Dynamical correlations of $S = 1/2$ quantum spin chains

by

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Abstract

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Chapter 1

Introduction

Quantum spin chains provide simple yet rich examples of strongly correlated systems. For a theoretical physicist, one-dimensional (1D) arrays of interacting spins that behave according to the rules of quantum mechanics are interesting because they are amenable to detailed analytical and numerical studies [1]. These studies have revealed that spin chains exhibit exotic properties which contradict our classical intuition about magnetic ordering. For instance, spin-1/2 chains with an isotropic antiferromagnetic exchange interaction do not order even at zero temperature, and their spectrum is best interpreted in terms of fractional excitations named spinons which are very different from spin waves in three-dimensional magnets. But spin chains are not confined to the theoretical realm. They also exist in the real world, in the form of chemical compounds in which, due to the lattice structure, the coupling between magnetic ions is highly anisotropic and strongest along one spatial direction [2]. Indeed, thanks to steady advances in materials science, the research field of 1D quantum magnetism has benefited from the interplay between theory and experiment that is essential in condensed matter physics. The interest in spin chain models is actually quite general, ranging from applications in quantum computation [3] to mathematical tools in string theory [4].

Given the long history of studies of spin chains, it is fair to say that most relevant static thermodynamic properties, such as specific heat and magnetic susceptibility, are well understood by now. However, despite various efforts, the problem of calculating dynamical properties, such as the dynamical structure factor probed directly in inelastic neutron scattering experiments, poses a challenge to standard theoretical approaches and has remained unsolved. The need to clarify some of the open questions concerning the dynamics of spin chains motivated the work reported in this thesis.
1.1 Heisenberg model

Electrons are charged spin-1/2 particles which carry an intrinsic magnetic moment. In the early days of quantum mechanics, Werner Heisenberg [5] pointed out that the spin-independent Coulomb interaction between two electrons in a diatomic molecule, with a properly anti-symmetrized wave function, gives rise to an exchange interaction that couples the electron spins. The generalization of this idea to a large number of electrons leads to an important mechanism for magnetism in solids [2]. The Heisenberg model describes a bilinear exchange interaction between nearest neighbor spins at fixed positions on a lattice

\[ H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \]  

(1.1)

where $J$ is the exchange integral and $\vec{S}_i$ denotes the spin operator at site $i$, which obeys commutation relations of angular momentum operators [6]. If these are electrons spins (total spin $S = 1/2$), there are two states for each lattice site, denoted by $\{ |\uparrow\rangle_i, |\downarrow\rangle_i \}$. The Hilbert space has dimension $2^N$, where $N$ is the number of lattice sites. The components of the spin operator can be represented by Pauli matrices $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ in the form $\vec{S}_i = \hbar \vec{\sigma}_i / 2$, corresponding to the generators of the SU(2) group. More generally, the $\vec{S}_i$ operators can represent atomic spins, which depend on the electronic configuration and can be integer or half-integer.

![Figure 1.1: Schematic representation of a spin chain with $N$ sites and periodic boundary conditions.](image)

The type of magnetic order (or the lack thereof) in the ground state of the Heisenberg model depends on the sign of the exchange coupling $J$, dimensionality and lattice structure. For $J < 0$, the exchange interaction favors a state in which all the spins point along the same direction. The ground state picks out a particular direction in space and spontaneously
break the rotational symmetry of the Hamiltonian. This is actually the true ground state of the ferromagnetic model. We speak of long-range order in the ground state since the correlation between spins stays finite at arbitrarily large distances. For $J > 0$, the spins at neighboring sites would like to point along opposite directions. In the classical picture, the ground state breaks translational invariance and the system splits up into two sublattices with opposite magnetization. This classical state is called Néel state and is illustrated in Fig. (1.1) for a one-dimensional lattice. Unlike the ferromagnetic case, this state is not an eigenstate of the Hamiltonian (1.1) because the sublattice magnetization is not a good quantum number. This suggests that quantum fluctuations play an important role in the antiferromagnetic model. Although the resulting physics can be quite interesting in two and three dimensions (see, for example, the search for spin liquid states in frustrated magnets [2]), the effects of quantum fluctuations become extreme in the 1D case. While the classical Néel state is a good starting point for linear spin wave theory [7] in many three-dimensional lattices at finite temperature, it fails dramatically in 1D. In fact, the Mermin-Wagner-Hohenberg theorem [8, 9] rules out finite temperature phase transitions in the isotropic model in one and two dimensions. Even at zero temperature, it can be shown that the quantum corrections to the sublattice magnetization diverge in 1D and destroy the long-range order of the ground state [7]. The impossibility of spontaneous breaking of a continuous symmetry in a 1D model with short-range interactions was also discovered by Coleman in the context of quantum field theory [10]. But, if the classical picture fails, how should we think about the ground state of the 1D quantum antiferromagnet?

1.2 An example of a Heisenberg spin chain

Before we say more about the theoretical analysis of the model, let us discuss a concrete realization of an antiferromagnetic spin chain. The Heisenberg model (1.1) can be obtained more realistically from the Hubbard model, which describes electrons hopping on a lattice and repelling each other when two electrons occupy the same site. At half-filling and in the limit of strong on-site repulsion, there is exactly one electron per lattice site and charge fluctuations can be neglected at energies much lower than the interaction strength. The orbital degrees of freedom are frozen and only the spin degrees of freedom at each lattice site have to be considered. Kinetic exchange
that results from virtual hopping processes lifts the spin degeneracy of the ground state and the low-energy effective model is the Heisenberg model with $J > 0$ (antiferromagnetic) [2]. This means that antiferromagnetism appears naturally in Mott insulators, as is indeed observed in real compounds.

Although bulk materials are three dimensional, the value of the exchange coupling $J$ can be different along different directions of the lattice. In the copper oxide compound Sr$_2$CuO$_3$ [11], the crystal structure is characterized by CuO$_4$ squares sharing oxygen corners (Fig. 1.2). The experimental interest in this compound was motivated by the discovery of high-temperature superconductivity in related doped cuprates. In Sr$_2$CuO$_3$ the copper ions are in a 3d$^9$ configuration and have spin 1/2. The overlap with the oxygen atoms in the 180 degree Cu-O-Cu bonds is responsible for a strong superexchange interaction [12]. The effective $J$ along the copper-oxygen chain is as large as $J/k_B = (2200 \pm 200) K$ [11]. On the other hand, the interchain coupling is very weak, resulting in a very low Néel temperature, $T_N \sim 5 K$, below which three-dimensional magnetic ordering sets in. Therefore, over a wide temperature range, $T_N < T < J/k_B$, Sr$_2$CuO$_3$ is well described by the one-dimensional Heisenberg model (1.1). Other examples of effective spin-1/2 Heisenberg chains with smaller values of $J$ include KCuF$_3$ ($J/k_B \approx 190 K$) [13] and copper pyrazine dinitrate, CuPzN ($J/k_B \approx 10 K$) [14].

### 1.3 The Bethe ansatz

As the semiclassical approach fails in 1D, understanding the one-dimensional antiferromagnet requires a whole new theoretical framework. Such framework actually appeared even before spin wave theory. In 1931, Hans Bethe [15] showed that the 1D Heisenberg model can be solved exactly, in the sense that one can construct the exact eigenstates and eigenvalues of the Hamiltonian (1.1). The key for Bethe’s solution was the fact that in the Heisenberg model any scattering among spin excitations can be factorized into a series of two-body scattering processes. The many-body wave functions are superpositions of plane waves with relative amplitudes fixed by the two-body phase shift. The allowed values of quasi-momenta for given boundary conditions are determined by solving coupled nonlinear equations known as the Bethe ansatz equations. The reduction to two-particle scattering is not a general property of interacting Hamiltonians, but is valid for the Heisenberg model because the latter is integrable, meaning that it has an infinite number of lo-
Chapter 1. Introduction

(a) Crystal structure of Sr$_2$CuO$_3$, a $S = 1/2$ Heisenberg chain compound. Adapted from Ref. [11].

(b) A cut on the bc plane showing the Cu-O chain. The chain oxygens mediate a superexchange interaction between the magnetic copper ions.

Figure 1.2:
Remarkably, integrability is not so unusual in one dimension. Other widely studied 1D models, such as the Lieb-Liniger model [17] (interacting Bose gas) and the Hubbard model [18], are also integrable. The Bethe ansatz is also applicable to these models.

The Bethe ansatz solution [19, 20] proves that the ground state of the spin-1/2 Heisenberg chain is unique and has total spin equal to zero (a singlet state) if the number of sites is even. The spectrum is gapless (or “massless”) in the thermodynamic limit. The elementary excitation is called a spinon and corresponds to a hole in the set of roots of the Bethe ansatz equations. A single spinon is a fractional excitation which carries spin 1/2 and cannot be created alone without changing the boundary conditions. In order for the total $S_z$ of the chain to change by an integer number, as required by superselection rules, the spinons have to be created in pairs. This implies, for instance, that the simplest triplet excitation lie in a two-parameter continuum (whose lower bound is known as the de Cloizeaux-Pearson dispersion [21]), in contrast with the single-magnon peak predicted by semiclassical spin wave theory. This has in fact been observed in inelastic neutron scattering experiments [14], in a clear demonstration of one-dimensional behavior.

The Bethe ansatz equations for the Heisenberg spin-1/2 chain have been extensively studied, in an attempt to extract useful properties of the model. Due to the complexity of the solution, this is not always possible. It suffices to say that, seventy seven years after the original paper, not even the completeness of the Bethe eigenstates for the XXZ model (without an assumption about the distribution of complex roots known as the string hypothesis) has been proved yet [22]. In the thermodynamic limit, the Bethe ansatz equations assume the form of integral equations for the density of quasi-momenta. Some exact results which have been obtained by manipulating these equations include the ground state energy [23], zero temperature susceptibility [24] and spin wave velocity [21]. An application of the Bethe ansatz equations for finite systems is the calculation of the finite size spectrum [25], which is important in conformal field theory [26]. It is also possible to compute finite temperature static properties (e.g. specific heat, finite temperature susceptibility) using a set of nonlinear integral equations known as Thermodynamic

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1 Actually, the definition of integrability is clear for classical models, but ambiguous in quantum mechanics because linearly independent conserved quantities can be constructed for any quantum model (see discussion in [16]). It is more useful to think of quantum integrability as the absence of diffraction or three-particle scattering, as is the case for the Bethe ansatz solvable models.
Bethe Ansatz (TBA) [27]. However, this procedure has been criticized for relying on the string hypothesis to describe the spectrum of the XXZ model. It is worth mentioning that models describing spin chains with higher values of $S$ are not integrable. The case $S = 1/2$ is therefore special since we have access to an exact solution with which approximate analytical and numerical results can be compared. However, according to the Lieb-Shultz-Mattis theorem [28], a gapless spectrum is generic in isotropic half-integer spin chains, unless parity symmetry is spontaneously broken and the ground state is degenerate. The theorem does not hold for integer values of $S$. In fact, Haldane [29] conjectured that integer spin chains should exhibit a finite gap to the lowest excited state, while the SU(2) symmetry remains unbroken. Haldane’s conjecture has been confirmed by numerical calculations as well as experimentally, and the existence of a gap was proven rigorously for the related bilinear biquadratic $S = 1$ Affleck-Kennedy-Lieb-Tasaki (AKLT) model [30]. The difference between integer and half-integer spin chains can be attributed to the effects of a topological term in the nonlinear sigma model [31].

1.4 Anisotropic spin chains

The generalization of the model (1.1) which introduces exchange anisotropy as well as a finite external magnetic field is the so-called XXZ model in a field

$$H = J \sum_{j=1}^{N} [S_{j}^x S_{j+1}^x + S_{j}^y S_{j+1}^y + \Delta S_{j}^z S_{j+1}^z - h S_{j}^z].$$

(1.2)

In comparison with the Heisenberg (or XXX) model, the symmetry of the XXZ model has been reduced from SU(2) to U(1) (rotation around the $z$ axis). The total magnetization $S^z = \sum_j S_j^z$ is still a good quantum number. Moreover, this model is also integrable by the Bethe ansatz [32, 33]. While some exact analytical results can be derived for the model with $h = 0$, in general the Bethe ansatz equations for the XXZ model at finite magnetic field have to be solved numerically [19].

The first reason to study the XXZ model is that one should not expect perfectly isotropic exchange interactions in real materials. On a lattice the

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$^2$A simple program to solve the Bethe ansatz equations for the XXZ model numerically can be found in the appendix of Ref. [1].
rotational symmetry of the spin interaction can be broken by spin-orbit or dipolar interactions. However, this effect is weak and bulk spin chain materials are very close to being isotropic [34]. But the second and most important reason why the XXZ model is interesting is because it appears as an effective model whenever a physical system can be described as a one-dimensional lattice with two states per site. One example is that of $S = 1/2$ two-leg ladders in the strong coupling limit $J_\perp \gg J_\parallel$, where $J_\perp$ and $J_\parallel$ are the couplings along the rungs and along the chain, respectively [35]. Two-leg ladders are similar to $S = 1$ chains in the sense that there is an energy gap to the triplet state on each rung. But an external magnetic field can lower the energy of the triplet state with total $S^z$ parallel to the field. Near the critical field, the singlet-triplet gap closes and the two low-lying states form a doublet which acts as an effective spin-1/2 degree of freedom. The effective model for a $S = 1/2$ ladder with $J_\perp \gg J_\parallel$ is the XXZ model with $\Delta = 1/2$ [36, 37]. Artificial systems which have phases described by effective XXZ models, with arbitrary values of $\Delta$, include Josephson junction arrays [38], linear arrays of qubits [39] and ultracold bosonic atoms (with two internal hyperfine states) trapped in optical lattices [40]. In the latter, it should be even possible to observe phenomena associated with the integrability of the 1D model, such as the absence of relaxation mechanisms [41].

The Bethe ansatz solution allows us to map out the phase diagram of the XXZ model by looking at the energy of the low-lying excitations as a function of exchange anisotropy $\Delta$ and magnetic field $h$ (Fig. 1.3). Along the zero field line in parameter space, the limits $\Delta \to -\infty$ and $\Delta \to +\infty$ correspond to the classical Ising ferromagnet and antiferromagnet, respectively. These are both known to have a gapped spectrum, with domain-wall-type excitations. We also know that the model is gapless at the Heisenberg point $\Delta = 1$, so we should expect quantum phase transitions by simply varying the anisotropy parameter $\Delta$. As a matter of fact, the Bethe ansatz reveals that the XXZ chain is gapless along an entire critical line $-1 < \Delta \leq 1$ (sometimes called easy plane anisotropy regime). There is a gapped ferromagnetic phase for $\Delta < -1$ and a gapped Néel phase for $\Delta > 1$. Including the magnetic field, one finds the ground state phase diagram represented in Fig. 1.3 [16]. There is a whole region where the spectrum of the spin chain is gapless. Starting from the gapless phase, the system enters the ferromagnetic phase if the field is increased above the saturation field. On the other hand, a finite magnetic field can close the gap for $\Delta > 1$.

The gapped, Ising-like phases of the XXZ spin chain can be understood
Figure 1.3: Phase diagram for the XXZ model as a function of anisotropy parameter $\Delta$ and magnetic field $h$. Between the gapped ferromagnetic (FM) and antiferromagnetic (AFM) phases, there is a critical regime characterized by quasi-long range order (QLRO). This is a Luttinger liquid phase which includes the Heisenberg antiferromagnet $\Delta = 1$. The exact value of the Luttinger parameter $K$ at special points along the zero field line are indicated.
with simple semiclassical pictures, but the gapless phase seems more exotic. Long-range order should not exist in this phase, which includes the Heisenberg model. What we would really like to know in order to characterize this phase and make connection with experiments is how spin-spin correlation functions decay at large distances. Unfortunately, this cannot be done by employing directly the Bethe ansatz solution. Even when we know the exact eigenstates and the spectrum, calculating correlation functions requires computing matrix elements (so-called form factors) between a unmanageable number of complicated wave functions (recall that the size of Hilbert space grows as $2^N$). This calls for an alternative, approximate yet more intuitive approach to the physics of one-dimensional magnets.

### 1.5 Field theory methods

Another reason to consider the anisotropic model is that the XXZ spin chain is equivalent to a model of interacting spinless fermions. This is made clear by the Jordan-Wigner transformation, which maps the $S_j^z$ operator onto a local density of fermions [1]. This way, the spin-up state is equivalent to a particle and the spin-down state to a hole. Under this transformation the $x$ and $y$ terms of the exchange interaction in (1.2) are mapped onto a kinetic energy (hopping) term, whereas the $z$ part translates into a density-density interaction term. As a result, the model with $\Delta = 0$, known as the XY model, is equivalent to free fermions on the lattice and can be solved very easily by performing a Fourier transform to momentum space. The ground state of the XY model is understood as a Fermi sea of the Jordan-Wigner fermions, whose density is fixed by the magnetization of the spin chain. In particular, the zero field case corresponds to a half-filled band, with one fermion per every other lattice site. Excitations with total $S^z = 0$ correspond to the creation of particle-hole pairs. This solution of the XY model makes it possible to calculate some correlation functions exactly [28, 42]. The correlation functions are found to decay very slowly (as power laws) in the large distance limit, which leads to the notion of quasi-long range order in 1D gapless systems.

The solution of the XY model also provides a convenient starting point for exploring the entire gapless phase once we find a way to treat the fermion-fermion interactions for $\Delta \neq 0$. In three dimensions, Landau’s Fermi liquid
theory [43] shows that the excitations of a system of interacting fermions are quasiparticles which resemble the "bare" electron in the Fermi gas and differ only by the renormalization of a few parameters such as the effective mass [44]. The situation is very different in one dimension, because again quantum fluctuations have a drastic effect and lead to the breakdown of Fermi liquid theory in 1D [45]. The method of choice to describe the low-energy excitations of an interacting 1D fermionic system is called bosonization [46]. This approach starts by taking the continuum limit and linearizing the dispersion of the particle-hole excitations about the Fermi points with momentum $\pm k_F$. One then introduces an effective bosonic field associated with the collective density fluctuations of the Fermi gas. The advantage of the bosonization method is that "forward" fermionic interactions can be treated exactly. Their effect is simply to renormalize the velocity and "stiffness" of the non-interacting bosons. The resulting free boson model is known as the Luttinger model [47]. There is no clear correspondence between the bosons of the Luttinger model and the exact eigenstates found in the Bethe ansatz. However, it is possible to define a kink in the bosonic field that carries spin-1/2 and for $\Delta = 1$ obeys semionic statistics, in close analogy with the spinons of the Heisenberg model [48].

The bosonization approach is asymptotically exact in the limit of low energies and long wavelengths. Haldane [49] introduced the concept of the Luttinger liquid, pointing out that the Luttinger model should be the fixed point of any gapless 1D system with a linear dispersion in the low-energy limit. Residual boson-boson interactions which perturb the Luttinger liquid fixed point are either irrelevant or drive the system into a gapped phase under the renormalization group. This is a powerful result. In our case, it means that we can write down an effective field theory that is valid in the entire gapless phase of the XXZ chain. All we need to do is to determine the two parameters of the Luttinger model, namely the renormalized spin velocity $v$ and the so-called Luttinger parameter $K$, as a function of $\Delta$ and $\hbar$ in the original lattice model (1.2). These parameters can be fixed by comparing the field theory predictions for the low-energy spectrum and susceptibility with the corresponding results obtained from the Bethe ansatz [19]. However, the bosonization approach is more general than the Bethe ansatz in the sense that it can be applied to nonintegrable models as well. This enables one to

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Assuming the interactions are repulsive. Attractive interactions lead to a superconducting (BCS) instability.
compute universal properties which are independent of integrability.

Since the low energy effective theory for the XXZ model is a free bo-
son model, it is possible to compute the asymptotic large distance behavior
of correlation functions [50]. The result is that the spin correlation func-
tions decay as power laws with non-universal exponents which depend on the
Luttinger parameter $K$. Since $K$ is known exactly from the Bethe ansatz
solution, these results are nonperturbative in the interaction strength (i.e.
anisotropy parameter) $\Delta$. In particular, the Luttinger liquid theory applies
to the (strongly interacting) Heisenberg point $\Delta = 1$, although at zero field
it is important to consider the effects of a marginally irrelevant bulk operator
[51]. A power law decay implies that the correlation length is infinite; in the
language of phase transitions, the effective theory is critical. A great deal of
information, particularly finite temperature correlation functions and finite
size spectrum, can be obtained using techniques of conformal field theory
[52]. A review of field theory methods for spin chains can be found in [53].

The combination of Bethe ansatz, field theory and various numerical
methods (such as Quantum Monte Carlo [54] and Density Matrix Renor-
malization Group [55]) has a long and successful history. It has provided
us with a deep understanding of several properties spin-1/2 chains, many
of which have been confirmed by experiments. To mention a few examples,
Eggert, Affleck and Takahashi [56] showed that the finite temperature sus-
ceptibility of the Heisenberg chain approaches the zero temperature value
with an infinite slope (a logarithmic singularity that results from the effect
of the marginally irrelevant bulk operator). This prediction was used to fit
the susceptibility and extract the effective exchange coupling constant $J$ for
$\text{Sr}_2\text{CuO}_3$ [11]. Another example is the contribution of the staggered part
of the correlation function to the spin-lattice relaxation rate $1/T_1$ and the
spin-echo decay rate $1/T_{2G}$ probed by nuclear magnetic resonance (NMR)
[57, 58]. Finally, a third example is the calculation of the temperature and
magnetic field dependence of the line width of the absorption intensity in
electron spin resonance (ESR) experiments on Cu benzoate [59].

$^4$The field theory approach also explains the phase transitions of the XXZ model. For $\Delta > 1$, umklapp scattering becomes relevant and the system goes through a Kosterlitz-
Thouless transition. The effective field theory for the Néel phase is the quantum sine-
Gordon model, which has massive excitations (solitons, anti-solitons and breathers). On
the other side of the phase diagram, the system enters the ferromagnetic phase when the
spin susceptibility diverges ($\chi \propto K \to \infty$).
1.6 The problem of dynamical correlation functions

Inelastic neutron scattering experiments yield access to dynamical spin correlation functions. This is because neutrons carry spin-1/2 and can interact (via a dipolar interaction) with individual ions in a magnetic material, transferring both energy and momentum to the lattice. It can be shown [60] that the cross section for non-spin flip scattering, measured in experiments with polarized neutron beams, is directly proportional to the longitudinal dynamical structure factor

\[ S_{zz}(q, \omega) = \frac{1}{N} \sum_{j,j'=1}^{N} e^{-i\mathbf{q} \cdot (\mathbf{j} - \mathbf{j}')} \int_{-\infty}^{+\infty} dt e^{i\omega t} \left\langle S_j^z(t) S_{j'}^z(0) \right\rangle, \tag{1.3} \]

where \( \langle \ldots \rangle \) denotes the expectation value in the ground state of the Hamiltonian (1.2) (at zero temperature). The cross section for spin flip scattering is proportional to the transverse dynamical structure factor.\(^5\) Unlike static thermodynamic quantities, the dynamical structure factors are given by the Fourier transform of *time-dependent* correlation functions.

The first neutron scattering experiments on \( S = 1/2 \) Heisenberg chains in 1973 [61] pointed to an asymmetric line shape, with a peak at lower energies. This was later confirmed by further experiments [14, 62]. Moreover, the data suggested a double peak structure at finite magnetic field. As mentioned in section 1.3, these results were a direct proof that spin wave theory could not be used to describe 1D antiferromagnets. Early theoretical approaches based on the Hartree-Fock approximation [63] and Holstein-Primakoff representation (a large \( S \) expansion) [64] led to unphysical results and failed to explain the asymmetry of the line shape of \( S_{zz}(q, \omega) \) for the Heisenberg chain.

The XY model can serve as a starting point for an appropriate quantum mechanical treatment of the dynamical structure factor in the gapless phase. The expression for \( S_{zz}(q, \omega) \) in (1.3) is equivalent to the Fourier transform

\(^5\)The longitudinal and transverse functions are equivalent for the Heisenberg model at zero field due to SU(2) symmetry, but not for the general anisotropic case. The transverse correlation function is more difficult to calculate because, while \( S_j^z \) maps onto a local density of fermions under the Jordan-Wigner transformation, the mapping of the operators \( S_j^x = S_j^x \pm iS_j^y \) involves a nonlocal string operator. For this reason, there are no analytic expressions for the transverse dynamical structure factor even for the XY model. I will not discuss the transverse structure factor in this thesis.
of the density-density correlation function of the fermions defined in the Jordan-Wigner transformation [28]. Since for the XY model these fermions are noninteracting, $S^{zz}(q, \omega)$ turns out to be given by the density of states for excitations with a single particle-hole pair. The exact line shape derived for the XY model at zero magnetic field (half-filling) is illustrated in Fig. 1.4. It shows a step discontinuity at the lower threshold of the two-particle continuum and a square-root divergence at the upper threshold. There is no spectral weight outside the two-particle continuum.

![Figure 1.4: Particle-hole excitation spectrum and exact line shape of $S^{zz}(q, \omega)$ for the XY model at zero magnetic field. Note the square root divergence at the upper threshold and the step discontinuity at the lower threshold of the continuum. The dashed lines represent the single boson dispersion at $q \sim 0$ and the approximate lower bounds for the continuum at $q \sim \pi$ obtained by linearizing the dispersion about the Fermi points $k_F = \pm \pi/2$.](image)

Luther and Peschel [50] applied bosonization to treat the effects of fermionic interactions and calculate time-dependent correlation functions for the XXZ model in the low energy limit. However, the result for the dynamical structure factor is somewhat disappointing. As discussed above, one of the very first steps in the bosonization procedure is the approximation of linear dispersion of the low lying excitations. Without this assumption, the model is not solvable. In the fermionic approach, the effect of a nonlinear dispersion is understood as the violation of the Ward identities which guarantee the
cancelation of bubble diagrams with more than two interaction lines [65]. In the bosonic language, band curvature terms introduce interactions between the bosons of the Luttinger model [49]. These interactions are irrelevant in the renormalization group sense, which means that they give subleading corrections to the large distance asymptotics of correlation functions. Yet, due to the linear dispersion approximation the Luttinger model does not capture the correct continuum of particle-hole excitations. The low-energy spectrum predicted by the Luttinger model is represented by the dashed lines in Fig. 1.4. There is a linear mode near \( q \sim 0 \), corresponding to a single boson with infinite lifetime, and a continuum near \( q \approx \pi \) for \( h = 0 \) bounded from below by two straight lines. The result of Luther and Peschel is consistent with this approximate spectrum. They found that \( S^{zz}(q, \omega) \) has two contributions at low energies: (i) for \( q \approx 0 \), the line shape is given by a delta function peak at the energy carried by the single boson, \( S^{zz}(q, \omega) \sim \delta(\omega - vq) \); (ii) for \( q \approx \pi \), there is a power law singularity at the (approximate) lower edge of the continuum, \( S^{zz}(q, \omega) \sim [\omega^2 - v^2(q - \pi)^2]^{K-1} \).

There are several reasons why the Luttinger liquid result for \( S^{zz}(q, \omega) \) is not satisfactory. First, the delta function peak in contribution (i) does not say anything about the line shape probed by experiments. It contains even less information than the exact solution for the XY model, where we know that \( S^{zz}(q, \omega) \) has well defined lower and upper thresholds. All this Luttinger liquid result predicts is that the line shape should become infinitely narrow in the limit \( q \to 0 \). This is indeed the case for the XY model, where it can be verified that the width of the particle-hole continuum vanishes as \( q^3 \) for \( h = 0 \) and \( q^2 \) for \( h \neq 0 \) [28]. Second, based on general arguments for interacting field theories, we expect that for \( \Delta \neq 0 \) a continuous spectrum should appear at energies above the “mass shell” of the bosonic excitations, \( \omega = vq \), corresponding to an incoherent contribution from multiple-particle states. There is no such contribution in the Luttinger liquid result (i). Third, result (ii) does tell us that there is a power law singularity at some lower threshold, which becomes a square root divergence for \( \Delta = 1 \) (\( K = 1/2 \) at the isotropic point). This is in qualitative agreement with the asymmetry of the line shape observed in experiments. However, the straight lines in Fig.

\[ ^{6} \text{For} \ h \neq 0, \text{the low energy continuum appears at} \ q \approx 2k_F = \pi + 2\pi \langle S_j^z \rangle, \text{where} \ k_F \text{is the effective Fermi momentum and} \ \langle S_j^z \rangle \text{is the average magnetization per site.} \]

\[ ^{7} \text{The theory predicts a power law singularity only at} \ T = 0. \text{At finite temperatures, the singularity is replaced by a rounded maximum near the lower edge of the continuum. This is what is seen in experiments.} \]
1.4 are not the real edges of the two-particle continuum, except at $q = \pi$. There is no guarantee that the Luttinger liquid exponent for the power law singularity is the correct one away from $q = \pi$. Furthermore, result (ii) does not predict the behavior of $S^{zz}(q, \omega)$ at higher energies, particularly at the upper threshold of the two-particle continuum, which is beyond the reach of this approximation.

In the lack of a useful field theory result, in 1979 Müller et al. [66] put forward an approximate analytic expression for $S^{zz}(q, \omega)$ for the Heisenberg chain. Their proposal (detailed in [67]) was inspired by the exact solution for the XY model, selection rules for classes of Bethe ansatz eigenstates, numerical results for short chains ($N \leq 10$) as well as known sum rules [68]. The formula which became known as the Müller ansatz assumes that almost all the spectral weight is confined within the thresholds of the (later named) two-spinon continuum. The line shape predicted by the Müller ansatz is plotted in Fig. 1.5. Note that, contrary to the result for the XY model, there is a power law divergence at the lower threshold and a step function at the upper threshold. The square root singularity at the lower threshold was chosen to agree with the field theory result of Luther and Peschel at $q \approx \pi$. As Müller et al. noted themselves, their formula could not be exact, not only because it cannot satisfy all the sum rules simultaneously, but also because it does not account for the spectral weight above the upper boundary of the two-spinon continuum, which was clearly seen in the numerical results. Nonetheless, the Müller ansatz proved quite useful in analyzing experimental data [69]. A generalization of the Müller ansatz for the XXZ chain in the gapless regime was presented in [70].

Later it was shown that the dynamical structure factor for the related Haldane-Shastry model (isotropic spin-1/2 chain with long range $1/r^2$ interaction) can be calculated exactly [71]. This model is equivalent to a gas of noninteracting spinons, therefore only two-spinon excitations contribute to $S^{zz}(q, \omega)$. Interestingly, the exact result for $S^{zz}(q, \omega)$ of the Haldane-Shastry model coincides with the Müller ansatz, although the expressions for the thresholds of the two-spinon continuum are different.

Substantial progress was made in 1996 when Bougourzi et al. [72] applied quantum group methods developed by Jimbo and Miwa [73] and calculated the exact two-spinon contribution to $S^{zz}(q, \omega)$ for the Heisenberg model at zero field. Their solution exploits the infinite symmetry of the XXZ chain in the massive Néel phase directly in the thermodynamic limit. The expression for the form factors for the two-spinon states are obtained by taking the
limit $\Delta \to 1$ from above. The two-spinon dynamical structure factor [74] is illustrated in Fig. 1.5. Although more complicated than the Müller ansatz, this result confirms a square root divergence, accompanied by a logarithmic correction, at the lower edge of the two-spinon continuum. At the upper edge, however, the two-spinon contribution vanishes in a square-root cusp. Note that this is still not the full solution for the Heisenberg chain, since four and higher spinon states also contribute to $S^{zz}(q, \omega)$, but there are no analytic formulas for the corresponding form factors. However, the exact two spinon result by itself is a good approximation because it accounts for 72.89% of the total spectral weight in the integrated intensity [74]. In fact, the two-spinon solution was shown to be in better agreement with experiments than the Müller ansatz [14], since the latter overestimates the spectral weight at the upper boundary of the two-spinon band.

The solution of Bougourzi et al. is not applicable in the gapless regime of the XXZ chain. Moreover, there are no such analytical results for the Heisenberg chain at nonzero magnetic field. However, more recently a method based on the Algebraic Bethe Ansatz (or Quantum Inverse Scattering Method [19]) was developed which allows one to derive determinant expressions for form factors between Bethe ansatz eigenstates for finite chains [75]. These expressions can be evaluated numerically for fairly large chains (of the order of a few hundred sites in most cases). By focusing on the dominant classes of eigenstates, the dynamical structure factors can be computed numerically for arbitrary values of anisotropy and field [76]. The main drawback of this approach are strong finite size effects.

Remarkably, the study of dynamical correlation functions had advanced more on the Bethe ansatz front than on the field theoretical one, which had been so fruitful in the calculation of thermodynamic properties and equal-time correlations. At the time the research reported here was started, a field theory interpretation of the emergence of a two-particle continuum with edge singularities having the Luttinger model as the starting point was still missing.

1.7 Beyond the Luttinger liquid paradigm

The calculation of the dynamical structure factor exposes a limitation of the Luttinger model as the effective field theory for the XXZ spin chain. The peak in the line shape of $S^{zz}(q, \omega)$ for small $q$ is infinitely sharp because the
Figure 1.5: Two approximations for the dynamical structure factor $S^{zz}(q, \omega)$ for the Heisenberg chain at zero magnetic field. Dashed line: Müller ansatz (analytic expression given in [67]). Solid line: exact two-spinon contribution (calculated numerically using equations in [74]).
Luttinger model is Lorentz invariant, implying that the bosonic excitations propagate ballistically with velocity $v$. Lorentz invariance is not a symmetry of the original lattice model; it only emerges in the low-energy limit. In order to obtain a peak with finite width, it is necessary to go beyond the free boson picture and treat irrelevant interactions properly. This turns out to be a nontrivial task, because simple perturbation theory in the irrelevant operators can lead to infrared divergences [77].

The problem of the finite width of the dynamical structure factor also appears in the context of electron transport in quasi-1D wires. The related quantity there is the imaginary part of the density-density correlation function. It was pointed out in [78] that, as a consequence of the linear dispersion approximation, the Luttinger model does not account for the leading contribution to the Coulomb drag response between quantum wires with different electronic densities. Following an alternative route to bosonization, Pustilnik et al. [79] studied the dynamical structure factor for spinless fermions with parabolic dispersion using perturbation theory in the interaction. This problem is analogous to the spin chain at finite magnetic field in the limit $\Delta \ll 1$. The fermionic approach to calculate $S^{zz}(q, \omega)$ treats band curvature exactly, but faces logarithmic divergences which appear in all orders of perturbation theory. The divergences can be dealt with by using a formalism developed in the study of X-ray edge singularities in metals [80]. Pustilnik et al. found that the most striking effect of interactions on the dynamical structure factor is to induce power-law singularities at the thresholds of the particle-hole continuum. The $q$-dependent exponents are not clearly related to any previously known exponents calculated in Luttinger liquid theory. Interestingly, an extrapolation of the results of Pustilnik et al. to strong interactions seemed very promising since the asymmetric line shape that results from their approach is reminiscent of the one expected for spin chains. However, the two-spinon result for the Heisenberg point suggests that the exponents should be independent of momentum in the zero field (particle-hole symmetric) case.

The limitations of the Luttinger model are even more critical when it comes to correlation functions at finite temperature. In general, one expects that at finite temperature inelastic scattering will generate a finite decay rate for the quasiparticles of an interacting system. In the Luttinger model, however, the dynamical structure factor for small $q$ remains a delta function peak for $T > 0$. This means that the bosonic modes still propagate ballistically in the scaling limit [57]. The question then is whether this remains true
once we include irrelevant interactions between the bosons. Surprisingly, the answer seems to depend on high-energy properties such as the integrability of the lattice model. One way to probe the propagation of excitations is by means of transport properties. It is now well accepted that the dc heat conductivity calculated using the Kubo formula [81] should be infinite for the XXZ model because the heat current operator is a nontrivial conserved quantity [82]. Indeed, experiments show that the mean free path for thermal transport in spin chain compounds is limited by spin defects, rather than intrinsic scattering between spinons [83].

The problem of spin transport (equivalent to charge transport in the fermionic version) is less clear. The spin current operator does not commute with the Hamiltonian, except in the trivial noninteracting case (the XY model). Nonetheless, Zotos et al. [82] have conjectured that the spin Drude weight, defined as the coefficient of the delta function peak in the conductivity at zero frequency, should be finite for integrable models. A finite Drude weight implies an infinite dc spin conductivity at finite temperatures. This means that the existence of nontrivial conserved quantities should protect the ballistic propagation of the excitations. So far it has not been possible to address this question using field theory methods because not much is known about the role of integrability in low-energy effective models. It has been suggested that, contrary to the conjecture, a finite Drude weight could be generic to 1D models which have the Luttinger model as fixed point [84]. However, this conclusion cannot be correct because, as pointed out in [85], the presence of certain irrelevant interactions neglected in [84] can make the Drude weight vanish, rendering the conductivity finite.

Evidence for a diffusive behavior in Heisenberg spin chains has been claimed in [86]. By doing oxygen NMR in Sr$_2$CuO$_3$, Thurber et al. were able to separate the contribution from the low-energy modes with $q \approx 0$ to the spin-lattice relaxation rate $1/T_1$. The Luttinger model predicts that $1/(T_1T)$ is given by a magnetic-field-independent constant at low temperatures. However, the experiment suggested that $1/(T_1T)$ diverges with decreasing field as $1/\sqrt{\omega_n} \propto h^{-1/2}$, where $\omega_n$ is the nuclear magnetic resonance frequency. This is a signature of diffusive behavior, which is well established in higher dimensions [87]. The frequency dependence of the NMR response is related to the long-time decay of short distance spin correlations, in particular the self-correlation function $\langle S_j^z(t)S_j^z(0) \rangle$. In one dimension, diffusive behavior is equivalent to a $1/\sqrt{t}$ decay of the self-correlation function. This is not
the result expected within the Luttinger model, but the long-time behavior is not necessarily determined by low-energy modes. Apparently, spin diffusion conflicts with the picture of ballistically propagation bosons which is the basis of the Luttinger liquid paradigm. It also seems to contradict the conjecture about ideal transport in integrable spin chains. If correct, this experimental result could change the way we think about excitations of 1D models. Understanding the behavior of time-dependent correlation functions at zero temperature constitutes an important step towards answering these questions.

1.8 Overview

This thesis is a theoretical study of various aspects of the longitudinal dynamical structure factor for the XXZ model at zero temperature. Our goal was to derive analytic formulas for the width, tail and edge singularities of $S_{zz}(q, \omega)$ which are nonperturbative in the anisotropy parameter $\Delta$ and therefore hold in the entire critical region of the phase diagram. This could only be accomplished by combining field theory methods with the exact Bethe ansatz solution in ways that had not been explored before.

The next chapters are organized as follows. Chapter 2 focuses on the broadening of the on-shell peak of $S_{zz}(q, \omega)$ at finite magnetic field and in the limit of small $q$. By treating the leading irrelevant operators which account for band curvature effects, I show that the width of the on-shell peak scales as $q^2$ in the interacting case, similarly to the exact result for the XY model. I relate the coefficient of the $q^2$ dependence to a coupling constant of the low-energy effective model which can be calculated using the Bethe ansatz solution. This provide a formula for the width of $S_{zz}(q, \omega)$ at finite field which is asymptotically exact in the limit of small $q$. Another important result in this chapter is that the line shape which arises from adding boson decay processes to the Luttinger model is not a Lorentzian. Within the approximation which neglects dimension-four and higher irrelevant operators, the peak has a rectangular shape with well-defined lower and upper thresholds. These are identified with the energy thresholds for the creation of particle-hole pair excitations in the Bethe ansatz solution. In Chapter 3, I show that the low-energy effective theory with irrelevant operators can also account for the spectral weight above the upper threshold of the particle-hole continuum. Besides deriving formulas for the high-frequency tail of $S_{zz}(q, \omega)$
at both zero and finite magnetic field, I show that integrability affects the line shape of $S^{zz}(q, \omega)$ at zero field in a noticeable way. This is because the conservation of the energy current operator rules out a boson decay process which, if present in the effective Hamiltonian, would modify the high-frequency tail near the upper threshold of the two-particle continuum. The question of what happens at the thresholds of the two-particle continuum is addressed in Chapter 4. I apply the afore mentioned analogy with the X-ray edge problem and derive an effective Hamiltonian to study the edge singularities of $S^{zz}(q, \omega)$. The results in this chapter are not restricted to low energies and small $q$. The main result there is the derivation of exact formulas for the singularity exponents in terms of phase shifts which can be extracted from the Bethe ansatz equations. This approach reproduces the singularities of the two-spinon dynamical structure factor for the Heisenberg chain as a special case. In addition, I show that the edge singularities govern the long-time behavior of the self-correlation function. I prove that the leading term in the long-time asymptotics is not the one given by the Luttinger liquid result, but involves high-energy particle-hole excitations near the top and bottom of the band. Finally, in Chapter 5 I make some concluding remarks and suggestions for future research.
Bibliography


Chapter 2

Broadening of the dynamical structure factor by boson decay

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