The eigenenergies for AFM domains can be obtained in a similar manner. The eigenvalues obtained in this fashion (various lines) are compared to the spectral weights obtained for $\beta t = 1$ and $k = 0, \pi/2, \pi$ in Figs 3.5 and 3.6. The integers labelling the lines show the length of the corresponding domains, also see Table 3.1. The agreement between these trapping energies and the location of the resonances in $A(k, \omega)$ is very good. The weights of these resonances vary strongly with $k$ but their energies are nearly dispersionless. For AFM coupling, the trapping energies in different domains are sometimes very similar, suggesting that here trapping occurs at the boundaries of the domain, not inside its bulk; this explains the broader features at $\omega/t \approx -3.7, -2.9$ and $-1.7$.

To better understand the momentum dependence, complete sets of spectral weights are shown in Figs. 3.7 and 3.8 for FM and AFM coupling, respectively. For simplicity we do not mark the trapping energies of the carrier in the various domains, but we have checked that the agreement is as good as in Figs 3.5 and 3.6 at all $k$.

\[ \text{Note that with the latter procedure one only finds the eigenenergies of trapped states which have a finite probability of the carrier being at the center of the domain.} \]
For FM coupling, we see the two bands that have evolved from the $T = 0$ peaks moving with increasing $k$ in a way that roughly mirrors the $T = 0$ dispersions shown in Fig. [3.1]. As $k$ increases, spectral weight is systematically shifted from the lower to the upper edge of each band. In addition we notice a small spectral weight transfer from the lower band to the upper band. This is in contrast to the FM $T = 0$ solution, where both peaks have equal spectral weight. For AFM coupling, the $\pi$-periodicity of the $T = 0$ dispersion is partially masked by the many additional resonances that appear on both sides of the $T = 0$ peaks, and the significant transfer of spectral weight from the lower to the upper band. The latter is similar to the behavior observed for the $T = 0$ solution. In both cases, the location of the various resonances does not change appreciably with $k$.

To understand the physical origin of these resonances, consider the analogy with the binary alloy model, which also shows such "peaky" structures in its total density of states (DOS), marking the bound states of the carrier inside small clusters of like-atoms [21, 28]. As is well known, in the presence of any amount of on-site disorder all eigenstates of a 1$d$ chain become localized. To find the DOS one can formally calculate the disorder averaged Green’s function (which regains invariance to translations) but this quantity has no physical meaning. This is because in any real system there is a given disorder distribution, and if all eigenstates are localized then the carrier occupies forever the same small region of space and self-averaging does not occur. In other words, if the carrier is trapped in a cluster of atoms it will stay trapped indefinitely.

Each configuration of the binary alloy can be mapped into a spin configuration of the Ising chain, by replacing atoms A/B by spins up/down.

<table>
<thead>
<tr>
<th>Color</th>
<th>Length</th>
<th>FM domain</th>
<th>AFM domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>black</td>
<td>1</td>
<td>...↑↑↓↑↑↑↑...</td>
<td>...↑↑↑↓↓↑...</td>
</tr>
<tr>
<td>blue</td>
<td>2</td>
<td>...↑↑↓↑↑↑↑...</td>
<td>...↑↑↑↑↑↑↑↑...</td>
</tr>
<tr>
<td>red</td>
<td>3</td>
<td>...↑↑↓↑↑↑↑...</td>
<td>...↑↑↑↑↑↑↑↑...</td>
</tr>
<tr>
<td>green</td>
<td>4</td>
<td>...↑↑↓↑↑↑↑...</td>
<td>...↑↑↑↑↑↑↑↑...</td>
</tr>
<tr>
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<td>...↑↑↓↑↑↑↑...</td>
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</tr>
<tr>
<td>cyan</td>
<td>2′</td>
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</tr>
<tr>
<td>yellow</td>
<td>3′</td>
<td>-</td>
<td>...↑↑↓↑↑↑↑...</td>
</tr>
</tbody>
</table>

Table 3.1: List of the shortest domains (underlined spins) that form in otherwise ordered backgrounds. The energies for trapping the carrier in these domains are shown in Figs [3.5] and [3.6].
3.4. Results

Figure 3.7: $A(k, \omega)$ for different values of $k$ and FM coupling, at $|J|/t = 0.5$, $J_0/t = 2.5$, $\beta t = 1.0$, $h = 0$, $\eta/t = 0.04$.

Small clusters of like-atoms then map into magnetic domains, and there are trapped states of the carrier inside them, as already shown. However, unlike the fixed disorder configuration, the spin configuration changes continuously through thermal fluctuations. A trapped carrier therefore has a finite lifetime linked to the persistence of that domain: eventually the local spin configuration changes and the carrier is released to move along the chain. This is why here the “peaky” structures indicate actual finite life-time resonances for extended eigenstates of well-defined momentum, not infinitely-lived localized states like in the alloy model. This is a significant qualitative difference.

We conclude this section by considering the role of the external magnetic field $h$. Its effects on the $k = 0$ spectral weight for FM coupling are shown in Fig. 3.9. We find that as $h$ increases, the initially large feature at the bottom of the lower band starts to disappear and most of its weight is moved to the bottom of the upper band. This is expected since the external field favors/disfavors the spin-up/down background responsible for this main...
3.4. Results

Figure 3.8: The same as in Fig. [3.7], but for AFM coupling.

feature (evolved from the $T = 0$ peak) of the upper/lower band. Interesting, however, most of the resonances in the lower band remain almost unchanged. The reason is that while $\beta h \ll 1$, the energy cost for a small domain is very low so their appearance is very likely. If $\beta h \gg 1$ the Ising chain is forced into the $m > 0$ ground state and only the higher $T = 0$ peak survives (not shown).

For AFM coupling the effect of $h$ is more dramatic (see Fig. [3.10]), as it forces the system into the $m > 0$ FM ground-state if $\beta h$ becomes large enough. Indeed, for large $h$ most of the weight is moved into the upper FM peak and most of the resonances disappear, except for the one at $\omega/t \approx -2.9$ that is still quite large. Its energy is very close to that of the first FM cluster listed in Table [3.1], and indeed it seems plausible that this is due to a single flipped spin which entraps the carrier. This domain is disfavored by $h$, but actually lowers the exchange energy with its neighbors.

Note that we used different field strengths for the FM and AFM cases. In the latter case much higher fields are needed to produce long range correlations since there is a competition between the exchange energy of neigh-
3.4. Results

Figure 3.9: Spectral functions $A(0, \omega)$ for different values of $h$, for FM coupling. Parameters are $|J|/t = 0.5$, $J_0/t = 2.5$, $\beta t = 1.0$, $\eta/t = 0.04$.

boring spins and the external field. A measure for this is the spin-spin correlation function $\langle \sigma_{-M_c} \sigma_{M_c} \rangle$, which for the parameters used in Figs 3.9 and 3.10 equals 0.41 (FM, if $h/t = 0.3$) and 0.64 (AFM, if $h/t = 2.0$). A value of $\langle \sigma_{-M_c} \sigma_{M_c} \rangle = 1$ means that the chain is completely ordered.

3.4.1 Analytic approximation

We now use the insights gained from the Monte Carlo results to propose an analytic approximation for the GF at low and medium temperatures. We present the derivation only for the case of FM coupling when $h = 0$; the other cases can be treated similarly.

The main idea is to only consider a limited number of spin configurations when performing the thermal average, to allow for its (quasi)analytic evaluation. Since our numerical results show the importance of small domains, the configurations we select are the two ordered configurations $|\text{FM}, \sigma \rangle$ with all spins pointing up or down, $\sigma = \uparrow, \downarrow$ together with the one-domain configurations:

$$
|n, n + l, \uparrow \rangle = 4^{-(l+1)} \hat{\sigma}_n^- \cdot \hat{\sigma}_{n+1}^- \cdot \ldots \hat{\sigma}_{n+l}^- |\text{FM}, \uparrow \rangle
$$

$$
|n, n + l, \downarrow \rangle = 4^{-(l+1)} \hat{\sigma}_n^+ \cdot \hat{\sigma}_{n+1}^+ \cdot \ldots \hat{\sigma}_{n+l}^+ |\text{FM}, \downarrow \rangle,
$$

(3.23) (3.24)
3.4. Results

where the domain starts at site $n$ and ends at $n + l$. The operator $\hat{\sigma}_i^\pm$ is the raising/lowering operator for the $i^{th}$ Ising spin. To preserve translational invariance we need to consider all possible locations of the domain within the Ising chain. All these one-domain states are weighed by the same Boltzmann factor $e^{-4\beta J}$ (we take the energy of the fully ordered FM states as reference).

As discussed, a physically meaningful result has equal contributions from the spin-down and spin-up sectors. We now discuss the spin-up contribution, which we denote by $G^\uparrow(k, \omega)$. The spin-down contribution $G^\downarrow(k, \omega)$ is then obtained by simply letting $J_0 \rightarrow -J_0$, and the GF is given by $G(k, \omega) = [G^\uparrow(k, \omega) + G^\downarrow(k, \omega)]/2$. By itself, the decomposition into an up-part and a down-part is not an approximation. The approximation stems from the fact that we are only considering the one-domain configurations when calculating $G^\uparrow(k, \omega), G^\downarrow(k, \omega)$.

By only considering domains up to a maximal length $L$ (for reasons discussed below), we thus approximate:

$$G^\uparrow(k, \omega) = \frac{1}{Z} \left[ G^{\uparrow FM}(k, \omega) + e^{-4\beta J} \sum_{l=0}^{L-1} G^{(l+1)}(k, \omega) + \ldots \right] \quad (3.25)$$

where $Z = 1 + e^{-4\beta J} L \cdot N + \ldots$. The thermodynamic limit $N \rightarrow \infty$ will
be taken at a later stage. The first contribution, from the ordered state, is
\[
G_{\uparrow}^{\text{FM}}(k, \omega) = \langle \text{FM}, \uparrow | c_{k} \hat{G}(\omega + \hat{H}) c_{k}^\dagger | \text{FM}, \uparrow \rangle
\]
\[
= \frac{1}{\omega - \varepsilon(k) - J_0 + i\eta}.
\]  
(3.26)
To find the contributions
\[
G_{\uparrow}^{(l+1)}(k, \omega) = \sum_{n} \langle n, n + l, \uparrow | c_{k} \hat{G}(\omega + \hat{H}) c_{k}^\dagger | n, n + l, \uparrow \rangle
\]  
(3.27)
from the states with a domain of length \(l\), we have to work harder. Using Dyson’s identity once we obtain:
\[
G_{\uparrow}^{(l+1)}(k, \omega) = G_{\uparrow}^{\text{FM}}(k, \omega) \left[ N - 2J_0 \sum_{m=0}^{l} f_{\uparrow,k}^{(l+1)}(m, \omega) \right],
\]  
(3.28)
where we defined the auxiliary GFs:
\[
f_{\uparrow,k}^{(l+1)}(m, \omega) = \sum_{n} \frac{e^{ikR_{n+m}}}{\sqrt{N}} \langle n, n + l, \uparrow | c_{k} \hat{G}(\omega + \hat{H}) c_{n+m}^\dagger | n, n + l, \uparrow \rangle.
\]  
(3.29)
Using Dyson’s equation again we find:
\[
f_{\uparrow,k}^{(l+1)}(m, \omega) = -2J_0 \sum_{m'=0}^{l} g_{\uparrow}^{\text{FM}}(m' - m, \omega) e^{ik(R_{n+m'} - R_m)} f_{\uparrow,k}^{(l+1)}(m', \omega)
\]
\[
+ G_{\uparrow}^{\text{FM}}(k, \omega),
\]  
(3.30)
where \(g_{\uparrow}^{\text{FM}}(m' - m, \omega) = \frac{1}{N} \sum_{q} e^{iq(R_{m'} - R_m)} G_{\uparrow}^{\text{FM}}(q, \omega)\) are easy to find analytically. This is a linear system of \(l + 1\) equations that is solved to find all \(f_{\uparrow,k}^{(l+1)}(m, \omega)\), which are then used in Eq. (3.28). Note that all \(f_{\uparrow,k}^{(l+1)}(m, \omega)\) are proportional to \(G_{\uparrow}^{\text{FM}}(k, \omega)\), since the latter quantity provides the inhomogeneous terms in this linear system.

When Eq. (3.28) is inserted in Eq. (3.25), if we group all terms proportional to \(G_{\uparrow}^{\text{FM}}(k, \omega)\) we see that its factor \(1/Z\) is canceled. Higher order terms corresponding to states with two or more domains (not included in this calculation) should similarly cancel the factor \(1/Z\) for the remaining terms in Eq. (3.25), or at least make the thermodynamic limit of the ratio meaningful. To \(\mathcal{O}(e^{-4\beta J})\) order and for \(N \to \infty\), we therefore find:
\[
G_{\uparrow}(k, \omega) \approx \left[ 1 - 2J_0 e^{-4\beta J} \sum_{l=0}^{L-1} \sum_{m=0}^{l} f_{\uparrow,k}^{(l+1)}(m, \omega) \right] G_{\uparrow}^{\text{FM}}(k, \omega).
\]  
(3.31)
3.4 Results

Eq. (3.31) obeys the sum rule \( \int_{-\infty}^{+\infty} d\omega A(k,\omega) = 1 \) if the second term has no poles in the upper half of the complex plane. This is because the second term is proportional to \( |G_{FM}^\uparrow(k,\omega)|^2 \) and therefore falls off like \( 1/\omega^2 \) as \( |\omega| \to \infty \).

One may use Eq. (3.31) to extract a low-\( T \) approximation for the self energy:

\[
\Sigma^\uparrow(k,\omega) \approx -2J_0 e^{-4\beta J} \sum_{l=0}^{L-1} \sum_{m=0}^{l} \frac{f_{\uparrow,k}^{(l+1)}(m,\omega)}{G_{FM}^\uparrow(k,\omega)},
\]

and define \( G^\uparrow(k,\omega) \approx \left( |G_{FM}^\uparrow(k,\omega)|^{-1} - \Sigma^\uparrow(k,\omega) \right)^{-1} \) instead of \( G^\uparrow(k,\omega) \approx G_{FM}^\uparrow(k,\omega) \left[ 1 + \Sigma^\uparrow(k,\omega)G_{FM}^\uparrow(k,\omega) \right] \) of Eq. (3.31). At low enough temperatures both give the same results, but at higher temperatures the former approximation leads to spurious poles in the spectral weight, as discussed in Chapter 3, so we use Eq. (3.31) in the following.

Results for FM and AFM coupling are shown in Figs. 3.11 and 3.12, respectively, for various lengths \( L \) of the largest domain included, at two temperatures. For comparison, the Monte Carlo results are also shown (shaded area) and the analytic approximation of Eq. (3.31) for domains with a maximal length of \( L \), for FM coupling \( |J|/t = 0.5 \), at \( J_0/t = 2.5 \), \( h = 0, \eta/t = 0.04 \), \( k = 0 \) and \( \beta t = 3 \) (top) and \( \beta t = 2 \) (bottom).
3.4. Results

regions). The quality of the approximation varies substantially with $L$. The top panel of Fig. 3.11 shows that for $\beta t = 3$ and $L = 5$, the weight of the resonances is underestimated and not all of them are reproduced by the approximation. For $L = 10$ the agreement between the approximation and the exact results is very good, but it worsens again for $L = 30$. Not only does the latter overestimate the weight of the resonances, but it also predicts negative spectral weight just below the bands. While this negative weight is needed to satisfy the sum rule, its presence is unphysical and signals a failure of the approximation. The same trends are observed for $\beta t = 2$ in the bottom panel of Fig. 3.11. Here the best agreement is obtained at $L = 3$, although resonances associated with longer domains are missing. They appear for $L = 5$, however so does the unphysical behavior. For even lower values of $\beta$ the approximation fails completely to capture the correct weight of the resonances, although, as shown in Figs 3.5 and 3.6, their locations are due to carrier trapping in domains.

The AFM approximation yields very similar results. The top panel of Fig. 3.12 shows that again for $\beta t = 3$ excellent agreement with the exact solution is reached for $L = 10$, while for larger values of $L$ the weight of the resonances is overestimated and unphysical behavior occurs if $L = 30$. For $\beta t = 2$ the agreement with the exact solution is best for $L = 4$ and unphysical behavior already occurs at $L = 6$. Again the approximation fails badly to capture the proper weight of various features, for smaller values of $\beta$ (higher $T$).

Naively, one may expect the approximation to improve when $L$ is increased since this means that a larger fraction of the possible configurations is considered. However, there are two factors which determine how a domain contributes to the thermal average. One is the additional energy cost of a domain, which is accounted for by the Boltzmann factor and in 1$d$ does not depend on the domain’s length. The other is the increase in entropy with increasing number of domains. As the temperature increases, minimization of the free energy $F = U - TS$ is increasingly driven by entropy maximization, resulting in more domains and thus shorter correlations. The order of magnitude for the maximal domain size should be given by the spin-spin correlation length $\xi$, which for $h = 0$ is given by $\xi^{-1} = -\log(\tanh(\beta|J|))$ (see Appendix B for a derivation). Indeed, we obtain $\xi \approx 4$ and $\xi \approx 10$ for $\beta t = 2$ and $\beta t = 3$, respectively (cf. Fig. 3.13). This compares well with the values of $L$ where the approximation performs well, see Figs. 3.11 and 3.12.

Another way to see why the approximation with $L \to \infty$ is bound to become wrong is to realize that all domains whose length is longer than the
3.4. Results

distance explored by the carrier within its lifetime are actually indistinguishable from the “other” ordered FM configuration, from the point of view of the carrier. In other words, all these configurations essentially contribute a $G_{\uparrow}^{\text{FM}}(k,\omega)$, and their inclusion gives the wrong weighting to the $|\text{FM},\downarrow\rangle$ contribution. Similarly, configurations with two long domains placed relatively close together will have states where the carrier is trapped in the short region between the domains, indistinguishable from having a short domain formed in the “other” ordered FM configuration. Adding many such contributions will affect the weights of these one-domain contributions, etc. These arguments suggest that a better approximation is:

$$G_{\uparrow}(k,\omega) = \left[ 1 - \sum_{l=0}^{N/2} w_l(\beta) \sum_{m=0}^l f_{\uparrow,k}^{(l+1)}(m,\omega) \right] G_{\uparrow}^{\text{FM}}(k,\omega)$$

and $G_{\downarrow}(k,\omega) = G_{\uparrow}(k,\omega)|_{J_0 \to -J_0}$, where $w_l(\beta)$ are adjusted to capture accurately the weight of resonances due to trapping into short domains. For low and medium temperatures we showed that $w_l(\beta) = 2J_0e^{-4\beta J}$ if $l \leq \xi$, and zero otherwise, gives very decent predictions. Clearly this cannot work at high temperatures of order $\beta t = 1$ where $\xi \to 0$. So far we have been unable to think of a reasonable form of $w_l(\beta)$ in this regime, but the comparisons displayed in Figs 3.5 and 3.6 suggest that it should exist.

Figure 3.12: The same as in Fig. 3.11 but for AFM coupling.
3.5 Conclusions

To summarize, we obtained numerically exact spectral functions for a simplified model of a carrier injected into a 1d Ising chain at finite $T$. The results highlight the importance of small domains that can trap the carrier, which were shown to be responsible for the resonances that appear as $T$ increases. A simple analytic approximation based on these ideas was found to perform well at low and medium temperatures. With further insights, it may be possible to generalize it to high temperatures, as well. Interestingly, chains with both FM and AFM coupling can be understood in similar terms, although generically one expects quite different phenomenology for a carrier injected into a FM vs AFM background.

As highlighted throughout, there are parallels between this problem and that of a carrier moving in a random binary alloy, where the importance of small clusters of like-atoms, equivalent to the small domains of our model, is well documented [1, 21, 28]. There are, however, also major differences: finite $J$ maps into correlations between the atoms of the alloy (usually these are ignored). The thermal average is also very different, both qualitatively and quantitatively, from a disorder average. It is therefore not a priori clear how much of the considerable amount of work devoted to finding analytic approximations for binary alloys can be used for the magnetic problem.

In terms of generalizations, one direction is to see how far these insights carry over to higher dimensions, where long-range magnetic order survives at
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finite $T$. For binary alloys it is known that the fine-structure of the spectral function is most dominant in $1d$ [28]. For our model, the energy cost scales with the domain size in $2d$ and $3d$, unlike in $1d$ and unlike for a binary alloy. This may well lead to a behavior that is different from that of the binary alloys and could cause the fine-structure associated with very small domains to remain present in higher dimensions, at least at low temperatures.

Another interesting direction is to allow for Heisenberg coupling between the carrier and the local moments (still with Ising coupling between the latter). In this case spin-flip processes become possible. The carrier can move small domains around (in fact, the spin-polaron[7, 95] can be thought of as a mobile bound state between the carrier and a one-site domain), or split longer domains into several smaller ones, etc. Understanding the consequences of such processes and their effect on the finite-$T$ spectral function would be very useful. Even more complicated is the case with Heisenberg coupling between the lattice spins. Clearly there is a lot of work, both numerical and analytical, to be done before these problems are solved.

Our results underline the importance of the local environment for the behavior of a charge carrier in a magnetic background, at least for this model and in low dimension. Incorporating these effects is difficult since mean-field approximations cannot capture them. The only real alternative is to obtain an understanding of which states of the environment contribute most to the temperature average, and to propose approximations based on taking the average over this limited set of states. Our work presents the first step in this process.
Chapter 4

On the equivalence of models with similar low-energy quasiparticles

4.1 Introduction

All physics knowledge is built on the study of models. Formulating a model for the system of interest is thus a key step in any project. Of course, “all models are wrong, but some of them are useful”[11]. This is because ideally, a model incorporates all relevant physics of the studied system so that its solution is useful to gain intuition and knowledge regarding some properties of interest. At the same time, models discard details assumed to be irrelevant for these properties. Even though this makes them “wrong”, it is a necessary and even desirable step if the solution is to not be impossibly complicated.

How to decide where lies the separation line between relevant and irrelevant aspects for a given system and set of properties of interest, is still an art. A general guiding principle, based on perturbation theory, is that high-energy states can be discarded (integrated out) if one is interested in low-energy properties. Consequently, it is assumed that models with identical low-energy spectra provide equivalent descriptions of a system, and therefore the simplest of these models can be safely used.

A prominent example is the modeling of cuprates. It is widely believed that the Emery model [29] can be replaced by the simpler $t$-$J$ model to study their low-energy physics [18, 59]. The justification was provided by Zhang and Rice [114] who argued that the low-energy states of the Emery model are singlets formed between the spin of a doping hole hosted on the four oxygens surrounding a copper and the spin of that copper, and that the resulting QP is described accurately by the $t$-$J$ model [4]. Whether this is true is still being debated [26, 27, 56].

In this Chapter we show that by itself, the condition that two models
have the same low-energy spectrum is not sufficient to guarantee that they describe similar low-energy properties, despite widespread belief to the contrary. Indeed, we identify three models that have identical $T=0$ QPs yet have very different low-energy behavior at any temperature $T \neq 0$. The qualitative differences are due to rare events controlled by thermal fluctuations, which lead to a pseudogap-type of phenomenology.

While our argument takes the form of a “proof by counterexample”, we also provide arguments that our findings are not merely an “accident” caused by our specific choice of models, but are more general in nature. Specifically, we comment on its validity in arbitrary dimensions and also for other types of magnetic coupling which differ from the examples that are our main focus.

4.2 Models

The models of interest are sketched in Fig. 4.1. Note that Model II was studied in detail in Chapter 3. All three models describe the interaction of the carrier with a background of local moments, and as such bear some similarity to those used in the Zhang-Rice mapping mentioned above. Model I is the parent two-band model, from which Models II and III are derived as increasingly simpler effective models. In Model I, one band hosts the spin $-\frac{1}{2}$ magnetic moments and a second band, located on a different sublattice, hosts the carrier. Model II is also a two-band model, but the carrier and local moments are located on the same sites. One can think of the states occupied by the carrier in this model as being local linear combinations of the carrier states in Model I, each centered at a spin site. In Model III, the carrier is locked into a singlet with its lattice spin, forming a “spinless carrier” analogous to the Zhang-Rice singlet.

Figure 4.1: Sketch of the three models. Large, red arrows represent the local magnetic moments, empty (filled) blue circles represent empty (filled) carrier sites. For Models I and II the carrier spin is represented by a blue arrow, for Model III the carrier is a spinless “hole” in the Ising chain.
4.2. Models

There are also significant differences between our models and the Zhang-Rice mapping: (i) we restrict ourselves to one dimension as this suffices to prove our claim. However, some comments on the extension of our results to higher dimensions can be found below; (ii) We concentrate on the case of a FM background because for models with an AFM background the $T = 0$ spectra are not identical. However, we also present some AFM results later on, to demonstrate that some of the features we discuss here are generic, not FM-specific; and (iii) all spin exchanges are Ising-like, i.e. no spin flipping is allowed. The latter constraint allows us to find numerically the exact solutions using a Metropolis algorithm, to uncover a surprising finite-$T$ behavior for Model III.

In all three cases, the interactions between the local moments are described by the Ising Hamiltonian:

$$
\hat{H}_I = -J \sum_i \hat{\sigma}_{i+\delta} \hat{\sigma}_{i+1+\delta} - h \sum_i \hat{\sigma}_{i+\delta},
$$

where $\delta = 1/2$ for Model I and $\delta = 0$ for Models II and III, and $\hat{\sigma}_{i+\delta}$ is the Ising operator for the local magnetic moment located at $R_{i+\delta} = i + \delta$ (we set $a = 1$). Its eigenvalues are $\sigma_i = \pm 1$. For $J > 0$ the ground state of $\hat{H}_I$ is FM, and it is AFM for $J < 0$. In the case of FM coupling, the external magnetic field $h$ can be used to favor energetically one of the two possible FM ground states of the $h = 0$ case.

For Models I and II, the kinetic energy of the carrier is described by a nearest-neighbor hopping Hamiltonian:

$$
\hat{T} = -t \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i+1,\sigma} + \text{h.c.} = \sum_{k,\sigma} \epsilon(k) c^\dagger_{k,\sigma} c_{k,\sigma}
$$

where $c^\dagger_{i,\sigma}$ is the creation operator for a spin-$\sigma$ carrier at site $R_i$ and $c_{k,\sigma} = 1/\sqrt{N} \sum_i e^{ikR_i} c^\dagger_{i,\sigma}$ are states with momentum $k \in (-\pi, \pi)$ and eigenenergy $\epsilon(k) = -2t \cos k$. The interaction between the carrier and the local moments is an AFM Ising exchange:

$$
\hat{H}_{\text{exc}}^{(I,II)} = \frac{J_0}{2} \sum_{i,\sigma} \sigma c^\dagger_{i,\sigma} c_{i,\sigma} (\hat{\sigma}_{i-\delta} + \hat{\sigma}_{i+\delta}).
$$

Note that flipping the sign of the carrier spin corresponds to letting $J_0 \rightarrow -J_0$, so we can assume without loss of generality that the carrier has spin-up and suppress the spin index. The total Hamiltonian for Models I and II is thus given by $\hat{H}^{(I,II)} = \hat{H}_I + \hat{T} + \hat{H}_{\text{exc}}^{(I,II)}$. 

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4.3 Method

Model III is the FM ($J > 0$) or AFM ($J < 0$) Ising version of the one-band $t$-$J$ model discussed extensively in the cuprate literature [18, 59]. The case of interest now has $N + 1$ electrons in the $N$ site system ($N \to \infty$), and double occupancy is forbidden apart from the site where the additional carrier is located and which can be viewed as hosting a “spinless carrier” whose motion shuffles the otherwise frozen spins. The Hamiltonian is $\hat{H}^{\text{(III)}} = \hat{P}\hat{T}\hat{P} + \hat{H}_I$, where the operator $\hat{P}$ projects out additional double occupancy. It is important to note that in contrast to Models I and II, here the spin-operators $\hat{\sigma}_i$ are related to the electron creation/annihilation operators via $\hat{\sigma}_i = \sum_\sigma \sigma c^\dagger_{i,\sigma} c_{i,\sigma}$.  

4.3 Method

We calculate the finite-$T$ spectral weight $A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega)$, where $G(k, \omega)$ is the one-carrier propagator. If the carrier is injected in the magnetic background equilibrated at temperature $T$, the GF is given by cf. Eq. (1.29)

$$G(k, \omega) = \sum_\sigma \frac{e^{-\beta E_I^\sigma}}{Z} \langle \{\sigma\}|c_{k,\uparrow} \hat{G}(\omega + E_I^\sigma) c^\dagger_{n,\uparrow}|\{\sigma\}\rangle$$

The sum is over all configurations $\{\sigma\} = (\sigma_1, \ldots, \sigma_N)$ of the Ising chain, with corresponding energies $\hat{H}_I|\{\sigma\}\rangle = E_I^\{\sigma\}|\{\sigma\}\rangle$, and $Z = \sum_\{\sigma\} \exp(-\beta E_I^\{\sigma\})$. The resolvent is $\hat{G}(\omega) = [\omega - \hat{H} + i\eta]^{-1}$, where $\eta \to 0^+$ ensures retardation. The shift by $E_I^\{\sigma\}$ in the argument of the resolvent shows that the poles of the propagator mark the change in the system’s energy, i.e. the difference between the eigenenergies of the system with the carrier present, and those of the undoped states into which it was injected. This reflects the well-known fact that electron addition states have poles at energies $E_{N+1,\alpha} - E_{N,\beta}$ [63].

After Fourier transforming to real space and using the invariance to translations of the thermally averaged system, we arrive at:

$$G(k, \omega) = \sum_\{\sigma\} \sum_n e^{ikR_n} \frac{e^{-\beta E_I^\{\sigma\}}}{Z} g_{0,n}(\omega, \{\sigma\}), \quad (4.4)$$

where $g_{0,n}(\omega, \{\sigma\}) = \langle \{\sigma\}|c_{0,\uparrow} \hat{G}(\omega + E_I^\{\sigma\}) c^\dagger_{n,\uparrow}|\{\sigma\}\rangle$ is the Fourier transform of the amplitude of probability that a state with configuration $\{\sigma\}$ and the carrier injected at site $n$ evolves into a state with the carrier injected at site 0. These real-space propagators are straightforward to calculate,
4.3. Method

as they correspond to a single particle (consistent with our assumption of a canonical ensemble with exactly one extra charge carrier in the system) moving in a frozen spin background. We emphasize that this is true only because of the Ising nature of the exchange between the background spins. Heisenberg coupling, on the other hand, would lead to spin fluctuations that would significantly complicate matters. Below we present the calculation of these real-space propagators for Model III. For Model II, the solution is described in detail in Chapter 3, and the same approach, with only minor modifications, applies to Model I.

It is convenient to introduce the following notation. When an extra electron is injected at site \( n \) of Model III it effectively removes the spin at this site. The spin \( \sigma_n \) will therefore be missing from the set \( \{\sigma\} \) which describes the state of the spin-chain before injection. Consequently we label the new state, after injection, as \( \{\sigma\} \setminus \sigma_n = |\ldots \sigma_{n-1} \circ \sigma_{n+1} \ldots \} \), where \( \circ \) denotes the effective “hole” created by the injection of the extra electron. The “hole” can propagate along the chain and in doing so reshuffles the spins. To capture the propagation of the “hole” we introduce a new index \( j \) corresponding to the number of sites that the “hole” has hopped to the left (\( j < 0 \)) or right (\( j > 0 \)). A general state is therefore given by \( \{\sigma\} \setminus \sigma_{n,j} = |\ldots \sigma_{n-1} \sigma_{n+1} \ldots \sigma_{n+j} \circ \sigma_{n+j+1} \ldots \} \). Note that this way of labelling states is not unique. For instance, if \( \sigma_0 = \sigma_1 = \ldots = \sigma_n \), then \( \{\sigma\} \setminus \sigma_{0,0} = |\{\sigma\} \setminus \sigma_{n,-n} \).

With this notation, the real-space propagators are \( g_{0,n}(\omega, \{\sigma\}) = \langle \{\sigma\} \setminus \sigma_{0,0} \rangle G(\omega + E_{\{\sigma\}}^f) |\{\sigma\} \setminus \sigma_n, 0 \rangle \). Their EOM are obtained by splitting the Hamiltonian in two parts, \( \hat{H} = \hat{H}_0 + \hat{V} \), and repeatedly using Dyson’s identity \( \hat{G}(\omega) = \hat{G}_0(\omega) + \hat{G}(\omega)\hat{V}\hat{G}_0(\omega) \). Choosing \( \hat{H}_0 = \hat{H}_f \) and suppressing the \( \omega \) and \( \{\sigma\} \)-dependence we obtain

\[
g_{0,0} = G_0(\omega + \Delta_0)[1 - tf_{0,1} - tf_{0,-1}], \tag{4.5}
\]
\[
f_{0,n} = -tG_0(\omega + \Delta_n)[f_{0,n+1} + f_{0,n-1}], \tag{4.6}
\]

where \( G_0(\omega) = (\omega + i\eta)^{-1} \), \( \Delta_n = E_{\{\sigma\}}^f - E_{\{\sigma\}\sigma_{0,n}}^f \) and \( f_{0,n} = \langle \{\sigma\} \setminus \sigma_{0,0} \rangle G(\omega + E_{\{\sigma\}}^f) |\{\sigma\} \setminus \sigma_{n,n} \rangle \). Note that \( f_{0,0} = g_{0,0} \). The exact form of \( \Delta_n \) depends on the sign of \( n \):

\[
\Delta_0 = -J\sigma_0(\sigma_{-1} + \sigma_1) \tag{4.7}
\]
\[
\Delta_n = \Delta_0 + J\sigma_{-1}\sigma_1 - J\sigma_n\sigma_{n+1}, \text{ for } n > 0 \tag{4.8}
\]
\[
\Delta_n = \Delta_0 + J\sigma_{-1}\sigma_1 - J\sigma_n\sigma_{n-1}, \text{ for } n < 0. \tag{4.9}
\]

The EOM (4.6) can be solved with the ansatz \( f_{0,n} = A_n f_{0,n-1} \), for \( n > 0 \) and \( f_{0,n} = B_n f_{0,n+1} \) for \( n < 0 \). Since the “hole” has a finite lifetime \( \propto 1/\eta \)
and \( f_{0,n} \) measures the probability that the “hole” injected at site 0 moves to site \( n \), one expects \( f_{0,n} \to 0 \) for \( n \to \infty \). We therefore introduce a sufficiently large cutoff \( M_c \) and require \( A_{M_c} = 0 = B_{-M_c} \). It is then straightforward to obtain

\[
A_n = \frac{-t}{\omega + \Delta_n + i\eta + tA_{n+1}}, \quad \text{(4.10)}
\]

\[
B_n = \frac{-t}{\omega + \Delta_n + i\eta + tB_{n-1}}, \quad \text{(4.11)}
\]

\[
g_{0,0} = \frac{1}{\omega + \Delta_0 + tB_{-1} + tA_1}, \quad \text{(4.12)}
\]

\[
f_{0,n} = A_n \ldots A_1 g_{0,0} \quad \text{for } n > 0, \quad \text{(4.13)}
\]

\[
f_{0,n} = B_n \ldots B_1 g_{0,0} \quad \text{for } n < 0. \quad \text{(4.14)}
\]

To calculate the \( g_{0,n} \) we make use of the fact that hopping reshuffles the spins. Therefore \( g_{0,n} \neq 0 \), only if \( \sigma_0 = \sigma_1 = \cdots = \sigma_n \). In that case, as mentioned above, the states \( |\{\sigma\} \setminus \sigma_0, n\rangle \) and \( |\{\sigma\} \setminus \sigma_n, 0\rangle \) are equal which means that \( g_{0,n} = f_{0,n} \).

The thermal average in Eq. (4.4) is then calculated for the infinite chain with a Metropolis algorithm which generates configurations \( \{\sigma\} \) of the undoped chain. To summarize, our method of solution consists of the following steps: (i) generate a configuration \( \{\sigma\} \) of the Ising chain using a Metropolis algorithm; (ii) Calculate all the \( g_{0,n}(\omega, \{\sigma\}) \) propagators for that specific configuration, and perform the sum over \( n \) in Eq. (4.4); (iii) repeat steps (i) and (ii) until convergence is reached. The details of this procedure were discussed in the previous chapter for Model II and additional information can be found in Section 1.6 and Appendix C; the generalization to Models I and III is straightforward. For Model III it is convenient to inject the carrier with an unpolarized total spin, to ensure that a “hole” is always created. Since for each configuration \( \{\sigma\} \) there is a configuration \( \{\bar{\sigma}\} \) with all the spins flipped, injecting an unpolarized carrier does not change the results, but merely speeds up the numerics.

### 4.4 Results

#### 4.4.1 FM results

At \( T = 0 \), the undoped Ising chain is in its FM ground state. The QPs of Models I and II have energy \( \mp J_0 + \epsilon(k) \) if the carrier is injected with its spin antiparallel/parallel to the background. Only the former case can be
meaningfully compared with Model III, which has a QP of energy $2J + \epsilon(k)$ ($2J$ is the cost of removing two FM Ising bonds). Thus, apart from trivial shifts, the three models have identical QPs, namely carriers free to move in the otherwise FM background.

Finite-\(T\) spectral weights $A(k = 0, \omega)$ for the different models are shown in Fig. 4.2. We emphasize that only the electron-addition part is discussed here. We do not consider the electron-removal states, which lie at energies well below those of the electron-addition states and must be identical for all three models because in all cases, one of the electrons giving rise to the magnetic moments is removed.

For Models I and II, shown in panels (a) and (b), at the lowest temperature one can see two peaks marking the contributions from injection of the carrier into the two ground states of the Ising chain (all spins up and all spins down, respectively). Indeed, these peaks are located at $\pm J_0 - 2t$, the lower one of which is marked by the vertical line. Note that we chose a large $J_0$ value to keep different features well separated and thus easier to identify. The insets show the spectral weights for $h = -0.1t$, which at low \(T\) suppresses the contribution from the up-spin FM state so that only the lower peak remains visible.

With increasing \(T\), both peaks broaden considerably on their higher-energy side, and many resonances become visible. As demonstrated in the previous chapter for Model II, these resonances are due to temporal trapping of the carrier inside small magnetic domains that are thermally generated at higher \(T\). The presence of these domains also explains the decreasing difference between the $h = 0$ and $h = -0.1t$ curves at higher \(T\). For $\beta J = 0.5$ both curves are shown in the main panels (the finite $h$ curve is shaded in). Indeed, the resonances appear in the same places and with equal weight in both curves, the only difference being a small spectral weight transfer from $J_0 - 2t$ to $-J_0 - 2t$, i.e. from the FM ground-state disfavored by $h < 0$ to the one favored by it. The weight for the former is no longer zero like for $T \to 0$, showing that at higher \(T\) the carrier is increasingly more likely to explore longer domains of spin-up local moments.

The main difference between Models I and II is that the latter also has a third finite-\(T\) continuum, centered around $\omega = 0$. It corresponds to injecting the carrier in small AFM domains, where its exchange energy vanishes because it sits between a spin-up and a spin-down local moment. Such energy differences are not possible in Model II, where the carrier interacts with a single moment so its exchange energy is $\pm J_0$.

From the analytical approximation of Section 3.4.1 we know that in the low-\(T\) limit the spectrum of Model II is well described by only considering...
4.4. Results

Figure 4.2: Spectral weight at $k = 0$ for a FM background and three different temperatures for (a) Model I with $J_0/t = 5, J/t = 0.5$; (b) Model II with $J_0/t = 5, J/t = 0.5$; (c) Model III with $J/t = 2.5$. Insets in panels (a) and (b) show the spectral weight in the presence of a magnetic field, while in (c) it shows the two continua appearing at low energies, for $\beta J = 0.5$. In all cases, the broadening is $\eta/t = 0.04$. The vertical lines show the energy of the $T = 0$ QP peak.
Figure 4.3: $A(k, \omega)$ for the three models with FM background at $\beta J = 0.5$. Other parameters are as in Fig. 4.2. The dispersionless low energy, low weight part of the spectrum of Model III is not shown. Red, vertical lines indicate the location of the $T = 0$ QP peaks.
4.4. Results

contributions from small domains of flipped spins with length $L$. Since only the FM bonds at the ends of the domain are broken the energy cost of such a domain is $4J$, independent of the domain length. Exactly the same domains exist in Model I, where they also cost an energy of $4J$ and are expected to give the largest contribution to the low-$T$ spectrum. To compare the effect of injecting the carrier in such a domain in Model I and Model II it is useful to rewrite $H_{\text{exc}}^{(I)}$ as follows

$$H_{\text{exc}}^{(I)} = J_0 \sum_i c_i^\dagger c_i \hat{\sigma}_i^{(I)},$$

(4.15)

where we defined $\hat{\sigma}_i^{(I)} = (\hat{\sigma}_{i-\delta} + \hat{\sigma}_{i+\delta})/2$. Note that $\hat{\sigma}_{i+\delta}$ belongs to both $\hat{\sigma}_i^{(I)}$ and $\hat{\sigma}_{i+1}^{(I)}$ which makes it difficult to reverse this transformation. Furthermore we suppressed the spin index of the carrier since as mentioned above we assume that is has spin-up.

Formally $H_{\text{exc}}^{(I)}$ in the rewritten form looks exactly the same as $H_{\text{exc}}^{(II)}$, the difference between them is that the new spin operator $\hat{\sigma}_i^{(I)}$ can take the values 1,0 and -1. With this transformation it becomes clear that when a carrier is injected into one of the domains mentioned above there is a small difference between the potential it experiences in Model I and in Model II. In Model II the carrier sees a potential step from $+J_0$ to $-J_0$ (or vice versa) at the edge of the domain. In Model I on the other hand the domain edges are stretched out over two sites and the carrier sees a potential step from $+J_0$ to 0 to $-J_0$ (or vice versa). The special case of a single site domain which corresponds to a potential dip from $+J_0$ to $-J_0$ and back to $+J_0$ in Model II becomes a potential dip from $+J_0$ to 0 and back to $+J_0$ in Model I. This explains the spectral weight at $\omega = 0$ in Model I. However, the sharpness of the domain edges in Model II compared to Model I does not change the nature of the low energy states. Consequently, if one is interested in the low-energy behavior, Models I and II are equivalent because their low-energy continua have similar origins and evolve similarly with $T$. This is true in the whole Brillouin zone (BZ), as can be seen from comparing panels (a) and (b) of Fig. 4.3.

The finite-$T$ evolution of the spectral weight of Model III is very different. Consider first the $k = 0$ case, shown in Fig. 4.2(c). The $T = 0$ peak at $2J-2t$ (marked by the vertical line) evolves with $T$ very similarly to the low-energy peaks of the other two models, broadening on its high-energy side and again displaying resonances due to temporal trapping inside small domains. The $k$ evolution of this feature, shown in Fig. 4.3(c), is also very similar to the low-energy continua of the other two models.
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Figure 4.4: When doping “removes” a thermally excited spin-down, the energy variation upon doping is \( E_b - E_a = -2dJ + \epsilon(k) \) and lies (at least partially) below the \( T = 0 \) QP ground-state energy of \( 2dJ - 2dt \).

However, for Model III this continuum is not the low-energy feature. Instead, in 1d there are three lower-energy continua centered at 0, \(-2J\) and \(-4J\), all of which are due to injection of the carrier into specific, thermally excited configurations of the background. For example, consider the \(-2dJ\) continuum which also appears in dimensions \( d > 1 \). As sketched in Fig. 4.4 it corresponds to the carrier being paired with a thermally excited spin. This lowers the exchange energy by \( 2dJ \), as \( 2d \) AFM bonds are broken. In contrast, \( T = 0 \) doping always leads to loss of exchange energy, because only FM bonds can be broken. This is why in Model III it can cost less energy to dope from a thermally excited state rather than the ground-state, and therefore why its finite-\( T \), low-energy properties are not controlled by the \( T = 0 \) QP.

The weight of these low-energy continua is very small, see inset of Fig. 4.2(c), because they are controlled by thermal activation. For example, in the limit \( T \to 0 \) the spectral weight of the continuum centered at \(-2dJ\) can be calculated to first order, as was shown in Chapters 2 and 3, by expanding Eq. (4.4) in powers of \( e^{-\beta 4dJ} \). The lowest order terms correspond to the two FM ground states which have all spins aligned, \( |\{\uparrow\}\rangle \) and \( |\{\downarrow\}\rangle \), respectively. The first order terms are given by states with a single flipped spin and are denoted by \( |\{\uparrow, \sigma_m = \downarrow\}\rangle \) and \( |\{\downarrow, \sigma_m = \uparrow\}\rangle \), where \( m \) indicates the location of the flipped spin. Since the flipped spin can be anywhere in the system there are \( N \) of these states for each ground state configuration. For simplicity we assume that the spin of the extra carrier is unpolarized, then it suffices to consider only \( |\{\uparrow\}\rangle \) and \( |\{\uparrow, \sigma_m = \downarrow\}\rangle \), the contribution from the other ground state will be exactly the same. Considering only these states in the trace of Eq. (4.4) we obtain:

\[
G(k, \omega) = \frac{1}{Z} [G^{(0)}(k, \omega) + e^{-\beta 4dJ} G^{(1)}(k, \omega)] + \mathcal{O}((e^{-\beta 4dJ})^2),
\]  

\(4.16\)

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where

\[
G^{(0)}(k, \omega) = [\omega - \epsilon_k - 2dJ + i\eta]^{-1}
\]

\[
G^{(1)}(k, \omega) = \sum_{n, \sigma} e^{ikR_n} \sum_m g_{0,n}(\omega, \{\uparrow, \sigma_m = \downarrow\})
\]

\[
Z' = \frac{Z}{e^{-\beta E_{FM}}} = (1 + Ne^{-\beta dJ} + \ldots)
\]

Note that \(G^{(0)}(k, \omega)\) is identical to the \(T = 0\) solution.

To evaluate \(G^{(1)}(k, \omega)\) we need to treat the case \(m = 0\) separately. In this case the extra carrier removes the flipped spin. This results in the breaking of 2d AFM bonds and therefore an energy gain of \(2dJ\). Furthermore as pointed out above only \(g_{0,0}(\omega, \{\uparrow, \sigma_0 = \downarrow\})\) contributes to the sum since the extra carrier was injected into a domain of length 1. Since the flipped spin was removed and all the remaining spins are aligned it is easy to calculate \(g_{0,0}(\omega, \{\uparrow, \sigma_0 = \downarrow\})\) which in the limit \(N \to \infty\) becomes

\[
g_{0,0}(\omega, \{\uparrow, \sigma_0 = \downarrow\}) = \int \frac{dq}{(2\pi)^{d}} \frac{1}{\omega - \epsilon_q + 2dJ + i\eta},
\]

\(i.e.\) a continuum of states centered at \(\omega = -2dJ\).

We are now left with calculating the remaining contributions to \(G^{(1)}(k, \omega)\) for which \(m \neq 0\). This is not a trivial problem, but since there is only one flipped spin in the system and we are summing over all “hole” locations, we can approximate \(g_{0,n}(\omega, \{\uparrow, \sigma_m = \downarrow\}) \approx g_{0,n}(\omega, \{\uparrow\})\). In doing so we neglect that the energy is lowered when the “hole” is adjacent to the flipped spin \(\sigma_m\). Reinserting into Eq. (4.18) we obtain

\[
G^{(1)}(k, \omega) \approx g_{0,0}(\omega, \{\uparrow, \sigma_0 = \downarrow\}) + (N - 1)G^{(0)}(k, \omega),
\]

where the factor \(N - 1\) in front of \(G^{(0)}\) is due to the sum over \(m\). Note that this factor ensures that the \(Z'\) in the Eq. for \(G(k, \omega)\) is approximately canceled. Similarly one expects contributions from states with two or more well-separated flipped spins to cancel the \(Z'\) in front of \(g_{0,0}(\omega, \{\uparrow, \sigma_0 = \downarrow\})\) (see the discussion in Chapters 2 and 3). Consequently the low-\(T\) expansion of the Green’s function gives:

\[
G(k, \omega) \approx G^{(0)}(k, \omega) + e^{-\beta dJ}g_{0,0}(\omega, \{\uparrow, \sigma_0 = \downarrow\}).
\]

\(i.e.\) the spectral weight below the \(T = 0\) QP which is given by \(g_{0,0}(\omega, \{\uparrow, \sigma_0 = \downarrow\})\) vanishes like the probability \(e^{-\beta dJ}\) to find a flipped spin.
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Figure 4.5: Rescaled spectral weight $e^{\beta J} [A(0, \omega) - A^{(0)}(0, \omega)]$ in the region of the continuum centered at $-2J$, for Model III with FM background and different values of $\beta$. For comparison the dashed, black line shows $-\text{Im}[g_{0,0}(\omega,\{\uparrow,\sigma_0=\downarrow\})]/\pi$ calculated with Eq. (4.20). Other parameters are $J/t = 2.5$ and $\eta/t = 0.04$.

To verify this behavior we show in Fig. 4.5 the rescaled spectral weight $e^{\beta J} [A(0, \omega) - A^{(0)}(0, \omega)]$, where $A^{(0)}(k, \omega) = \delta(\omega - \epsilon_k - 2J)/\pi$ is the $T = 0$ QP peak. From Eq. (4.22) it is clear that at sufficiently low $T$ the resulting curves should equal $-\text{Im}[g_{0,0}(\omega,\{\uparrow,\sigma_0=\downarrow\})]/\pi$, which is shown by the dashed, black line in Fig. 4.5. Indeed we find that the three curves in Fig. 4.5 for $\beta J = 1.5$, 2.0 and 2.5, respectively, collapse onto each other and onto the curve for $-\text{Im}[g_{0,0}(\omega,\{\uparrow,\sigma_0=\downarrow\})]/\pi$. Close to the upper edge of the continuum the agreement starts to falter. This is because in addition to the $T = 0$ peak there are other peaks in the spectral weight (see Fig. 4.2) whose tails contribute to the $-2J$ continuum and are not subtracted. Multiplying with $e^{\beta J}$ amplifies these tails. Similarly the oscillating features in Fig. 4.5 are finite size effects which are amplified by the factor $e^{\beta J}$.

Similar calculations can be performed for the other low-energy features. All their spectral weights vanish as $T \to 0$ because they all originate from doping the carrier into a thermally excited environment, which become less and less likely to occur in this limit.

The finite-$T$ behavior of Model III is thus qualitatively different from that of Models I and II. For the latter, the $T = 0$ QP peak also marks the lowest energy for electron-addition at any finite temperature, whereas for Model III we observe the appearance of electron-addition states well below the $T = 0$ QP peak. Their spectral weight vanishes as $T \to 0$, which is very
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Figure 4.6: $A(k=0, \omega)$ for Model III with FM background, for different values of $J$ at a temperature $\beta J = 0.5$. The dashed red lines show the location of the $T = 0$ QP peak. Full blue lines mark the energies $-2J \pm 2t$. Parts of the spectra have been rescaled for better visibility.

reminiscent of pseudogap behavior and offers a simple and general scenario for how it can be generated. These low-energy states vanish from the spectrum as the temperature is lowered not because a gap opens and/or the electronic properties are somehow changed, but simply because these states describe doping into thermally excited local configurations, and the probability for the doped carrier to encounter them vanishes as $T \to 0$.

As should be clear from these arguments, the appearance of these low-energy continua is not a consequence of the large $J/t$ values used so far for Model III. Indeed, Fig. 4.6 shows that similar behavior is observed for smaller $J$ values (parts of these spectral weights have been rescaled for better visibility). With decreasing $J$ the different continua overlap, but shoulders marking some of their edges are still clearly visible and marked by dashed lines. In all cases, at finite $T$ spectral weight appears below the $T = 0$ QP.

For the experimental observation of pseudogap behavior it is of importance whether the chemical potential falls into the region of the spectrum that exhibit pseudogap behavior or remains at the $T = 0$ peak. Since we are working in a canonical ensemble this is not a priori clear. However, we expect that at finite $T$ the chemical potential will move away from the $T = 0$ peak towards the low-energy states that become available.
4.4. Results

Figure 4.7: $T = 0$, AFM solutions. Top panels: contour plots of $A(k, \omega)$. Bottom panels: Cross sections at $k = 0$. (a) and (d) Model I with $J_0/t = 5$, $|J|/t = 0.5$; (b) and (e) Model II with $J_0/t = 5$, $|J|/t = 0.5$; (c) and (f) Model III with $|J|/t = 2.5$. To improve visibility of the continuum a hard cutoff at $A(k, \omega) = 0.1$ was used for the Model III contour plot. In all cases $\eta/t = 0.04$.

peak, marked by the full line.

It should also be clear that this phenomenology is not restricted to FM backgrounds, either: one can easily think of excited configurations in an AFM background whose exchange energy would be lowered through doping, in a $t$-$J$ model similar to Model III. We have verified numerically that at finite $T$, features lying below the corresponding $T = 0$ QP peak indeed appear in the spectral weight of AFM chains. These results are presented below. This phenomenology is therefore quite general.

4.4.2 AFM results

Just like in the FM case, there are also two ground states of the undoped AFM Ising chain: either the odd or the even lattice hosts the up local moments. Of course, both AFM ground states yield the same QP properties. However, the QPs that result when a carrier is injected in the three models are different even at $T = 0$, for the AFM backgrounds. This is shown in
4.4. Results

Fig. 4.7, where contour plots of the $T = 0$ spectral weight $A(k, \omega)$, and cross sections at $k = 0$, are shown.

For Model I, the energy shifts due to the Ising exchange with the spins to the left and right of the extra electron exactly cancel out and the QP behaves like a free electron with dispersion $\epsilon(k)$. For Model II, interaction with the AFM background opens a gap in the QP spectrum and halves its BZ. The upper and lower bands have dispersion $\pm \sqrt{J_0^2 + \epsilon^2(k)}$, respectively. For Model III, the $T = 0$ spectral function is independent of $k$ and has a coherent QP peak at $\omega = 4|J| - 2\sqrt{J_0^2 + t^2}$ and a continuum for $4|J| - 2t < \omega < 4|J| + 2t$. The QP peak corresponds to a bound state with the extra electron confined at its injection site. Propagation of the extra electron along the chain reshuffles the Ising spins and gives rise to the continuum centered at $4|J|$. One can therefore think of this continuum as the electron+magnon continuum. Mathematically, the $k$-independence follows directly from the fact that for Model III, $g_{0,n}(\omega, \{\sigma\}) = 0$ when $n > 0$, if $\{\sigma\}$ is the AFM ground state.

The finite-$T$ spectral functions for $k = 0$ are shown in Fig. 4.8. For all three models the peaks broaden and spectral weight appears below, as well as above the $T = 0$ QP peak. This is in contrast to the FM case, where in Models I and II, at $k = 0$, spectral weight appears only above the $T = 0$ QP peak. For Model I the energy difference between the low-energy states and the $T = 0$ peak is controlled by $J_0$, because at finite $T$ the extra electron can be injected into small domains where the Ising exchange interaction with the spin to the left no longer cancels that with the spin to the right. For Model II on the other hand injecting the extra electron into a small FM domain merely enhances its mobility and leads to an energy change of the order of $t$. As the temperature increases more weight is transferred to these low-energy features, and the low-energy behavior of Model II starts to resemble that of Model I even though they have different $T = 0$ QPs.

For Model III, at finite $T$ new features appear, centered at $-2d|J|$ and $0$. Just as for the FM case, they are due to the injection of the extra electron into specific, excited, local configurations of the chain. If the electron is injected into a small FM domain embedded in an otherwise AFM ordered background, the energy is lowered by $2d|J|$. As long as the electron stays within the FM domain reshuffling of the spins does not result in a further change in energy. This explains the appearance of spectral weight at $\omega \sim -2d|J|$. This is true for any dimension $d$ and consequently the appearance of spectral weight at $-2d|J|$ is a generic feature of Model III. Coming back to the specific case of $d = 1$, if the electron leaves the FM domain, then reshuffling of the spins recreates an FM bond and destroys one
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Figure 4.8: AFM Spectral weight at $k=0$ for three different temperatures for (a) Model I with $J_0/t = 5$, $|J|/t = 0.5$; (b) Model II with $J_0/t = 5$, $|J|/t = 0.5$; (c) Model III with $|J|/t = 2.5$, the inset shows spectral weight below the $T=0$ QP peak for $\beta|J| = 2.5$. In all cases, the broadening is $\eta/t = 0.04$. The vertical lines show the energy of the $T=0$ QP peak.
of the AFM bonds. The total change in energy (injection and reshuffling) is therefore zero, explaining the continuum centered around $\omega \sim 0$. Besides the appearance of these new, low-energy continua, resonances appear close to the $T = 0$ QP peak and within the high-energy continuum (not visible in Fig. 4.8 due to the scale). They are likely caused by injection of the electron into an AFM domain and subsequent scattering off domain walls which can only exist at finite $T$.

**4.5 Discussion and conclusions**

In this work, we identified models that have identical $T = 0$ low-energy QPs (for couplings favoring a FM background), and yet exhibit very different low-energy behavior at finite $T$, proving that the former condition does not automatically guarantee the latter.

In particular, the finite-$T$ behavior in Model III is controlled by rare events, where the carrier is injected into certain magnetic configurations created by thermal fluctuations. Their energies are higher than that of the undoped ground-state, however the spectral weight measures the change in energy upon carrier addition (or removal), and this may be lower at finite $T$ than at $T = 0$. This is the case for Model III because here doping removes a magnetic moment from the background while its motion reshuffles the other ones. It is not the case for Models I and II where the carrier can do neither of these things. This difference is irrelevant at $T = 0$ because of the simple nature of the undoped FM ground-state, but becomes relevant at finite $T$.

We showed that such transfer of finite-$T$ spectral weight well below the $T = 0$ QP peak is independent of the size of the magnetic coupling $J$ and occurs for both FM and AFM coupling. Furthermore, we provided arguments that this behavior is expected to occur in any dimension.

One may wonder how much of an influence the Ising nature of the spins plays for the spectral weight transfer to energies below the $T = 0$ QP peak in Model III. A way to get an estimate of this is by using a FM XY model where the angles between the spins can take any value. The Hamiltonian of

![Figure 4.9: Spiral spin configuration in a 1d XY model.](image)
the classical XY chain is given by
\[ \hat{H}^{XY} = -J \sum_i \cos(\theta_{i+1} - \theta_i) \] (4.23)

For this model the GS of the spin chain is the state in which all spins are completely aligned, \( i.e. \) all angles \( \theta_i = 0 \). This state is identical to the GS of Model III. There are many types of excited states in the XY model, but if one injects the "hole" into a spiral configuration where neighboring spins are rotated with respect to each other by a fixed angle \( \theta \) (see Fig. 4.9) one can use the same formalism as above to calculate the real-space GF \( g^{XY}_{00}(\omega) \) for this configuration. By setting the denominator of \( g^{XY}(\omega) \) to zero the QP energy of the lowest "hole" state is obtained. It is given by
\[ E^{XY}(\theta) = 3J \cos(\theta) - J \cos(2\theta) - \sqrt{J^2(\cos(\theta) - \cos(2\theta))^2 + 4t^2} \] (4.24)

Note that for \( \theta = 0 \) we recover the result of the FM, \( T = 0 \) QP peak whose energy is \( E^{XY}(0) = 2J - 2t \).

The question we are trying to answer is whether there are values of \( \theta \) for which \( E^{XY}(\theta) < E^{XY}(0) \). Such states would have the same effect as the single spin down domains which we identified as giving contributions
to the spectral weight below the $T = 0$ peak for Model III. Of course, this is trivially satisfied by $\theta = \pi$ which produces AFM order. The real question is therefore whether there are also smaller values of $\theta$ for which this occurs. That this is indeed the case is verified in Fig. 4.10(a) where we show $E^{XY}(\theta) - E^{XY}(0)$ for different values of $J$. Clearly a critical value, $\theta_c$, exists for which the energy of a ”hole” injected into a spiral is identical to that of a ”hole” injected into the ordered XY chain. Chains with $\theta > \theta_c$ will contribute to spectral weight below the $T = 0$ QP peak. The dependence of $\theta_c$ on $J$ is shown in panel (b) of Fig. 4.10. One can show that $\theta_c \to 0$ in the limit $J \to \infty$. Note that $\theta_c < \pi/2$ even for relatively small values of $J$.

Note that we did not consider the energy it requires to create such a spiral which will scale with the system size, since every spin is rotated by an angle $\theta$. The Boltzmann weight of such a spiral will consequently be very small. However, the above discussion does show that domains which can lead to spectral weight below the $T = 0$ QP peak also exist for more complicated types of coupling, as long as the carrier is injected into the same band which hosts the spins.

It is also interesting to discuss in how far these results would be altered if the interaction between the extra electron and the local magnetic moments was of Heisenberg instead of Ising type. For Models I and II we showed in Chapter 2 that for Heisenberg $J_0$ and FM coupling between local magnetic moments, the formation of a spin-polaron becomes possible. As we pointed out this can also lead to the transfer of spectral weight to energies far away from the $T = 0$ QP peak. However, this mechanism is quite different from the mechanism that leads to the appearance of spectral weight below the $T = 0$ peak in Model III. First of all the spin-polaron only exists when $|J_0|$ is sufficiently large, whereas in Model III spectral weight appears below the $T = 0$ peak for all values of $J$. Another difference is that the spin-polaron states in Models I and II are not necessarily the low-energy features, even at $T = 0$. Instead it is possible that the $T = 0$, low-energy states belong to the $c+m$ continuum. In this case a mapping from Model I/II to Model III becomes impossible, because the $T = 0$, low-energy feature of Model III is a single QP peak instead of a continuum. If the extra electron is injected with its spin parallel to the local magnetic background the $T = 0$ spectrum for Models I and II is a single QP peak, but again the mapping to Model III is impossible, because Model III requires the extra electron to have opposite spin, otherwise it cannot be hosted by the half-filled band. Consequently the mapping from Model I/II to Model III is only meaningful if the low-energy feature of Model I/II is the spin-polaron. The spin-polaron then corresponds to the effective “hole” in Model III and as discussed above, at finite $T$, Model
4.5. Discussion and conclusions

III predicts additional features to appear below it. For Model I/II, on the other hand, we cannot completely rule out the possibility of additional features appearing below the spin-polaron state, but we discussed in Chapter 2 that such features would correspond to a bound state between the extra electron and multiple magnons and are extremely unlikely. The main conclusions from this Chapter should therefore remain true for Heisenberg $J_0$, as well.

While far from being a comprehensive study, these results and our discussion clearly demonstrate that the appearance of finite-$T$ spectral weight well below the $T = 0$ QP peak, due to the injection of the carrier into a thermally excited local environment making it behave very unlike the $T = 0$ QP, is a rather generic feature for $t$-$J$ like models. The weight of these finite-$T$, low-energy features must vanish when $T \to 0$ because the probability for such excited environments to occur vanishes, therefore these models exhibit generic pseudogap behavior.
Chapter 5

Summary and outlook

The theme of this thesis is unusual finite-$T$ signatures in the one-electron spectral function of models of doped magnetic insulators. In all the models studied in this thesis a single charge carrier interacts with a magnetic background. The most sophisticated model we studied is the so-called s-f(d) model, in Chapter 2. There we used a low-$T$ expansion to investigate how thermal magnons change the spectrum of a spin up carrier when it is injected into a magnetic background with positive magnetization. We found that apart from the usual broadening of the $T=0$ QP peak, spectral weight is shifted to spin-polaron states. In the case of AFM $J_0$ this results in the transfer of spectral weight to a continuum at energies well below the $T=0$ QP peak. Furthermore spectral weight was transferred to the c+m continuum spanned by the energies $\{E_\uparrow(k - q + q') - \Omega_{q'} + \Omega_q\}_{q,q'}$ and we discussed that in general one expects continua to appear at all energies $\{E_\uparrow(k + \sum_{i=1}^{m} q'_i - \sum_{i=1}^{m} q_i) - \sum_{i=1}^{m} \Omega_{q'_i} + \sum_{i=1}^{m} \Omega_{q_i}\}_{q_1,...,q_m}$.

Unfortunately we were unable to calculate higher order corrections to the low-$T$ expansion from Chapter 2. It was furthermore found that the approximation breaks down when $T$ becomes too large and produces a spurious pole in the spectral function.

Consequently we chose a very different approach in Chapter 3. By simplifying the model to a 1$d$ chain for which both the spin-spin interaction, as well as the carrier-spin interaction are of Ising type we were able to obtain exact, numerical results. These results highlight the importance of small magnetic domains which can temporarily entrap the carrier and lead to a distinctive fine-structure in the carrier spectrum. As discussed, a somewhat similar situation occurs in binary alloys, where charge carriers can become trapped in small domains of like atoms. However, spin-spin correlations and the absence of true disorder set the magnetic case apart from binary alloys.

The results from the Monte Carlo simulation allowed us to develop an analytical approximation which takes into account the contributions of the simplest magnetic domains of length $L$. For this approximation to work one needs to introduce a cutoff for $L$ which should be of the order of the spin-spin correlation length. The numerical results furthermore suggest that a
similar approximation should work even at higher $T$ if one takes into account a $T$ dependent prefactor for the contribution of each domain. However, the form that such a prefactor should have is not obvious. It is likely that a similar approach could work for the low-$T$ expansion of Chapter 2, i.e. by multiplying the self-energy Eq. 2.10 with a $T$ dependent prefactor one should be able to account for the incomplete cancellation of the factor $1/Z$ and avoid the appearance of the spurious pole. But of course the same problem of guessing the form of the prefactor exists here, as well. A possible extension to the work in this thesis could be to try to improve on these approximations.

The study of simplified 1$d$ models was continued in Chapter 4 where we found that at finite $T$, $t-J$-like models in which the carrier is injected into the same band as the spins are generically different from multi-band models in which the carrier is hosted by a separate band. The reason for this is that in $t-J$-like models the injected carrier removes a spin and can therefore lower the energy of the spin chain. Since the spectral function measures energy differences, this results in the appearance of spectral weight below the $T = 0$ QP peak. The crucial point here is that this difference may not be obvious at all from the $T = 0$ spectrum. Of course we showed in Chapter 2 that spectral weight below the $T = 0$ QP peak can also appear in a two-band model, but there the mechanism for this was a Heisenberg exchange which allowed for the emission and absorption of magnons. As discussed, this is quite different from the mechanism that leads to low-energy QP weight in the $t-J$-like model from Chapter 4.

Another important point raised in Chapter 4 is that of pseudogap-like behavior. Since the spectral weight below the $T = 0$ QP weight in $t-J$-like models depends on the presence of certain thermally excited configurations (domain walls, in our case) it will disappear as $T \to 0$. One can think of this as a type of pseudogap opening up.

To summarize, in this thesis new methods for the study of finite-$T$ effects in doped magnetic insulators were developed. All of these methods explicitly take into account the local environment of the carrier and its interactions with magnons or magnetic defects. This sets them apart from mean-field like approaches, but also limits their applicability to more complicated models. A recurring theme was the expansion in powers of the Boltzmann factor which we used for the analytical approximations in Chapters 3 and 4 and for the low $T$ expansion in Chapter 2. Furthermore two different mechanisms for the transfer of spectral weight to energies below the $T = 0$ QP peak were found. This shows that finite-$T$ effects in doped magnetic insulators can lead to quite unusual behavior.
Let us now comment on possible extensions of this work. As already mentioned one could try to obtain higher order terms for the low-$T$ expansion from Chapter 2 which hopefully fix the appearance of the spurious pole. However, including states with more than one magnon is very difficult since one needs to take into account magnon-magnon interactions. Even for the Ising model these interactions exist since for $S = 1/2$ two magnons cannot be on the same site. One could try to avoid this problem by transforming the spins to bosonic operators, this would be similar to the approach from Ref. [5].

Instead we believe that it is more promising to further investigate the claims we made in Chapter 4. There we provided arguments which suggest that even though our calculations were carried out in $1d$ and the exchange was of Ising-type our main conclusions remain true for higher dimensions and more complicated magnetic backgrounds, as well. The claim that this is true for higher dimensions can be checked with a very similar calculation to that in Chapter 4. However, numerically a calculation in $2d$ or even $3d$ will be much more costly and one will need to restrict the system size substantially. A quantum Monte Carlo simulation could be used to test our claim for Heisenberg exchange interactions, but to ensure that the results are comparable one needs to work in the canonical ensemble, while often quantum Monte Carlo simulations use the grand canonical ensemble. A different approach could be to do a similar calculation for a more complicated model with classical spins, e.g. a Potts model [55, 85, 107] or the XY-model.

While in this thesis we focused on the interaction of the extra charge carrier with magnons and domain walls, more sophisticated models of the magnetic background would also allow one to study its interaction with other types of magnetic excitations such as magnetic vortices or skyrmions which appear in higher dimensions. A brief discussion of the type of effects that this could lead to was presented at the end of Chapter 4 for a 1d spin-spiral. A more thorough investigation of these ideas and an extension to higher dimensions would be interesting.

In conclusion, much more work is needed before the evolution of the spectral weight with temperature is fully understood, for doped magnetic semiconductors. Our results, however, clearly show that this is a topic full of interesting and unexpected physics, and that therefore simplistic ideas and treatments are likely to fail. This is demonstrated, particularly, by the fact that even for the highly simplified models studied in Chapters 3 and 4 and even for FM order, which is the simplest type of magnetic order, the temperature evolution of the spectral weight is far from trivial.
Bibliography


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Appendix A

Derivation of the lowest $T \neq 0$ self-energy term

We present this calculation for the Heisenberg FM; the Ising case is treated similarly. To find $G^{(1)}_{\uparrow}(k, q, q', \omega)$, we divide $\hat{H} = \hat{H}_0 + \hat{V}$ where $\hat{H}_0 = \hat{T} + \hat{H}_z$ and $\hat{V} = \hat{H}_{S}^{xy} + \hat{H}_{\text{exc}}$, and use Dyson’s identity $\hat{G}(\omega) = \hat{G}_0(\omega) + \hat{G}(\omega)\hat{V}\hat{G}_0(\omega)$ where $\hat{G}_0 = [\omega - \hat{H}_0 + i\eta]^{-1}$ is the resolvent for $\hat{H}_0$. This procedure is similar to that used in Ref. [7] for the $T = 0$ spin-polaron. Applying Dyson’s identity once we obtain:

$$G^{(1)}_{\uparrow}(k, q, q', \omega) = G^{(0)}_{\uparrow}(k + q' - q, \omega + \Omega_{q'} - \Omega_q) \left[ \delta_{q, q'} - \frac{J_0}{2N} \sum_Q G^{(1)}_{\uparrow}(k, Q, q', \omega) + J_0 \sqrt{\frac{S}{2N}} F(k, q, \omega) \right]$$

The first term on the right-hand side is just the diagonal term. The second term accounts for the energy shift that occurs when the up-carrier is on the same site as the magnon, and the third term contains a new propagator $F(k, q', \omega) = \langle \Phi(q') c_{k, \uparrow} \hat{G}(\omega + \Omega_{q'}) c_{k + q, \downarrow} | \text{FM} \rangle$. This term accounts for spin-flip processes where the up-carrier absorbs the magnon, turning into a down-carrier with momentum $k + q$. Using Dyson’s identity again, we get an EOM for $F(k, q', \omega)$:

$$F(k, q', \omega) = J_0 \sqrt{\frac{S}{2N}} G^{(0)}_{\uparrow}(k + q, \omega + \Omega_{q'} + J_0 S) \times \sum_Q G^{(1)}_{\uparrow}(k, Q, q', \omega).$$

The diagonal element vanishes since the bra and ket are orthogonal. The energy shift $-J_0 S/2$ of the spin-down carrier is absorbed into the argument of $G^{(0)}_{\uparrow}$, leaving only the spin-flip process which links $F$ back to $G^{(1)}_{\uparrow}$.

These two coupled equations can now be solved as follows. We insert
Eq. (A.2) into Eq. (A.1) to obtain:

\[
G_\uparrow^{(1)}(k, q, q', \omega) = G_\uparrow^{(0)}(k + q' - q, \omega + \Omega q' - \Omega q) \{ \delta_{q,q'} \\
- \frac{J_0}{2} f(k, q', \omega) \left[ 1 - J_0 SG_\uparrow^{(0)}(k + q, \omega + \Omega q' + J_0 S) \right] \},
\]

(A.3)

where \( f(k, q', \omega) = \frac{1}{N} \sum_Q G_\uparrow^{(1)}(k, Q, q', \omega) \). Using Eq. (A.3) in the definition of \( f(k, q', \omega) \) yields:

\[
f(k, q', \omega) = \frac{1}{N} G_\uparrow^{(0)}(k, \omega) \left[ 1 + \frac{J_0}{2} g(k, q', \omega) \right. \\
\left. \times \left( 1 - J_0 SG_\uparrow^{(0)}(k + q', \omega + J_0 S) \right) \right]^{-1},
\]

with \( g(k, q', \omega) = \frac{1}{N} \sum_Q G_\uparrow^{(0)}(k + q' - Q, \omega + \Omega q' - \Omega Q) \). Note that \( g(k, q', \omega) \) can be calculated numerically since \( G_\uparrow^{(0)}(k, \omega) \) is a known function.

All that is left to do is to insert the above expression into Eq. (A.3) and calculate \( \sum_q e^{-\beta \Omega q} G_\uparrow^{(1)}(k, q, q, \omega) \), to find the expression listed in Section III.
Appendix B

Exact solution of the undoped Ising chain

Here we review the exact solution of the undoped Ising chain. All quantities of interest to us are obtained from the partition function:

$$Z = \sum_{\{\sigma\}} e^{-\beta E_i(\{\sigma\})}, \quad (B.1)$$

where the sum is over all configurations of lattice spins. The sum can be rewritten as:

$$Z = \text{Tr}(T^N) = \lambda_+^N + \lambda_-^N,$$

where the transfer matrix is $T_{\sigma,\sigma'} = e^{\beta(J\sigma\sigma' + h/2(\sigma + \sigma'))}$, and its eigenvalues are:

$$\lambda_{\pm} = e^{\beta J} \left[ \cosh(\beta h) \pm \sqrt{\sinh^2(\beta h) + e^{-4\beta J}} \right]. \quad (B.2)$$

The bulk value of the magnetization $m = \frac{1}{N} \sum_i \langle \sigma_i \rangle_T$ is:

$$m = \lim_{N \to \infty} \frac{1}{N^3} \frac{\partial \ln Z}{\partial h} = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}. \quad (B.3)$$

The correlation between spins is given by

$$\langle \sigma_n \sigma_m \rangle_T = \frac{\sinh^2(\beta h) + e^{-4\beta J}e^{-|m-n|/\xi}}{\sinh^2(\beta h) + e^{-4\beta J}}, \quad (B.4)$$

where the correlation length is $\xi = -1/\log(\lambda_-/\lambda_+)$. (For AFM coupling one needs to factor out $(-1)^{|m-n|}$ to ensure the real-valuedness of $\xi$).
Appendix C

Implementation of the Metropolis algorithm

The general theory behind the Metropolis algorithm is discussed in Chapter 1.6. In this appendix we merely discuss the specifics of our implementation. All the data that is shown in this appendix is for the model from Chapter 3 which is identical to Model II from Chapter 4.

Let us start by commenting on the effect of integrating out the complimentary set of spins \{M_c\}^C with the partition function \(Z_{\text{bath}}(\beta, \sigma_{-M_c}, \sigma_{M_c})\). Since it only depends on \(\sigma_{-M_c}\) and \(\sigma_{M_c}\) \(Z_{\text{bath}}(\beta, \sigma_{-M_c}, \sigma_{M_c})\) only changes the acceptance probability \(P_{\text{acc}}\) when a proposal to flip one of these two spins is made. It can therefore be incorporated into the general metropolis algorithm quite easily.

The thermal average in Eq. (4.4) is then calculated for the infinite chain with a Metropolis algorithm which generates configurations \{\sigma\} of the undoped chain.

We now discuss the measures taken to reduce correlations between individual measurements and to ensure convergence. In our implementation in a single Monte Carlo step an attempt to flip each of the \(2M_c + 1\) spins is made exactly once. To do this a list with the site indices in random order is used. After every Monte Carlo step the list is randomized again. The goal of this procedure is to reduce correlations between states.

To reduce correlations even further we investigate the autocorrelation function of the magnetization \(C^m_n\). To do this we run a Monte Carlo simulation for \(N\) steps and measure the magnetization at every step. The autocorrelation function can than be calculated as follows

\[
C^m_n = \frac{(N - l)^{-1} \sum_{i=1}^{N-l} (m_i - \bar{m})(m_{i+n} - \bar{m})}{N^{-1} \sum_{i=1}^{N} (m_i - \bar{m})^2}, \tag{C.1}
\]

where \(\bar{m}\) denotes the mean of the magnetization. Note that for AFM \(J\) the magnetization needs to be calculated separately for the odd and even sublattice.
Figure C.1: The autocorrelation of the magnetization for different values of $\beta$ and FM coupling. The dashed lines indicate when it has fallen off to 0.1. Parameters are $|J|/t = 0.5$, $J_0 = 2.5$ and $h = 0$.

The autocorrelation function is then used to determine how many Monte Carlo steps need to be performed between two consecutive measurements to ensure that they are no longer correlated. In Fig. C.1 we show the autocorrelation function for different values of $\beta$ and FM $J$. Note that for large $\beta$ correlations die off very slowly. When calculating the GF we only perform measurements after every $n$th Monte Carlo step, where $n$ is chosen in such a way that correlations have fallen off to at least 0.1, in some cases even 0.05. It needs to be pointed out that different observables may have different autocorrelation times. However, in a simple model like ours it is unlikely that the autocorrelation time of the GF varies drastically from that of the magnetization.

To assess the convergence of the spectral weight we perform a blocking analysis as is shown in Fig. C.2 for the prominent feature of the FM spectral weight at $\omega/t = -4.5$ (cf. Fig. 3.4). In this case the smallest blocks contained 800 measurements, but we also used blocks which contained only 100 measurements and in turn increased the number of blocks. The data from Fig. C.2 shows that the spectral weight at this value of $\omega$ is well converged (the relative error is $\sim 0.6\%$) and that correlations are insignificant. Note that for less prominent features the relative errors can be much larger. This is unavoidable since these features occur when the carrier is trapped in
Appendix C. Implementation of the Metropolis algorithm

Figure C.2: Blocking analysis of the relative error of \( A(k = 0, \omega = -4.5t) \) for FM \( |J| = 0.5 \) (cf. Fig. 3.3). Other parameters are \( k = 0, J_0/t = 2.5, h = 0 \) and \( \eta/t = 0.04 \).

Figure C.3: The FM spectral function \( A(0, \omega) \) for \( |J_0|/t = 2.5, |J|/t = 0.5, h = 0 \) and \( \eta/t = 0.04 \). The error bars correspond to the largest error from the blocking method.
magnetic clusters which are unlikely to occur and therefore longer sampling times are needed to increase their accuracy.

To provide the reader with a better feeling of the convergence of the whole spectrum we show in Fig. C.3 a plot of $A(0, \omega)$ for $\beta/t = 1.0$ with errorbars corresponding to the largest error from the blocking method. This figure also shows the same spectrum, but with a negative value for $J_0$. Physically the sign of $J_0$ is irrelevant and therefore we can use a comparison between the two spectra as a consistency check. Note that $A(k, \omega)$ obeys the sum rule $\int_{-\infty}^{\infty} d\omega \ A(k, \omega) = 1$. Consequently the difference between the two spectra which is purely of statistical nature must average to zero.