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SU(3) Lattice Gauge Theories and Spin Chains

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Abstract

I modelli su reticolo con simmetrie $SU(n)$ sono attualmente oggetto di studio sia dal punto di vista sperimentale, sia dal punto di vista teorico; particolare impulso alla ricerca in questo campo è stato dato dai recenti sviluppi in campo sperimentale per quanto riguarda la tecnica dell'intrappolamento di atomi ultrafreddi in un reticolo ottico. In questa tesi viene studiata, sia con tecniche analitiche sia con simulazioni numeriche, la generalizzazione del modello di Heisenberg su reticolo monodimensionale a simmetria $SU(3)$. In particolare, viene proposto un mapping tra il modello di Heisenberg $SU(3)$ e l'Hamiltoniana con simmetria $SU(2)$ bilineare-biquadratica con spin 1. Vengono inoltre presentati nuovi risultati numerici ottenuti con l'algoritmo DMRG che confermano le previsioni teoriche in letteratura sul modello in esame. Infine è proposto un approccio per la formulazione della funzione di partizione dell'Hamiltoniana bilineare-biquadratica a spin-1 servendosi degli stati coerenti per $SU(3)$.

Contents

Introduction

SU(n) gauge theories are of fundamental importance in the description of a wide variety of physical phenomena: the interactions of a great zoology of elementary particles can be described by means of those symmetries. Some well known examples are SU(3), which is the gauge-symmetry of QCD, and SU(6), which has been proposed to describe spinful quarks.

One way to extrapolate information about a lattice theory is to map it into a field theory defined on a continuous space, using a semiclassical approximation. For gauge theories, also the opposite happens, since often these theories are studied not only in the continuum, but also on a discretized lattice. In this way, it is possible to analyze gauge theories from a statistical mechanical point of view, with all the tools and techniques that statistical mechanics provides [31]. In this sense, the definition of gauge theories on a lattice constitutes a bridge between high energy physics, which requires a deep knowledge of continuous gauge theories, and condensed matter physics, whose one of main topics of interest is the study of theories defined on a discretized space. This parallelism has become recently even more important, due to the striking progresses in the field of experiments with ultracold atoms in an optical lattices [8] [24]. Trapping fermionic alkaline-earth atoms (usually some isotopes of Ytterbium or Strontium) in an optical lattice, it is possible to realize a physical system whose effective Hamiltonian presents a SU(n) symmetry. This experimental technique is very powerful since by tuning the parameters of the system it is possible to reproduce a wide variety of Hamiltonians. In this sense, these experiments may be used in order to simulate high energy phenomena on a lattice, constituting in this way a good example of quantum simulator.

From a theoretical point of view, the formalism usually used in the definition of spin chains - that is, 1-dimensional lattice models with SU(2) symmetry - can be easily generalized to SU(n) degrees of freedom, and, in this sense, it is possible to formulate SU(n) generalizations of the SU(2) quantum Hamiltonians which has been studied so much in the literature [7, 19, 22, 27]. These generalizations are based on the substitution of SU(2) generators in the explicit formulation of the Hamiltonian with the proper ones of the SU(n) group. One typical example is the

case of the antiferromagnetic Heisenberg model, which has been generalized for a set of SU(n) degrees of freedom [1–3, 38, 39].

SU(2) Heisenberg model has been studied thoroughly since it is very useful in order to describe magnetic quantum systems with nearest-neighbour interactions. In the study of the path integral formulation of the partition function for the SU(2) chain, the presence of a topological term, the so called Berry Phase, is of outmost importance in order to determine the behaviour of the system. Indeed, this topological term is the one that, through the continuum limit semiclassical approximation, makes the system critical or massive depending on the value (half-integer or integer) of the spin, as argued by Haldane [27]

An analogous statement holds for SU(n) antiferromagnetic Heisenberg Hamiltonians: a topological term appears in the path integral of the partition function, and the value it takes has a great influence on the behaviour of the system. The main difference between the SU(2) and a generic SU(n) Heisenberg model is that the possible irreducible representations for SU(n) - the equivalent of the spin for SU(2) - have a reacher structure than the ones for the SU(2) case, making the semiclassical approximation more complex. In this sense, the choice of the SU(n) representation is of fundamental importance in order to determine the behaviour of the system.

The focus of this thesis is on the SU(3) generalization of the quantum antiferromagnetic Heisenberg Model. As highlighted before, SU(3) is the gauge group of QCD. In particular, the quarks up, down and strange are organized according to the fundamental representation of SU(3), while their respective antiparticles form an antifundamental representation of the same group. In this sense, when studying a quantum "spin" Hamiltonian with SU(3) degrees of freedom on the sites of the lattice, in the fundamental or antifundamental representation, a good picture is to interpret the degrees of freedom on the chain as interacting particles (antiparticles) confined on a lattice. If we want to stick to this picture, that is, if we are interested in the fundamental and antifundamental representations of the SU(3) group, there are two possible inequivalent formulations of the Heisenberg Hamiltonian. In the first, on each site there is a particle (fundamental representation), while in the second particles and antiparticles are alternated on odd and even sites respectively (so, fundamental and antifundamental representations are alternated). This, of course, changes not only the explicit formulation of the Hamiltonian, but also the quantum numbers of the system.

The SU(3) Heisenberg antiferromagnetic model with the fundamental representation on the whole chain has been studied in literature; it has been shown to be critical with central charge $c = 2$ [2, 5], as confirmed by numerical results [5]. One interesting feature of this model is that it can be mapped into a spin-1 chain [5], the well known Lai-Sutherland model, which had already been inferred to present

a SU(3) symmetry [2]. This correspondence makes it possible to apply all the known results about the Lai-Sutherland chain to the SU(3) Hamiltonian.

As highlighted before, the choice of the representations of the SU(3) group used in the defintion of the SU(3) antiferromagnetic Heisenberg problem, is of main importance for the behaviour of the system. Indeed, if we chose to use not the fundamental representation on each site, but to alternate fundamental and antifundamental representations on odd and even sites of the chain, the physics of the system changes dramatically. A model which has been argued to have a SU(3) symmetry with alternated representations is the spin-1 biquadratic chain [14]; this system has been proved analytically to be gapped [29, 30], though its gap is so small that numerical studies on this model have often been tricky, since it could easily seem to be in a critical phase in a finite-length numerical study [11, 42].

In this work, an explicit mapping between SU(3) operators and spin-1 matrices is proposed. It makes evident the correspondence between the antiferromagnetic SU(3) Heisenberg model and spin-1 chains in both the formulation of the SU(3) Hamiltonian. Since both the Lai-Sutherland model and the biquadratic chain are particular cases of a more general spin-1 Hamiltonian depending on a parameter α, this mapping could be useful in order to study how the SU(3) symmetry appears and disappears varying α. In this perspective, we propose a path integral formulation of the partition function of the more general spin-1 system, formulated in terms of SU(3) generators, which could, in principle, be the starting point to find the continuum field theory underlying the spin system for any value of the parameter α.

It should be stressed that the SU(3) Heisenberg model with alternated representations has not been investigated numerically in the literature in its usual formulation, though there are many numerical works about its spin-1 analogue, the biquadratic chain [11, 14, 42]. In this work, we present some new numerical results obtained with the DMRG algorithm. Since the map we propose allows us to apply all the known results about the biquadratic spin-1 chain to the SU(3) model under study, we compare our results with the one expected from the spin-1 chain. Our estimates of the gap and of the ground-state energy are in perfect correspondence with the theoretical ones, confirming once again the equivalence between the SU(3) and the spin-1 system.

This thesis is organized as follows:

- Since our aim is to study SU(n) lattices models, an introduction to SU(n) group is given in the first chapter, with particular emphasis on SU(3), which is the group we are more interested in.

- Chapter 2 is devoted to the description of the SU(2) Heisenberg Chain; the methodology described in order to find the partition function of the model

in its path integral formulation and the continuum limit turns out to be very useful, since the SU(n) Hamiltonian can be treated in an analogous way.

- In Chapter 3 an introduction to the experimental and theoretical approach to SU(n) systems is provided, in order to stress the importance of the problem and to give an highlight on the results known about this wider class of systems.

- The possibility of defining more than one non-equivalent SU(3) Heisenberg Hamiltonians is discussed in Chapter 4. The possible formulations of a SU(3)-symmetric Heisenberg Hamiltonian are described, and some highlights on their structure and feature is given. An explicit mapping between spin-1 operators and SU(3) generators is given, which allows us to apply all the known results about a wide set of spin-1 chains to SU(3)-symmetric systems. New numerical results about the SU(3) antiferromagnetic Heisenberg model with alternate representations on even and odd sites are discussed. Finally, an alternative approach to the path integral formulation of the SU(3) Heisenberg model is proposed and discussed.

Chapter 1

SU(n) groups

In this chapter SU(n) groups are defined and introduced [26]. Some basic general features of this class of groups is described and a notation quite common in physics is introduced. SU(2) and SU(3) are described in more detail, due to their fundamental importance in many fields of physics; for SU(3) particular importance is given to its representations. Moreover, when studying SU(n) groups and their representations, Young Tableau provide a powerful method to describe and catalogue representations for these groups; they will be described briefly in the last section of this chapter.

1.1   Some general properties

The SU(n) symmetry group is the group given by $n \times n$ unitary matrices with determinant equal to one. It may be shown that it is a simple Lie group (and so, it is also semisimple). It is clear that the definition itself provides a representation of the group (in terms, of course, of $n \times n$ special unitary matrices), which is called defining representation. The generators of the defining representation can be found considering that every $n \times n$ unitary matrix U can be expressed in the following form:

$$U = \mathrm{e}^{M}, \tag{1.1.1}$$

with M a $n \times n$ antihermitian matrix, which by definition has n^2 independent real parameters. If we require $\det(U)$ to be equal to one, M has to be traceless because:

$$\det(U) = \det(\mathrm{e}^{M}) = \mathrm{e}^{\mathrm{Tr}[M]} = 1 \qquad \Rightarrow \qquad \mathrm{Tr}[M] = 0 \tag{1.1.2}$$

Antihermitian traceless matrices depend on $n^2 - 1$ real parameters; it means that also U depends on the same number of parameters, which constitutes the dimension of the Lie group, equal to the number of its generators (in each of its

representations). The Lie algebra $\mathfrak{su}(n)$ is given by the set of $n \times n$ traceless anti-hermitian matrices. Every traceless hermitian matrix can be expressed by a linear combination of the generators of SU(n), weighted by $n^2 - 1$ real parameters:

$$M = \sum_{i=1}^{n^2-1} \theta_i I_i \qquad \theta_i \in \mathbb{R} \qquad (1.1.3)$$

It should be noticed that the unitary group has precisely the same generators of SU(n) plus the Identity (as we said before, U(n) is a Lie group of dimension n^2); it is only the presence or absence of the identity operator in the set of generators of the algebra that makes the difference between the unitary group and its special subgroup.

The generators of SU(n) follow the $\mathfrak{su}(n)$ algebra (the explicit values of the structure constants depend upon the specific group):

$$[I_i, I_j] = c_{ijk} I_k \qquad (1.1.4)$$

Quite often however, relation (1.1.1) is rewritten in the form - which resembles a rotation in the complex plane:

$$U = \mathrm{e}^{iH} \qquad (1.1.5)$$

Due to the presence of the imaginary unity at the exponential, H is an hermitian traceless matrix, still depending on $n^2 - 1$ real parameters, so that we can write it, analogously as in (1.1.3):

$$H = \sum_{i=1}^{n^2-1} \theta_i F_i \qquad \theta_i \in \mathbb{R} \qquad (1.1.6)$$

The F_i in (1.1.6) are a set of $n^2 - 1$ hermitian traceless $n \times n$ matrices which fulfill the commutation relations:

$$[F_i, F_j] = iC_{ijk} F_k \qquad (1.1.7)$$

It is quite common to refer to the F_i in (1.1.6) and (1.1.7) as generators of SU(n), though this definition is slightly different from the formal one; quite analogously, we will refer to (1.1.7) as $\mathfrak{su}(n)$ algebra, though the formal definition is given by (1.1.4).

It is worth noticing that:

$$SU(n) \subseteq SU(m) \qquad n, m \in \mathbb{N} \qquad n \leq m \qquad (1.1.8)$$

That is beacuse it is always possible to write a $m \times m$ unitary matrix starting from a $n \times n$ one:

$$U_{m \times m} = \begin{pmatrix} U_{n \times n} & \mathbf{0}_{(m-n) \times n} \\ \mathbf{0}_{n \times (m-n)} & \mathbb{I}_{(m-n) \times (m-n)} \end{pmatrix}$$

The associate $m \times m$ hermitian matrix is then in the form:

$$H_{m \times m} = \begin{pmatrix} H_{n \times n} & \mathbf{0}_{(m-n) \times n} \\ \mathbf{0}_{n \times (m-n)} & \mathbf{0}_{(m-n) \times (m-n)} \end{pmatrix}$$

1.2 SU(2) symmetry group

1.2.1 Generators and commutation relations

SU(2) is the group of 2×2 special unitary matrices. From section (1.1), we know that the numbers of the generators of SU(2) is equal to $n^2 - 1\big|_{n=2} = 3$. The most common choice for the generators of the defining (or fundamental) representation is:

$$F_i = \frac{1}{2}\sigma_i \qquad i \in \{1, 2, 3\} \tag{1.2.1}$$

In (1.2.1), σ_i are the well known Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.2.2}$$

The F_i matrices follow the $\mathfrak{su}(2)$ algebra:

$$[F_i, F_j] = i\varepsilon_{ijk}F_k \qquad i, j, k \in \{1, 2, 3\} \tag{1.2.3}$$

ε_{ijk} is the Levi-Civita completely antisymmetric tensor. The Casimir operator of the group for the defining representation is:

$$F^2 = F_1^2 + F_2^2 + F_3^2 \tag{1.2.4}$$

By definition, it commutes with all the generators:

$$[F^2, F_i] = 0 \tag{1.2.5}$$

More generally, the Casimir operator of SU(2) may be expressed in any representation as the square sum of the three generators.

1.2.2 SU(2) and spin

SU(2) symmetry group is one of the most important groups in physics, because spin degrees of freedom can be described in terms of the SU(2) group. The most simple case is the one of $\frac{1}{2}$-spin, which corresponds to the fundamental representation; $\frac{1}{2}$-spin operators, up to some constants, are the Pauli matrices:

$$S_i = \frac{1}{2}\hbar\sigma_i \tag{1.2.6}$$

Of course, $\mathfrak{su}(2)$ algebra (1.2.3) holds for these operators.

Different representations correspond to different values of the Casimir operator, that is, different values for the total square spin. The three spin operators do not commute, due to the $\mathfrak{su}(2)$ algebra, so they can not be diagonalized at the same time; spin states are labeled by the eigenvalues of the Casimir operator S^2 (labeled with S), and of just one of the spin operators, usually S_3 (labeled with s); s may only assume values between $-S$ and $+S$ in steps equal to one [23].

$$
\begin{aligned}
S^2|S,s\rangle &= \hbar^2 S(S+1)|S,s\rangle \\
S_3|S,s\rangle &= \hbar s|S,s\rangle
\end{aligned}
\tag{1.2.7}
$$

Often in physics representations of SU(2) are labelled by means of spin. When calculating the direct product of SU(2) representations, the Clebsh-Gordan series describes how spin combine into different ones, for example:

$$\left\{\frac{1}{2}\right\} \otimes \left\{\frac{1}{2}\right\} = \{0\} \oplus \{1\} \tag{1.2.8}$$

The $\{0\}$ representation corresponds to a 1-dimensional SU(2) representation, with a unique spin state $|0,0\rangle$, while the $\{1\}$ representation corresponds to a 3-dimensional representation of SU(2), and so on; from a physical point of view, the global spin of a system formed by two $\frac{1}{2}$-spin particle can have $S=1$ or $S=0$.

The SU(2) generators may also be expressed in a form which is very useful when applied to spin: S_1 and S_2 can be substituted by two other operators S_+ and S_-, defined as

$$
\begin{aligned}
S_+ &= S_1 + iS_2 \\
S_- &= S_1 - iS_2
\end{aligned}
\tag{1.2.9}
$$

These two operators are called ladder operators [23]; they have the following peculiar feature:

$$S_\pm|S,s\rangle = \hbar\sqrt{S(S+1) - s(s\pm 1)}|S,s\pm 1\rangle \tag{1.2.10}$$

The action of S_+ and S_- on a state gives the null vector in case lowering or raising the S_3 eigenvalue s makes it have a value which is not allowed in the representation we have chosen. $\mathfrak{su}(2)$ algebra can be written, in terms of these operators, as:

$$\begin{aligned} [S_\pm, S_3] &= i\hbar S_\pm \\ [S_+, S_-] &= 2\hbar S_3 \end{aligned} \qquad (1.2.11)$$

In the following, when dealing with spin operators, we will consider $\hbar = 1$.

1.3   SU(3) symmetry group

1.3.1   Generators and commutation relations

SU(3) is the group of 3×3 special unitary matrices; the number of its generator is equal to $n^2 - 1\big|_{n=3} = 8$. The most common choice for the generators in the defining (or fundamental) representation of the group is:

$$F_i = \frac{1}{2}\lambda_i \qquad (1.3.1)$$

In (1.3.1), λ_i are the so called Gell-Mann Matrices; their explicit formulation is:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$\lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \qquad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \qquad (1.3.2)$$

It can be easily seen how λ_1, λ_4 and λ_6 can be obtained from σ_1 - the first one of the Pauli Matrices (1.2.2) - just shifting in the proper way its elements inside a $3{\times}3$ matrix. The same happens for λ_2, λ_5, λ_7, which can be easily related to σ_2. λ_3 and λ_8 play the role of σ_3, being diagonal traceless matrices.

The eight generators fulfill the $\mathfrak{su}(3)$ algebra:

$$[F_i, F_j] = i f_{ijk} F_k \qquad (1.3.3)$$

The structure constant of $\mathfrak{su}(3)$ can be calculated [26] and their value is:

$$f_{123} = 1 \qquad f_{147} = f_{246} = f_{257} = f_{345} = \frac{1}{4}$$

$$f_{156} = f_{367} = -\frac{1}{2} \qquad f_{458} = f_{678} = \frac{\sqrt{3}}{2}, \qquad (1.3.4)$$

all the others being null or obtainable by a cyclic permutation of the indices of these ones.

As SU(2) is a subgroup of SU(3), it is easy to find that particular combinations of the Gell-Mann Matrices fulfill the $\mathfrak{su}(2)$ algebra. Let us now define a set of operators, which resemble in form the ladder operators usually found when studying SU(2) symmetric systems, and which will be very helpful in the study of SU(2) as subgroup of SU(3):

$$X = X^\dagger = \lambda_3 \qquad\qquad Y = Y^\dagger = \sqrt{3}\lambda_8$$

$$T = \frac{\lambda_1}{2} - i\frac{\lambda_2}{2} \qquad\qquad T^\dagger = \frac{\lambda_1}{2} + i\frac{\lambda_2}{2}$$

$$U = \frac{\lambda_6}{2} - i\frac{\lambda_7}{2} \qquad\qquad U^\dagger = \frac{\lambda_6}{2} + i\frac{\lambda_7}{2}$$

$$V = \frac{\lambda_4}{2} + i\frac{\lambda_5}{2} \qquad\qquad V^\dagger = \frac{\lambda_4}{2} - i\frac{\lambda_5}{2} \qquad (1.3.5)$$

The matrices (1.3.5) commute as described in table (1.1).

$[X,Y] = 0$	$[Y,T] = [Y,T^\dagger] = 0$	$[T,U] = -V^\dagger$
$[T,U^\dagger] = 0$	$[T,V] = U^\dagger$	$[T,V^\dagger]$
$[T^\dagger,U] = 0$	$[T^\dagger,U^\dagger] = V$	$[T^\dagger,V] = 0$
$[T^\dagger,V^\dagger] = -U$	$[U,V] = -T^\dagger$	$[U,V^\dagger] = 0$
$[U^\dagger,V] = 0$	$[U^\dagger,V^\dagger] = T$	$[T,T^\dagger] = -X = -2T_3$
$[X,T] = -2T$	$[X,T^\dagger] = 2T^\dagger$	$[X,U] = U$
$[Y,U] = -3U$	$[X,U^\dagger] = -U^\dagger$	$[Y,U^\dagger] = 3U^\dagger$
$[U,U^\dagger] = \frac{X}{2} - \frac{Y}{2} = -2U_3$	$[X,V] = V$	$[Y,V] = 3V$
$[X,V^\dagger] = -V^\dagger$	$[Y,U^\dagger] = -3V^\dagger$	$[V,V^\dagger] = \frac{X}{2} + \frac{Y}{2} = -2V_3$

Table 1.1: Commutation relations for the U, V, T operators

It must be noticed that we have chosen a notation slightly different from the usual one (in which $Y = \lambda_8$, keeping the factor $\frac{1}{\sqrt{3}}$ present in the definition of the eighth Gell-Mann Matrix, and the relations in tab.(1.1) change consequently). From (1.1) it is easy to verify that three $\mathfrak{su}(2)$ algebras live in SU(3), having as ladder operators U and $U^\dagger$, V and $V^\dagger$, T and $T^\dagger$ respectively. Being ladder operators,

we expect these six operators to act upon some quantum numbers, making them higher or lower; the quantum numbers we are looking for are the eigenvalues of the X and Y matrices. From (1.1), it is apparent that X and Y are two commuting operators; this means that these two matrices can be simultaneously diagonalized, and their eigenvalues are, in this sense, good quantum numbers. We will name these eigenvalues as x and y respectively, and by means of them we will label the states of the defining representation of SU(3). Indeed, it can be shown that $T(T^\dagger)$ lowers (raises) x by two, $U(U^\dagger)$ raises (lowers) x by one and lowers(raises) y by three, $V(V^\dagger)$ raises (lowers) x by one and raises (lowers) y by three. It must kept in mind that these quantum numbers have a limited set of possible values, corresponding to different eigenvalues of X and Y; when the action of a ladder operator on a state would lower or raise a quantum number to a value which is not in the set of the allowed ones, the resulting state is null, exactly as happens in the case of the ladder operators of a $\mathfrak{su}(2)$ algebra.

From commutation relations in table (1.1), it is quite evident that the rank of the group is equal to two. Since SU(3) is a simple Lie group, Racah's theorem states that this group is provided with two Casimir operators, which, in the fundamental representation, are:

$$K_1(F_1, \ldots, F_8) \;=\; \sum_{i=1}^{8} F_i^2 \tag{1.3.6}$$

$$K_2(F_1, \ldots, F_8) \;=\; \sum_{i,j,k=1}^{8} d_{ijk} F_i F_j F_k \tag{1.3.7}$$

The coefficients d_{ijk} appearing in (1.3.7) are related to the anticommutation relations between Gell-Mann matrices, and may be found keeping in mind that:

$$\{\lambda_i, \lambda_j\} = \frac{4}{3}\delta_{ij}\mathbb{I} + 2d_{ijk}\lambda_k \tag{1.3.8}$$

Of course, the formulation (1.3.6) and (1.3.7) can be generalized to more complex representations of the group.

1.3.2   SU(3) representations

Before giving some explicit examples of irreducible SU(3) representations, it is useful to have some general insight of how these representations may be built. Our starting point is constituted by the U, V, and T algebras. SU(3) multiplets can be constructed from SU(2) multiplets of each of the three subalgebras U, V and T; due to the commutation relations (1.1), these SU(2) multiplets should be coupled one to another in order to obtain a SU(3) multiplet. Moreover, being these three

$\mathfrak{su}(2)$ algebras completely equivalent - there is no reason to prefer one to the others - we expect this symmetry to be reflected in the graphic depiction on a plane of the states of any representation (with the two cartesian axes corresponding to the eigenvalues of the generators which play the role of X and Y in that representation), which should have the shape of a regular hexagon or triangle, due to the way the ladder operators act on the states and on the symmetry of their action [26].

Of course the simplest representation fulfilling all these requirements is the singlet $\{1\}$, constituted by one unique state with quantum numbers ($x = 0, y = 0$), as can be seen in fig.(1.1).
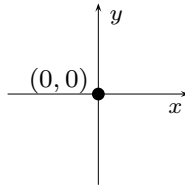

Figure 1.1: Singlet representation of the SU(3) group

The two basic multiplet representations of SU(3) are given by the fundamental representation $\{3\}$ (fig. (1.2))and the and the antifundamental one $\{\overline{3}\}$ (fig. (1.3)). In the case of $\{3\}$, it is apparent how the three states, which in the particle physics language are called up (u), down (d) and strange (s) respectively, are labeled by the eigenvalues of the operators X and Y: as we said before, the F_i defined in (1.3.1) from the Gell-Mann matrices are the generators of the fundamental (defining) representation. Through the ladder operators, T ($T^\dagger$), U ($U^\dagger$) and V ($V^\dagger$) described in the previous section it is possible to get from one state to another as in fig. (1.2).

The antifundamental representation is defined as the conjugate of the fundamental one. Its generators can be found explicitly in a quite straightforward way [26]. As we have seen from (1.1.1), (1.1.2) and (1.1.6), a SU(3) transformation in its defining (fundamental) representation, can be written as:

$$U = \mathrm{e}^{iH}, \qquad\qquad H = \sum_{a=1}^{8} \theta_a F_a, \qquad\qquad \theta_a \in \mathbb{R} \qquad\qquad (1.3.9)$$

Its conjugate transformation may be written as:

$$\overline{U} = U^* = \mathrm{e}^{-iH^*} \qquad\qquad H^* = \sum_{a=1}^{8} \theta_a F_a^*, \qquad\qquad \theta_a \in \mathbb{R} \qquad\qquad (1.3.10)$$
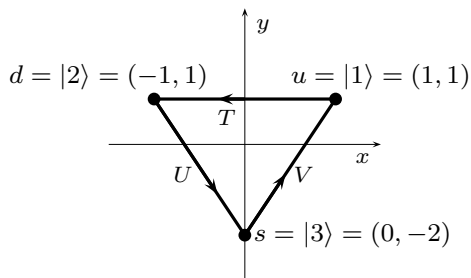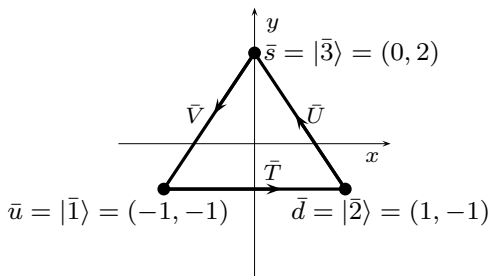
Figure 1.2: Representation $\{3\}$ Figure 1.3: Representation $\{\overline{3}\}$

From (1.3.10) it is quite straightforward to take as generators for the antifundamental representation the set of matrices $\overline{F} = \frac{\overline{\lambda}_i}{2}$, which may be defined starting from Gell-Mann matrices as:

$$\overline{\lambda}_i = -\lambda_i^* \qquad\qquad i \in \{1, ..., 8\} \qquad\qquad (1.3.11)$$

In this new set of generators, the role of X and Y is played by

$$\overline{X} = \overline{\lambda}_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad\qquad \overline{Y} = \sqrt{3}\overline{\lambda}_8 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad (1.3.12)$$

From fig. (1.3) it is now clear that the states of the antifundamental representation are labeled by the eigenvalues of $\overline{X}$ and $\overline{Y}$, precisely as happens for the fundamental one; quite analogously, $\overline{T}$ $(\overline{T}^\dagger)$, $\overline{U}$ $(\overline{U}^\dagger)$ and $\overline{V}$ $(\overline{V}^\dagger)$ (defined as in (1.3.5) substituting λ_i with $\overline{\lambda}_i$) make it possible to shift from one state to another as represented in fig. (1.3).

Being the fundamental and the antifundamental representations one the conjugate of the other (the states of the $\{\overline{3}\}$ can be found by changing the sign of the coordinates of the ones of the $\{3\}$), often the states of the antifundamental representation are referred to as antiparticles, and are called antiup ($\overline{u}$), antidown ($\overline{d}$) and antistrange ($\overline{s}$) respectively.

Irreducible representations of different dimensions are related one to the other through Clebsch-Gordan series. Some examples are:

$$\begin{aligned} \{3\} \otimes \{\overline{3}\} &= \{1\} \oplus \{8\} \\ \{3\} \otimes \{3\} &= \{6\} \oplus \{\overline{3}\} \end{aligned} \qquad (1.3.13)$$

In figures (1.4), (1.5), (1.6), (1.7), (1.8) some of the lowest dimensional representations are depicted; x and y on the two axes represent the eigenvalues of the

d-dimensional operators that play the role of X and Y in the d-dimensional representation depicted. If there are one or more circles around a certain point of the graph, it means that there are more than one state with the same coordinates. Of course, there is no upper limit to the dimension of irreducible representations that we can find.
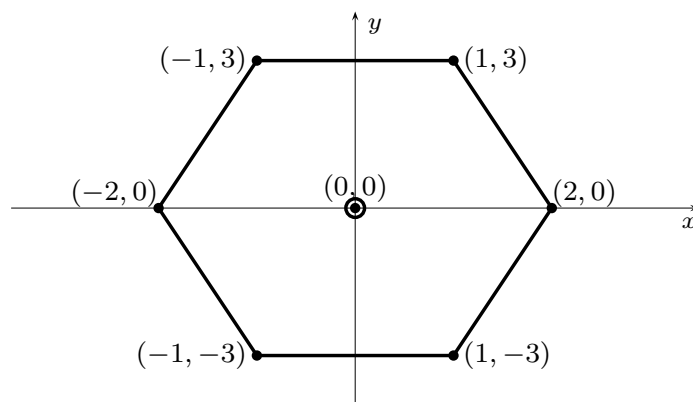

Figure 1.4: Representation {8}
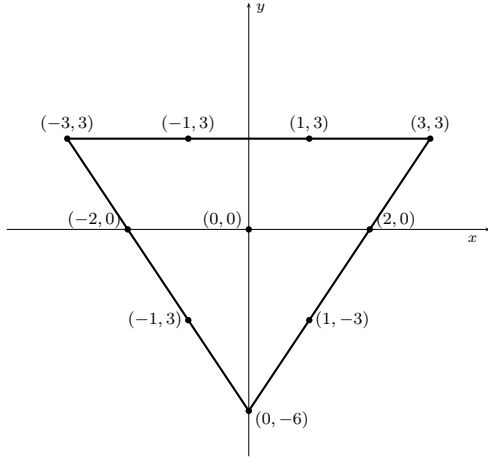
Figure 1.5: Representation {10}

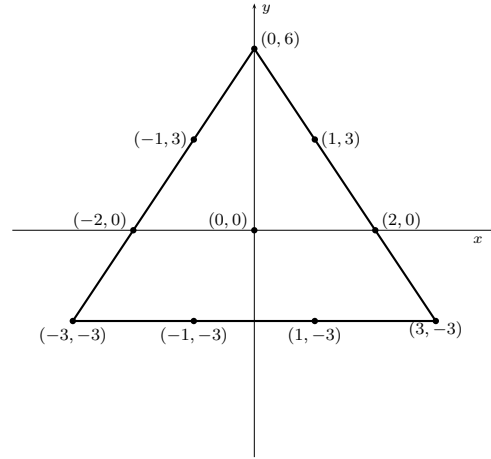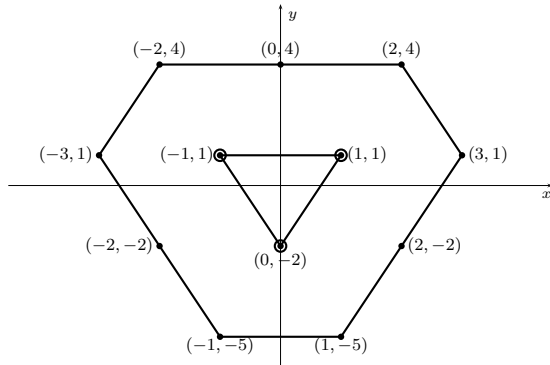Figure 1.6: Representation {$\overline{10}$}
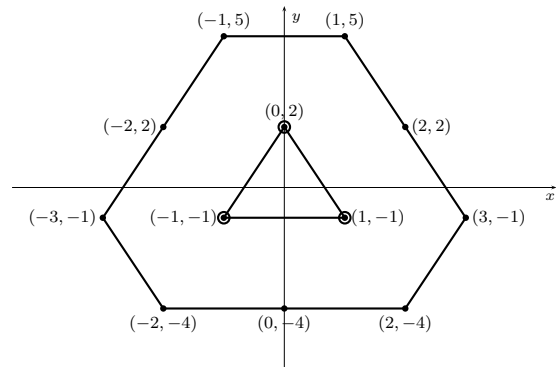

Figure 1.7: Representation {15}

Figure 1.8: Representation {$\overline{15}$}

1.4 Young Tableau

Young tableau are a useful and powerful method to describe different representations of the permutation group S_n and of SU(n) through a graphic depiction in accordance with a set of simple rules. Though they were born in the context of the study of permutations, they can be transposed also to the case of SU(n); since they are so easy to use and interpret,Young diagrams give us one efficient tool to manipulate SU(n) representation. In this section, Young tableau will be described both in the context of S_n and SU(n) [26]; for the SU(n) case particular stress will be put on the method for the evaluation of direct products between representations [26].

1.4.1 Young Tableau and the permutation group

Given a set of n objects (particles, numbers, . . .) a permutation is a transformation of the set which interchanges some (or all) objects of the set between themselves. If only two objects are exchanged one with the other, the permutation is called transposition; we can define a transposition operator P_{ij}, which exchanges the i-th object with the j-th one. Every permutation can be obtained by a combination (product) of transpositions; the way this combination may be defined is not unique, but every possible set of transposition by which we can obtain a certain permutation is formed by an odd or even number of transpositions. Thanks to this property, it is possible to define a sign for the permutation, which is equal to 1 if the permutation is even or -1 if it is odd. The set of all possible permutations of n objects is a group, and it is called permutation group S_n: indeed, it is quite evident that, once we have defined the identity element $\mathbb{I}$ which leaves the set unaltered, all the requirements necessary to define a group, stated in section (A.1), hold.

An explicit physical formulation may be useful to visualize the permutation group. Let us define a two-particles wave function $\psi(1, 2)$, which will be a function of all the degrees of freedom of the two identical particle; with the numbers 1, 2, . . . we denote the whole set of degrees of freedom. The transposition operator P_{12} will act on this state in the following way:

$$P_{12}\psi(1, 2) = \psi(2, 1) \tag{1.4.1}$$

In (1.4.1), we have exchanged the two particles or, equivalently, the first particle has assumed all the degrees of freedom that were of the second, and viceversa. It is possible to define a symmetric and an antisymmetric (under exchange of the degrees of freedom) wave function (ψ_s, ψ_a):

$$\psi_s = \psi(1, 2) + \psi(2, 1) \qquad\qquad \psi_a = \psi(1, 2) - \psi(2, 1) \tag{1.4.2}$$

It is easy to verify that these two wave function are really symmetric or antisymmetric:

$$P_{12}\psi_s = \psi_s \qquad\qquad P_{12}\psi_a = -\psi_a \qquad\qquad (1.4.3)$$

Of course, it is possible to define symmetric or antisymmetric wave functions with an arbitrary number of particles, and given a generic wave function $\psi(1, 2, ..., n)$ through a proper set of transpositions we can symmetrize or antisymmetrize it.

Let us now define what a Young tableaux (or Young diagram) is using as example the states in (1.4.2) We denote with a column of m boxes a state which is completely antisymmetric under the exchange of m indices, while a column with n_c row will represent a state which is completely symmetric under the exchange of n_c indices. The two two-particles wave functions (1.4.2) are then represented by:

$$\psi_s = \boxed{} \qquad\qquad \psi_a = \boxed{\begin{array}{c} \\ \end{array}} \qquad\qquad (1.4.4)$$

Of course, this notation can be generalized to any number of particles, but with a *caveat*: the number of boxes should always be equal to the number of particles. There are also more complicated cases than the one of completely (anti)symmetrized wave functions, because it is possible to have mixed symmetry states, which are (anti)symmetric only under the exchange of some particles and only in a certain number. For example, for three particle states, there are three possible cases:

$$\psi_s = \boxed{} \qquad \psi_{mix} = \qquad \psi_a = \qquad (1.4.5)$$

In (1.4.5) ψ_{mix} is a state symmetric under exchange of two of the three particles, and antisymmetric under the exchange of one of these two with the third. It should be noticed that, no matter how many particles we are considering, the completely symmetric and the completely antisymmetric states are unique: there is just one way to symmetrize or antisymmetrize completely a state. To have all the possible states which fulfill a certain n-particles (mixed) symmetry, it is enough to take the correspondent Young Tableaux and to fill it with all possible numbers from 1 to n, taking into consideration also the combinations with repeated numbers, but sticking to the following requirements - which describe the so called standard form for a Young diagram:

- The numbers must not decrease along a row, from left to right;

- The numbers must increase along a column, from top to bottom;

- The number of boxes in a column must not be lower than the number of boxes in the following one, from left to right.

It should be noticed that if we stick to these requirements properly, we do not have all the possible states. For example, for three-particles wave function, these two states are allowed:

$$\begin{array}{|c|c|}\hline 1 & 2 \\\hline 3 \\\cline{1-1}\end{array} \qquad \begin{array}{|c|c|}\hline 1 & 3 \\\hline 2 \\\cline{1-1}\end{array} \tag{1.4.6}$$

These ones, however, are not:

$$\begin{array}{|c|c|}\hline 1 & 2 \\\hline & 3 \\\hline\end{array} \qquad \begin{array}{|c|c|}\hline 1 & 3 \\\hline & 2 \\\hline\end{array} \tag{1.4.7}$$

They describe a wave function symmetric under the exchange of particles 1 and 2 and antisymmetric under exchange of particles 2 and 3, and symmetric under the exchange of particles 1 and 3 and antisymmetric under exchange of 3 and 2, respectively. However, these two states can be obtained by using the group operators P_{ij} on the two states (1.4.6) respectively: we have found two invariant subspaces of S_3. In this sense, the standard form of Young tableau lets us catalogue all irreducible representations of S_n through all the possible allowed combinations of n boxes. When we fill the boxes of a certain diagram in all the proper ways with numbers from 1 to n, we get a series of states which form a basis for an irreducible representation of the group characterized by certain (anti)symmetry properties, though we should also consider configurations of the diagram which are not allowed in order to have all the states of the representation: the number of possible allowed ways we can fill a given tableaux is equal to the dimension of the correspondent representation.

Given a permutation group S_n, it is possible to catalogue all its Young diagrams through a set of numbers q_i, each of them corresponding to the number of boxes in the i-th row; for example, the tableau for S_3 (1.4.5) may be characterized as (3,0,0), (2,1,0), (1,1,1) respectively. Another way to characterize the Yang tableaux of S_n is using not q_i, but another set p_i defined as $p_i = q_i - q_{i+1}$. States (1.4.5) may then be described by (3,0,0), (1,1,0), (0,0,1).

It is possible to define the conjugate Young diagram of a given one: each row becomes a column and each column becomes a row. It is clear that the dimensions of the representations related to a Young tableaux and to its conjugate one are the same: conjugate diagrams correspond to different representations with the same

dimension. To exemplify, let us consider the four possible representations of S_4:

$$\text{(1.4.8)}$$

The conjugation relations for these Young Tableau are:

$$\Longleftrightarrow$$

$$\Longleftrightarrow$$

$$\Longleftrightarrow \qquad \text{(1.4.9)}$$

The completely symmetric and the completely antisymmetric states are one the conjugate of the other; moreover, we can see that the last diagram in (1.4.9) is self-conjugate.

1.4.2   Young Tableau and SU(n)

In the previous paragraph, we have seen how Young diagrams work in the case of the permutation group S_N. Quite an analogous treatment may be applied to the case of SU(n), on the basis of the following theorem: every state formed by N particles, belonging to the permutation group S_N and generated by composing single-particle states of a n-dimensional SU(n) multiplet belongs also to an irreducible representation of SU(n) [26]. This theorem has a series of consequences; firs of all, it means that we can apply the Young tableau method to SU(n), keeping in mind that a diagram representing a SU(n) multiplet may have columns with a maximum of n boxes - that is, we can have a maximum of n rows. The reason is quite clear: if we have a state formed by particles of a n-dimensional multiplet, it makes no sense to try to antisymmetrize a state with $n + 1$ particles. Moreover, since the completely antisymmetric state is uniquely defined, columns with exactly n boxes may be omitted, because they do not contribute to the dimension of the

irreducible representation of SU(n) we are describing by means of the diagram. For example, let us consider SU(3): in (1.4.10) we see how a state with three-boxes columns may be reduced to an equivalent one.

$$\tag{1.4.10}$$

In this formulation, every tableaux represents an irreducible representation of SU(n), whose dimension will be equal to the numbers of way to fill the N boxes of the diagram with the numbers from 1 to n in a standard configuration; in this sense, every box will correspond to a particle, and the number inside it labels the state the particle is in.

We will call fundamental representations of SU(n) the representations related to Young tableau with only one of the p_i different from zero. The fundamental representations for SU(2), SU(3), SU(4) are:

SU(2) : $\qquad$ (1.4.11)

SU(3) : $\qquad$ (1.4.12)

SU(4) : $\qquad$ (1.4.13)

For the SU(3) case (1.4.12), these two representations are the ones that in section (1.3.2) we called fundamental and antifundamental respectively.

In the case of SU(n), we can define the conjugate of a Young diagram in a slightly different way than what we did for the permutation group. Let us consider a diagram characterized by a set of integers number p_i as defined in the previous section; its conjugate representation is the one with the same set p_i but in opposite order, that is:

$$(p_1, ..., p_{n-1}) \Longrightarrow (p_{n-1}, ..., p_1) \tag{1.4.14}$$

One simple example of conjugation is:

 $(p_1 = 2, p_2 = 1)$ $\quad \Longrightarrow \quad$ $(p_1 = 2, p_2 = 1)$ $\quad$ (1.4.15)

From the comparison of (1.4.9) and (1.4.15) it is quite evident that the definition of conjugation we have given when studying the permutation group and the one considered for the SU(n) case are not equivalent at all.

As our main interest is in the SU(3) symmetry group, let us now introduce the Young tableau for some of its representations. First of all, there are the fundamental and antifundamental representations (1.4.12); it is clear that they are one the conjugate of the other. For the octet representation we will have the diagram:

$$\{8\} \qquad\qquad (1.4.16)$$

This tableaux may be filled, as we expect, in eight different ways according to a standard configuration:

$$(1.4.17)$$

The other three-boxes tableau we may have for a SU(3) symmetry are:

$$\{10\} \qquad\qquad (1.4.18)$$

$$\equiv \textcircled{1} \qquad\qquad \{1\} \qquad\qquad (1.4.19)$$

It is not difficult to verify that (1.4.18) and (1.4.19) have dimensions equal to 10 and 1 respectively (for (1.4.19) it is due to the fact that for a SU(3) symmetry we can omit columns with 3 boxes).

It is clear that, for more complex representations, it may be exceedingly long to calculate how many standard configurations are possible for a given tableaux. What we need is a general formula allowing us to calculate the dimension of a diagram in a quicker way. Firstly, let us notice that for a representation of SU($n+1$), only n integers $\{p_1, ..., p_n\}$ are needed to characterize its tableaux, since columns with $n + 1$ boxes may be omitted. When we want to study the same diagram in the context of SU(n), all that we need to do is to eliminate the last p_i, that is, all columns with n boxes: in SU(n) the same diagram is defined by a set $\{p_1, ..., p_{n-1}\}$. A recursion formula may be proved, on the basis of these considerations; if we denote with $D_n(p_1, ..., p_{n-1})$ the dimension of the tableaux represented by the set $(p_1, ..., p_{n-1})$ interpreted as diagram for SU(n), we have:

$$D_{n+1}(p_1, ..., p_n) = \frac{1}{n!}(p_n + 1)(p_n + p_{n-1} + 2)...(p_n + ... + p_1 + n)D_n(p_1, ..., p_{n-1})$$
$$(1.4.20)$$

Thanks to (1.4.20) it is possible to calculate the dimension of a Young tableaux (that is, an irreducible representation) in SU($n + 1$) using the knowledge of the dimension of the same diagram in SU(n).

This formula may well be simplified for the case of SU(3). First of all, let us notice that the only possible diagrams for SU(2) are the ones with just one row of p_1 boxes. Since we can fill the boxes only with 1s and 2s, the diagrams in a standard form will have a set of numbers 1 followed by a set of numbers 2. There are exactly ($p_1 + 1$) configurations of this type: the one with just numbers 1 and no numbers 2, and p_1 configurations, in which the number two is repeated from a certain box to the end of the row:

We can then arrive to the conclusion that:

$$D_2(p_1) = p_1 + 1 \tag{1.4.21}$$

Thanks to (1.4.21) it is possible to apply (1.4.20) to the SU(n) case, in particular also to the SU(3) one. What we find is:

$$D_3(p_1, p_2) = \frac{1}{2}(p_2 + 1)(p_1 + p_2 + 2)D_2(p_1) = \frac{1}{2}(p_2 + 1)(p_1 + p_2 + 2)(p_1 + 1) \tag{1.4.22}$$

This formula gives us a simple way to calculate the dimension of the representation of SU(3) related to a given Young tableaux.

It is worth stressing that, in the context of SU(3), the two integer numbers p_1 and p_2 characterizing a representation may be also used to evaluate the Casimir operator K_1 defined in (1.3.6) for that representation: it can be shown that the following relation holds:

$$K_1 = \frac{p_1^2 + p_2^2 + p_1 p_2}{3} + p_1 + p_2 \tag{1.4.23}$$

(1.4.23) provides a simple way to calculate one of the Casimir operators of SU(3), which helps us to recognize different multiplet representations of the group.

We now turn to the description of how Young diagrams may be used to evaluate direct products: Young tableau provide indeed a powerful and efficient method to

find the direct product between representations of SU(n), and so to calculate the related Clebsch-Gordan series. Let us consider two Young tableau for two representations of SU(n), for example two octets of SU(3), and let us study their inner product:

$$\boxed{} \otimes \boxed{} = \{8\} \otimes \{8\} \tag{1.4.24}$$

The idea is to label all the boxes of the second representation with letters $\{a, b, \dots\}$, giving the same label to boxes in the same row in increasing order from top to bottom of the diagram, and then to juxtapose the boxes of the second tableaux to the first tableaux in all possible ways in order to obtain new Young diagrams with the following constraints:

- The new tableaux must be in a standard form;

- There must be no columns with more than n boxes;

- The letters of the alphabet $\{a, b, \dots\}$ in the boxes from the second diagram must increase from top to bottom of a column;

- The letters of the alphabet $\{a, b, \dots\}$ in the boxes from the second diagram must not decrease from left to right of a row;

- If we count from right to left of each row of the new tableau, as we go down from top to bottom of the diagram, the number of times the $(k+1)$-th letter has been repeated must never exceed the number of repetition of the k-th one;

For example, in the case (1.4.24), we get:

$$\boxed{} \otimes \boxed{\begin{smallmatrix}a&a\\b\end{smallmatrix}} = \boxed{\begin{smallmatrix}&&a&a\\&b\end{smallmatrix}} \oplus \boxed{\begin{smallmatrix}&a&a\\&\\b\end{smallmatrix}} \oplus \boxed{\begin{smallmatrix}&&a\\&a&b\end{smallmatrix}} \oplus \boxed{\begin{smallmatrix}&&a\\&a\\b\end{smallmatrix}} \oplus \boxed{\begin{smallmatrix}&&a\\&a&b\end{smallmatrix}} \oplus \boxed{\begin{smallmatrix}&&a\\&b\\a\end{smallmatrix}}$$

$$= \boxed{} \oplus \boxed{} \oplus \boxed{} \oplus \boxed{} \oplus ① \oplus \boxed{} \tag{1.4.25}$$

$$\{8\} \otimes \{8\} = \{27\} \oplus \{10\} \oplus \{\overline{10}\} \oplus \{8\} \oplus \{1\} \oplus \{8\} \tag{1.4.26}$$

Chapter 2

SU(2) Antiferromagnetic Heisenberg Model

This chapter is devoted to the study of the Antiferromagnetic Heisenberg Model and of its behaviour. Firstly, the model is defined and its Hamiltonian formulated; secondly coherent states for the SU(2) symmetry group are introduced [7,35]. We then turn to the study of the path integral formulation for the partition function [7,22]. The discrete system under analysis can be mapped into a continuous one, under a continuum limit [19,22], and the continuous model we find is described [37]. The well known Haldane Conjecture [27] is formulated and described through a Renormalization Group transformation [22,34].

2.1 An introduction to the model

Let us consider a chain, that is, a 1-dimensional lattice, with constant lattice spacing a. On each site of the chain we suppose that there is a single particle with a certain quantum spin S, and that only the spin degree of freedom of the particles matters in the definition of our system. The simplest interaction between particles on a spin chain is a nearest-neighbour interaction, that is, a two-body interaction between particles situated on sites one next to the other. One of the most important models for a spin chain of this kind is the Heisenberg model, whose Hamiltonian is:

$$\hat{H} = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{2.1.1}$$

$\mathbf{S}_i$ denotes the spin operators acting on the i-th site of the chain; the Hamiltonian can be formulated as:

$$\hat{H} = J \sum_i \left(S_1^i S_1^{i+1} + S_2^i S_2^{i+1} + S_3^i S_3^{i+1} \right) \tag{2.1.2}$$

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It is clear that this hamiltonian is isotropic along each of the three axes. Of course, it can be generalized, for example, assuming some kind of anisotropy or introducing an external magnetic field; in the following we will consider only the simple formulation (2.1.1).

Another characteristic that is very important for the behaviour of this physical system is the sign of the coupling constant J: if $J > 0$ the model is antiferromagnetic, if $J < 0$ it is ferromagnetic. Depending on the sign of J, the states of the spectrum dispose themselves differently: if the chain is ferromagnetic, the lowest energy states are the one with a ferromagnetic order, that is with the spins aligned, while in the antiferromagnetic case states with a Neel order, that is, with a staggered disposition of the spins on the chain, are favoured. Changing the sign of J, the lowest energy states become the most excited and viceversa. Moreover, it should be noticed that, depending on the value S of the spin on each site, the $\mathbf{S}_i$ constitute a different representation of the SU(2) group on each site; the Young diagram of a representation of given S is a row of $2S$ boxes:

$$\underbrace{\boxed{\ \ }\boxed{\ \ }\boxed{\ \ }\overset{\cdots}{\underset{\cdots}{}}\boxed{\ \ }\boxed{\ \ }\boxed{\ \ }}_{2S \text{ boxes}} \tag{2.1.3}$$

We are interested in the case of an Heisenberg Antiferromagnetic SU(2) spin chain, with a S-spin particle on each site. Our starting point is the partition function of the model, which determines the thermodynamic behaviour of the system:

$$Z = \mathrm{Tr}\left[\mathrm{e}^{-\beta \hat{H}}\right] \tag{2.1.4}$$

This quantity will be studied thoroughly in the following using a path integral formulation; to define a path integral, the so called coherent states will be needed. The next section is devoted to the introduction and the description of this set of states and of its properties.

2.2   Coherent states for SU(2)

It is a result of group theory [7] that every operator G of the SU(2) S-spin representation can be expressed as:

$$G = \mathrm{e}^{i\phi S_3}\mathrm{e}^{i\theta S_2}\mathrm{e}^{i\chi S_3} \tag{2.2.1}$$

θ, ϕ and χ determine univocally the matrix G. Their range is $\theta \in [0, \pi]$, $\phi \in [0, 2\pi[$, $\chi \in [0, 2\pi[$. The set of coherent states can be found applying the operator (2.2.1) to the highest weight state, that is, for SU(2), the maximally polarized state $|S, S\rangle$; since in quantum mechanics states are defined up to a phase, χ can be

fixed arbitrarly. The coherent state $|\Omega\rangle$ can be parametrized by a classical three-dimensional real unimodular vector $\boldsymbol{\Omega} = (\Omega_1, \Omega_2, \Omega_3)$, with:

$$\Omega_i = \frac{1}{S}\langle\Omega|S^i|\Omega\rangle \tag{2.2.2}$$

The explicit expression for $\boldsymbol{\Omega}$ is:

$$\boldsymbol{\Omega} = \Big(\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)\Big) \tag{2.2.3}$$

It should be noticed that (2.2.3) does not depend upon χ, as expected: two angles are enough to define the coherent states for SU(2). It can be proved [7] that the set of states $|\Omega\rangle$, depending on θ and ϕ, are overcomplete; the resolution of the identity is:

$$\frac{2S+1}{4\pi}\int d\boldsymbol{\Omega}|\Omega\rangle\langle\Omega| = \frac{2S+1}{4\pi}\int d\phi d\theta \sin(\theta)|\Omega\rangle\langle\Omega| = \mathbb{I} \tag{2.2.4}$$

It can be easily verified that the quantum state $|\Omega\rangle$ is normalized to one.

A many-particle coherent state, as the ones we will consider in the following, may be defined as:

$$|\Omega\rangle = \otimes_i|\Omega_i\rangle \tag{2.2.5}$$

In (2.2.5), $|\Omega_i\rangle$ denotes the single-particle coherent states of each of the particle contributing to the final state, each one depending on its angles θ_i, ϕ_i and χ_i. The resolution of the identity (2.2.4) can be easily generalized for a set of many-particles coherent states.

2.3 The path integral formulation

Let us now go back to the partition function (2.3.13); the first step of our analysis is to formulate this quantity by means of a path integral [7,22]. To do so, it is useful to notice that:

$$Z = \mathrm{Tr}\left[\mathrm{e}^{-\beta\hat{H}}\right] = \lim_{N\to\infty}\mathrm{Tr}\left[\left(\mathrm{e}^{-\frac{\beta}{N}\hat{H}}\right)^N\right] \tag{2.3.1}$$

In (2.3.1) we have only divided β in N intervals and taken the limit for $N \to \infty$. The trace can be expressed in a more explicit way through the coherent states of our system at temperature β:

$$Z = \lim_{N\to\infty}\int\left(\prod_i d\boldsymbol{\Omega}_i(\beta)\right)\langle\Omega(\beta)|\left(\mathrm{e}^{-\frac{\beta}{N}\hat{H}}\right)^N|\Omega(\beta)\rangle \tag{2.3.2}$$

Let us now introduce N resolutions of the identity, and, ignoring constant factors preceding Z, we find:

$$Z = \lim_{N \to \infty} \int \left(\prod_{i,\tau} d\boldsymbol{\Omega}_i(\tau) \right) \prod_{\tau=\epsilon}^{\beta} \langle \Omega(\tau+\epsilon)|e^{-\epsilon \hat{H}(\tau)}|\Omega(\tau) \rangle \qquad (2.3.3)$$

In (2.3.2) $\epsilon = \frac{\beta}{N}$, τ is an integer multiple of ϵ and we are assuming $|\Omega(\beta)\rangle = |\Omega(0)\rangle$. Since ϵ can be regarded as a very small quantity, we can now proceed to a Taylor expansion of the exponential to the first order in ϵ:

$$Z = \lim_{N \to \infty} \int \left(\prod_{i,\tau} d\boldsymbol{\Omega}_i(\tau) \right) \prod_{\tau=\epsilon}^{\beta} \langle \Omega(\tau+\epsilon)|(1 - \epsilon \hat{H})|\Omega(\tau) \rangle) \qquad (2.3.4)$$

It is now convenient to define the classical hamiltonian H as a normalized expectation value of the operator $\hat{H}$:

$$H(\tau) = \frac{\langle \Omega(\tau+\epsilon)|\hat{H}|\Omega(\tau) \rangle}{\langle \Omega(\tau+\epsilon)|\Omega(\tau) \rangle} \qquad (2.3.5)$$

Substituting (2.3.5) in (2.3.4), and exponentiating the hamiltonian again it is easy to obtain:

$$\begin{aligned}
Z &= \lim_{N \to \infty} \int \left(\prod_{i,\tau} d\boldsymbol{\Omega}_i(\tau) \right) \prod_{\tau=\epsilon}^{\beta} e^{-\epsilon H(\tau)} \langle \Omega(\tau+\epsilon)|\Omega(\tau) \rangle \\
&= \lim_{N \to \infty} \int \left(\prod_{i,\tau} d\boldsymbol{\Omega}_i(\tau) \right) \prod_{\tau=\epsilon}^{\beta} e^{-\epsilon H(\tau)} (1 + \epsilon \langle \dot{\Omega}(\tau)|\Omega(\tau) \rangle) \\
&= \lim_{N \to \infty} \int \left(\prod_{i,\tau} d\boldsymbol{\Omega}_i(\tau) \right) \prod_{\tau=\epsilon}^{\beta} e^{-\epsilon H(\tau) + \epsilon \langle \dot{\Omega}(\tau)|\Omega(\tau) \rangle} \qquad (2.3.6)
\end{aligned}$$

We now have to evaluate the scalar product $\langle \dot{\Omega}(\tau)|\Omega(\tau) \rangle$; it can be shown that the following result holds for the coherent states we defined in section (2.2) [7]:

$$\langle \dot{\Omega}(\tau)|\Omega(\tau) \rangle = \sum_j \langle \dot{\Omega}_j(\tau)|\Omega_j(\tau) \rangle = \sum_j i \dot{\phi}_j \cos(\theta_j) \qquad (2.3.7)$$

Moreover, also the hamiltonian H can be evaluated; keeping in mind that the quantum hamiltonian $\hat{H}$ is (2.1.1), H is defined as (2.3.5) and that (2.2.3) holds, it is quite straightforward to find, at the zeroth order in ϵ:

$$H(\tau) = JS^2 \sum_i \boldsymbol{\Omega}_i(\tau) \cdot \boldsymbol{\Omega}_{i+1}(\tau) \qquad (2.3.8)$$

We now have all we need to turn to a path integral formulation of the partition function. First of all, we define an integration measure for our integral:

$$D\mathbf{\Omega} = \lim_{N\to\infty} \prod_{i,\tau} d\mathbf{\Omega}_i(\tau) \tag{2.3.9}$$

Since ϵ is vanishing small, we can consider τ as a continuous variable; the final expression we find keeping in mind all we have done so far is:

$$Z = \oint D\mathbf{\Omega}\, e^{-\int_0^\beta d\tau H(\tau) + iS \sum_i \omega(\Omega_i)} \tag{2.3.10}$$

$$\omega(\Omega_i) = -\int_0^\beta d\tau \dot{\phi}_i(\tau)\cos(\theta_i(\tau)) \tag{2.3.11}$$

The term $S\sum_i \omega(\mathbf{\Omega}_i)$ is called Berry phase, and will contribute in a fundamental way to the description of the model, since it will give some topological information about it. Of course, formulation (2.3.11) may be summarized as:

$$Z = \oint D\mathbf{\Omega}\, e^{-\mathcal{S}(\mathbf{\Omega})} \tag{2.3.12}$$

$$\mathcal{S} = \int_0^\beta d\tau H(\tau) - iS \sum_i \omega(\Omega_i) \tag{2.3.13}$$

$\mathcal{S}$ is the action for our model, which will be of great importance in the following for the understanding of the behaviour of this system. Of course, this procedure can be done precisely in the same way for any other spin-model, substituting $\hat{H}$ with the appropriate quantum hamiltonian.

2.3.1 Geometrical interpretation of the Berry phase

The Berry phase is not explainable in terms of the Hamiltonian of our system: its form is due to the structure of the coherent states, and a geometrical interpretation of this quantity by means of the classical spin vectors $\mathbf{\Omega}_i(\tau)$ can be given [7]. Each one of the $\mathbf{\Omega}_i(\tau)$ is bounded, by its own nature of unimodular vector, to move upon a spherical surface of unitary radius; at any change of τ it changes direction, but not lenght, describing a trajectory upon this sphere, which can be parametrized using the parameter τ. In this picture, of course the angles $\theta(\tau)_i$ and $\phi(\tau)_i$ constitute the latitude and the longitude respectively of the points on the sphere belonging to the trajectory. Since $|\Omega(\beta)\rangle = |\Omega(0)\rangle$ the trajectories on the sphere are closed ones; this implies that it is possible to express $\omega(\mathbf{\Omega}_i)$ of the Berry phase in an equivalent formulation:

$$\omega(\mathbf{\Omega}_i) = -\int_0^\beta d\tau \dot{\phi}_i(\tau)\cos(\theta_i(\tau)) = \int_0^\beta d\tau \left(1 - \dot{\phi}_i(\tau)\cos(\theta_i(\tau))\right) \tag{2.3.14}$$

(2.3.14) can be easily recognized as the area on the spherical surface enclosed by the trajectory described by $\boldsymbol{\Omega}_i(\tau)$. It is then possible to use Stoke's theorem, and to express $\omega(\boldsymbol{\Omega}_i)$ as [7]:

$$\omega(\boldsymbol{\Omega}_i) = \int_0^\beta d\tau \, \mathbf{A}_i(\boldsymbol{\Omega}_i) \cdot \dot{\boldsymbol{\Omega}}_i$$
$$\nabla \times \mathbf{A}_i \cdot \boldsymbol{\Omega}_i = 1 \tag{2.3.15}$$

$\mathbf{A}_i$ is a vector potential, similar to the one usually defined in the context of classical electromagnetism. Of course, there is a gauge freedom in the choice of $\mathbf{A}_i$, and many equivalent formulations are possible for it.

2.4 The continuum limit approximation

The Heisenberg model, being defined on a lattice, describes the 1-d space as discrete; what we would like to do now is to study the continuum limit approximation of this model, in which space is treated as continuous. In order to do so, we shall consider a semiclassical approximation, which holds only in the large-S limit [7, 19, 22]. Firstly, we express the classical spin vector $\boldsymbol{\Omega}_i(\tau)$ through the so called Haldane Ansatz:

$$\boldsymbol{\Omega}_i = (-1)^i \mathbf{m}_i \sqrt{1 - \frac{a^2}{S^2}\mathbf{l}_i \cdot \mathbf{l}_i} + \frac{a}{S}\mathbf{l}_i \tag{2.4.1}$$

In (2.4.1), $\mathbf{m}_i$ is called Néel field, and constitutes the slowly varying part of the classical vector; its norm is equal to one, precisely as $\boldsymbol{\Omega}_i$, and it keeps track of the staggered Néel order which is favoured by the antiferromagnetic coupling through the term $(-1)^i$, which gives a different sign on odd and even sites. $\mathbf{l}_i$ is the canting field, and it is supposed to be very small: it constitute a correction to the main term constituted by $\mathbf{m}_i$, to which it is orthogonal. These two fields have then the following properties:

$$\mathbf{m}_i \cdot \mathbf{m}_i = 1 \qquad\qquad \mathbf{m}_i \cdot \mathbf{l}_i = 0 \tag{2.4.2}$$

In the continuum limit, the lattice constant a becomes vanishing small, and sums over the sites are replaced by integration over a continuous space variable x. $\mathbf{m}_i$ becomes then $\mathbf{m}(x)$, and $\mathbf{l}_i$ becomes $\mathbf{l}(x)$; we are allowed to have a Taylor expansion for $\mathbf{m}_{i+1}$ and for $\frac{a}{S}\mathbf{l}_{i+1}$ to the second order in a:

$$
\begin{aligned}
\mathbf{m}_{i+1} &= \mathbf{m}(x) + a\frac{\partial \mathbf{m}(x)}{\partial x} + \frac{1}{2}a^2\frac{\partial^2 \mathbf{m}(x)}{\partial x^2}\\
\frac{a}{S}\mathbf{l}_{i+1} &= \frac{a}{S}\mathbf{l}(x) + \frac{a^2}{S}\frac{\partial \mathbf{l}(x)}{\partial x}
\end{aligned}
\tag{2.4.3}
$$

Moreover, due to (2.4.2), it is clear that

$$\mathbf{m} \cdot \frac{\partial \mathbf{m}}{\partial x} = 0 \tag{2.4.4}$$

The continuum limit Hamiltonian is found taking (2.4.3) and (2.4.4) into consideration, and Taylor expanding to the second order in a: since the classical Hamiltonian is in the form (2.3.8), one gets - ignoring constant factors - [19]:

$$\int_0^\beta d\tau H(\tau) = J \int_0^\beta d\tau dx \left(-\frac{a}{2}\mathbf{m} \cdot \frac{\partial^2 \mathbf{m}}{\partial x^2} + 2\frac{a}{S^2}\mathbf{l}(x) \cdot \mathbf{l} \right) \tag{2.4.5}$$

After an integration by parts, we find the final form for the continuum limit of the Heisenberg Hamiltonian:

$$\int_0^\beta d\tau H(\tau) = \int_0^\beta d\tau dx \frac{Ja}{2} \left(S^2 \frac{\partial \mathbf{m}}{\partial x} \cdot \frac{\partial \mathbf{m}}{\partial x} + 4\mathbf{l} \cdot \mathbf{l} \right) \tag{2.4.6}$$

Let us now turn to the Berry phase (2.3.11): to have the continuum form for the effective action $\mathcal{S}$ (2.3.13), it also has to be formulated for a continuous 1-dimensional space, as we have just done for the hamiltonian. Though it will be trickier from an analytical point of view, the idea is exactly the same: to substitute the Haldane Ansatz (2.4.1) for $\mathbf{\Omega}_i$ in the Berry phase and to evaluate it consequentely. First of all we notice that, since $\mathbf{l}_i$ is the small rapidly varying part of the Haldane Ansatz, and plays the role of a correction, one is allowed decompose $\mathbf{\Omega}_i$ as:

$$\begin{aligned}
\mathbf{\Omega}_i &= \mathbf{\Lambda}_i + \delta\mathbf{\Lambda}_i \\
\mathbf{\Lambda}_i &= (-1)^i \mathbf{m}_i \\
\delta\mathbf{\Lambda}_i &= \frac{a}{S}\mathbf{l}_i
\end{aligned} \tag{2.4.7}$$

In the previous expression, $\mathbf{\Lambda}_i$ is the dominating part of the field, that is, the one depending on $\mathbf{m}_i$ in the Haldane Ansatz (2.4.1) (we have regarded the square root term as negligible, since $\mathbf{l}_i$ is a small fluctuation), and $\delta\mathbf{\Lambda}_i$ is the correcting term depending only on $\mathbf{l}_i$; consequentely, it is possible to write:

$$\omega(\mathbf{\Omega}_i) = \omega(\mathbf{\Lambda}_i) + \delta\omega(\delta\mathbf{\Lambda}_i) \tag{2.4.8}$$

To evaluate $\delta\omega(\delta\mathbf{\Lambda}_i)$, it is better to use the formulation (2.3.15) of the Berry phase, which uses a vector potential $\mathbf{A}_i$; after some algebra [19], one can find that the variation of ω is:

$$\delta\omega(\mathbf{\Lambda}_i) = \int_0^\beta d\tau \delta\mathbf{\Lambda}_i \cdot \left(\mathbf{\Lambda}_i \times \frac{\partial \mathbf{\Lambda}_i}{\partial \tau} \right) \tag{2.4.9}$$

Substituting (2.4.7) in this expression, we find:

$$\delta\omega(\mathbf{l}_i) = \frac{a}{S}\int_0^\beta d\tau\, \mathbf{l}_i \cdot \left(\mathbf{m}_i \times \frac{\partial \mathbf{m}_i}{\partial\tau}\right) \tag{2.4.10}$$

Let us now formulate the Berry phase in the continuum approximation:

$$S\sum_i \omega(\mathbf{\Omega}_i) = \Gamma(\mathbf{m}) + \int dx\,d\tau\, \mathbf{l} \cdot \left(\mathbf{m} \times \frac{\partial\mathbf{m}}{\partial\tau}\right) \tag{2.4.11}$$

$\Gamma(\mathbf{m})$ is the continuum limit for $S\sum_i \omega(\mathbf{\Lambda}_i)$. To calculate it, it is important to keep in mind the staggering factor $(-1)^i$ in (2.4.7):

$$S\sum_i \omega(\mathbf{\Lambda}_i) = S\sum_i (-1)^i \omega(\mathbf{m}_i) = S\sum_i \left(\omega(\mathbf{m}_{2i}) - \omega(\mathbf{m}_{2i+1})\right) \tag{2.4.12}$$

Expanding in a Taylor series, keeping only the first derivative of $\mathbf{m}$, one finds, turning to the continuum expression [7, 19]:

$$\begin{aligned}
\Gamma(\mathbf{m}) &= \frac{S}{2}\int dx\, \frac{\delta\omega}{\delta\mathbf{m}} \cdot \frac{\partial\mathbf{m}}{\partial x} \\
&= \frac{S}{2}\int dx\, \left(\mathbf{m}_i \times \frac{\partial\mathbf{m}_i}{\partial\tau}\right) \cdot \frac{\partial\mathbf{m}(x)}{\partial x} \\
&= \frac{\vartheta}{4\pi}\int dx\,d\tau \left(\frac{\partial\mathbf{m}}{\partial\tau} \times \frac{\partial\mathbf{m}}{\partial x}\right) \cdot \mathbf{m} \tag{2.4.13} \\
\vartheta &= 2\pi S \tag{2.4.14}
\end{aligned}$$

Getting all we did so far together, the action $\mathcal{S}$ has the form:

$$\begin{aligned}
\mathcal{S} &= \mathcal{S}_1 + \mathcal{S}_2 \tag{2.4.15} \\
\mathcal{S}_1 &= \int dx\,d\tau\, \frac{Ja}{2}\left(S^2\frac{\partial\mathbf{m}}{\partial x} \cdot \frac{\partial\mathbf{m}}{\partial x} + 4\mathbf{l}\cdot\mathbf{l}\right) \\
&\quad - i\int dx\,d\tau\left(\mathbf{m}\times\frac{\partial\mathbf{m}}{\partial\tau}\cdot\mathbf{l}\right) \tag{2.4.16} \\
\mathcal{S}_2 &= -i\Gamma(\mathbf{m}) \tag{2.4.17}
\end{aligned}$$

Let us keep in mind that our partition function is in now in the form:

$$Z = \int D\mathbf{l}\,D\mathbf{m}\,\delta(\mathbf{m}\cdot\mathbf{m} - 1)\mathrm{e}^{-\mathcal{S}} \tag{2.4.18}$$

Our final step is to perform the integration of the rapidly varying variable $\mathbf{l}$; in order to do so, it is enough to notice that $\mathcal{S}_1$ can be rearranged in order to make it possible a gaussian integration, just completing the square:

$$2aJ\mathbf{l}\cdot\mathbf{l}-i\mathbf{m}\times\frac{\partial\mathbf{m}}{\partial\tau}\cdot\mathbf{l} = \left(\sqrt{2Ja}\mathbf{l} - i\frac{\mathbf{m}}{2\sqrt{2}Ja}\times\frac{\partial\mathbf{m}}{\partial\tau}\right)^2 + \frac{1}{8Ja}\left(\mathbf{m}\times\frac{\partial\mathbf{m}}{\partial\tau}\right)^2 \quad (2.4.19)$$

We can now integrate the $\mathbf{l}$ variable of our path integral - which will give only a constant multiplicative factor before Z, that can be ignored -. Let us notice that:

$$\mathbf{m}\cdot\frac{\partial\mathbf{m}}{\partial\tau} = 0 \;\Rightarrow\; \left(\mathbf{m}\times\frac{\partial\mathbf{m}}{\partial\tau}\right)^2 = \frac{\partial\mathbf{m}}{\partial\tau}\cdot\frac{\partial\mathbf{m}}{\partial\tau} \quad (2.4.20)$$

The path integral we have is then [7, 19, 22]:

$$Z = \int D\mathbf{m}\,\delta(\mathbf{m}\cdot\mathbf{m} - 1)\mathrm{e}^{-\tilde{\mathcal{S}}-i\Gamma(\mathbf{m})} \quad (2.4.21)$$

$$\tilde{\mathcal{S}} = \int dx d\tau \tilde{\mathcal{L}} \quad (2.4.22)$$

$$\tilde{\mathcal{L}} = \frac{1}{2g}\left(v\left(\frac{\partial\mathbf{m}}{\partial x}\right)^2 + \frac{1}{v}\left(\frac{\partial\mathbf{m}}{\partial\tau}\right)^2\right) \quad (2.4.23)$$

$$g = \frac{2}{S} \qquad v = 2Jsa \quad (2.4.24)$$

The Lagrangian (2.4.23) can be recognized as the one of the so called O(3) non-linear σ model (NLσM) in its euclidean formulation; this gives us an hint of what is the physical interpretation of the procedure described so far. What we have now is a path integral of the exponential of the action of a field theory in its euclidean formulation: this object corresponds to the euclidean (Wick-rotated) generating functional for the field theory found through the continuum limit, evaluated with no external sources. We have then taken advantage of the correspondence between quantum statistical mechanics and quantum field theory, mapping the original spin chain in one dimension into a field theory in 1+1 dimensions (the role of time is played by the temperature τ) with well known characteristics.

The next section will provide an outline of the features of the classical O(3)NLσM and of its most important topological properties [37].

2.5 The O(3) non-linear σ model

The O(3) non-linear σ model describes three free real scalar fields (m_1, m_2, m_3), which can be expressed as a vector field $\mathbf{m}$, in 1+1 dimensions [37]; the

vector field $\mathbf{m}(x,\tau)$ is supposed to have modulus equal to one at any point of our 2-dimensional space-time:

$$\mathbf{m}(x,\tau) = \begin{pmatrix} m_1(x,\tau) \\ m_2(x,\tau) \\ m_3(x,\tau) \end{pmatrix} \qquad \mathbf{m}(x,\tau) \cdot \mathbf{m}(x,\tau) = \sum_{i=1}^{3} (m_i(x,\tau))^2 = 1 \quad (2.5.1)$$

Due to constraint (2.5.1), $\mathbf{m}$ can vary only on a sphere: this two-dimensional spheric surface constitutes an internal space for the possible configurations of the vector field, which must not be confused with the 1+1 dimensional space in which the fields m_i live.

The Lagrangian has the following form [37]:

$$\mathcal{L} = \frac{1}{2} \sum_{\mu=1}^{2} \sum_{i=1}^{3} \frac{\partial m_i}{\partial x^\mu} \frac{\partial m_i}{\partial x_\mu} = \frac{1}{2} \sum_{\mu=1}^{2} \frac{\partial \mathbf{m}}{\partial x^\mu} \cdot \frac{\partial \mathbf{m}}{\partial x_\mu} \qquad (2.5.2)$$

In (2.5.2), $x_1 = x$, $x_2 = \tau$ and Lorentz convention for up and down indices is used. In order to find the equation of motion, we should minimize the action, imposing that it encodes the constraint (2.5.1) by means of a Lagrange multiplier:

$$\mathcal{S} = \int dx d\tau \left(\mathcal{L}(x,\tau) - \lambda(x,\tau)(\mathbf{m} \cdot \mathbf{m} - 1) \right) \qquad (2.5.3)$$

The equation of motion is then:

$$(\Box + \lambda)\mathbf{m} = 0 \qquad (2.5.4)$$

It can be further simplified using the constraint (2.5.1):

$$\mathbf{m} \cdot (\Box + \lambda)\mathbf{m} = 0 \Rightarrow \lambda = -\mathbf{m} \cdot \Box\mathbf{m} \Rightarrow (\Box - \mathbf{m} \cdot \Box\mathbf{m})\,\mathbf{m} = 0 \qquad (2.5.5)$$

If we do not want to take into account the time dependence of the solutions of the equation of motion, but only to consider the static set of solutions, we can formulate the static equation of motion as:

$$\left(\frac{\partial^2}{\partial x^2} - \left(\mathbf{m} \cdot \frac{\partial^2 \mathbf{m}}{\partial x^2} \right) \right)\mathbf{m} = 0 \qquad (2.5.6)$$

Of course it is possible to turn to the hamiltonian formulation from the lagrangian formulation; the energy one can easily find for a static field is [37]:

$$E = \frac{1}{2} \int dx d\tau \left(\frac{\partial \mathbf{m}}{\partial x} \cdot \frac{\partial \mathbf{m}}{\partial x} + \frac{\partial \mathbf{m}}{\partial \tau} \cdot \frac{\partial \mathbf{m}}{\partial \tau} \right) \qquad (2.5.7)$$

Let us now consider the case $E = 0$; of course the partial derivatives in (2.5.7) must be equal to zero, which implies that $\mathbf{m}$ must not depend on the point of the space time we are calculating it in: $\mathbf{m}$ is, in this case, a three dimensional vector which remains constant through all the motion. Solution of this kind are clearly infinite degenerate, since, as we said before, due to the condition (2.5.1), $\mathbf{m}$ is bounded on the spherical surface S_2 of the internal space of the field: each point of the sphere corresponds to a proper zero-energy state, and what we have is a family of continuously degenerate minimum states. It is also possible to study the statical states with finite non zero energy, $0 < E < \infty$. To avoid divergencies in the expression (2.5.7), $\frac{\partial \mathbf{m}}{\partial x}$ is required to go to zero quickly enough at infinite, which means that (with $r = \sqrt{x^2 + \tau^2}$):

$$\lim_{r \to \infty} \mathbf{m} = \mathbf{m}_0 \tag{2.5.8}$$

In (2.5.8) $\mathbf{m}_0$ is a constant field belonging to the sphere S_2, to which $\mathbf{m}$ tends no matter from which direction we approach infinity. This limit has a consequence of fundamental importance: since at infinity our three-dimensional real field has precisely the same value not depending on the way we study its limit, the coordinate space (x, τ) can be compactified into a sphere with one of the pole coinciding with the point at infinity (in which the value of the field is univocally defined). Being $\mathbf{m}(x)$ a map between the physical coordinates and its inner space, which is a S_2 surface itself, it turns out that we have found, through the field, a mapping between the sphere of physical coordinates $S_{2,\text{phys}}$ and the internal space sphere $S_{2,\text{int}}$. To summarize, a finite energy solution with no dependence on the time variable τ is a mapping between two spheres:

$$\mathbf{m} : S_{2,\text{phys}} \to S_{2,\text{int}} \tag{2.5.9}$$

Mappings between spheres S_2 have an important topological property: they can be classified into homotopy sectors [37]. An homotopy sector is a set of maps which may be regarded as equivalent since one can be deformed into the other with continuity; mappings belonging to different homotopy sectors, on the contrary, are not smoothly deformable one into the other. It is a result of topology that, in the case (2.5.9), the homotopy sectors are in infinite countable number and can be labelled through an integer number $\mathcal{Q} \in \mathbb{Z}$; indeed, they form a group (called $\pi_2(S_2)$) which is isomorphic to $\mathbb{Z}$. The number $\mathcal{Q}$ is called winding number, or Pontraygin index, and it is equal to the number of times $S_{2,\text{int}}$ is wrapped by the $S_{2,\text{phys}}$ through the mapping $\mathbf{m}$. It can be shown [37] that the Pontraygin index assumes the form:

$$\mathcal{Q} = \frac{1}{4\pi} \int dx d\tau \left(\frac{\partial \mathbf{m}}{\partial \tau} \times \frac{\partial \mathbf{m}}{\partial x} \right) \cdot \mathbf{m} \tag{2.5.10}$$

Going back to the Heisenberg antiferromagnetic chain, what we have is that the term $\Gamma(\mathbf{m})$ in (2.4.13) and (2.4.14) is just the general expression of the winding number of the O(3) non-linear σ model, preceded by a factor $2\pi S$. Since we have to consider all the possible homotopy sectors in the path integral representing the partition function - that is, all possible paths for $\mathbf{m}$ -, the final form for Z is:

$$Z = \sum_{\mathcal{Q} \in \mathbb{Z}} \int D\mathbf{m}\delta(\mathbf{m} \cdot \mathbf{m} - 1)\mathrm{e}^{-\int d\tau dx \mathcal{L}} \; \mathrm{e}^{2\pi i S \mathcal{Q}} \qquad (2.5.11)$$

$\mathrm{e}^{2\pi i S \mathcal{Q}}$ is then a topological term. Its influence on the evaluation of the partition function depends on whether we are dealing with integer or semi-integer spin: if S is an integer number, the topological phase is just equal to one, and so it doesn't matter for the final result, while if S is semi-integer the sum over $\mathcal{Q}$ becomes staggered, since the topological phase is equal to $(-1)^{\mathcal{Q}}$, making much more difficult to predict through the path integral formulation of Z the behaviour of the system. Though the problem of the evaluation of Z for the Heisenberg chain is not resolved yet, there are very strong hints that a solution is possible; let us then turn to a deeper analysis of Z and of what it tells us about the system under examination.

2.6 A Renormalization Group transformation

The action we are dealing with is (2.4.22); of course, a redefinition of the space-time variables is always possible, in order to find:

$$\tilde{\mathcal{S}} = \int dx d\tau \frac{1}{2g}\Big((\partial_\tau \mathbf{m})^2 + (\partial_x \mathbf{m})^2\Big) \qquad (2.6.1)$$

We have chosen a rescaling of the variables which would absorb the velocity v in (2.4.23), in order to have exactly the euclidean formulation of lagrangian (2.5.2). We are interested in a semiclassical analysis of Z, that is a low-energy perturbative treatment of our action; this is possible only if the coupling constant g is reasonably small, that is (see (2.4.24)) if the spin S is sufficiently large. This kind of analysis corresponds to the assumption that the quantum perturbations are small, allowing us to consider our partition function as a semiclassical object; moreover, since the winding number can not be modified by local fluctuations, being a topological property of the system, the topological term may be ignored in the following part of our reasoning.

The new form for the action $\tilde{\mathcal{S}}$ has the relevant property of being invariant under rescaling of the variable by means of the same constant α; this kind of

symmetry is called scale invariance:

$$
\begin{cases}
x \to \alpha x \\
\tau \to \alpha \tau \\
\mathbf{m} \to \mathbf{m}
\end{cases}
\Rightarrow \tilde{\mathcal{S}} \to \tilde{\mathcal{S}}
\tag{2.6.2}
$$

The model described by the action (2.6.1) is in 1+1 dimensions; it can be easily generalized to an arbitrary number d of dimensions, but being careful with the coupling constant (which is adimensional in the case of a bidimensional system, but becomes dimensional when turning to a higher number of dimensions) [22]:

$$
\tilde{\mathcal{S}}_d \;=\; \frac{1}{2u a_0^{d-2}} \int d^d x (\partial_{\mathbf{x}} \mathbf{m})^2 = \int dx^d \tilde{\mathcal{L}}_d
\tag{2.6.3}
$$

$$
u \;=\; g a_0^{2-d}
\tag{2.6.4}
$$

In (2.6.4) a_0 is the (small) typical length scale of the system, and $\mathbf{m}$ is still composed by three components. Since, as stressed before, we are interested in a low-energy expansion, what we would like to do is to obtain an effective action for the model, keeping in the evaluation of the path integral only the low-energy fluctuation (that is, the one with small momentum $\mathbf{p}$, also called infrared); the faster (more energetic) modes of the fluctuations (called ultraviolet) may be integrated away through a so called Renormalization Group transformation. In general, a transformation of this kind consists in an appropriate variation of the coupling parameters of the system which keeps the form of the action invariant, living therefore unvaried the physical observables of the theory; the fluctuation of a scale we are not interested in will be averaged and only the relevant one kept [22].

Let us suppose that the third component of $\mathbf{m}$ describes only fast fluctuations, and so it may be regarded as small. Due to the fact the the module of $\mathbf{m}$ is equal to one, we can parametrize the first two components of this classical field by means of the third one and of an angle $\gamma \in [0, 2\pi]$; moreover, also the m_3 will be riparametrized by means of a scalar field ψ:

$$
m_1 = \sqrt{1 - m_3^2} \cos(\gamma)
\tag{2.6.5}
$$

$$
m_2 = \sqrt{1 - m_3^2} \sin(\gamma)
\tag{2.6.6}
$$

$$
m_3 = \sqrt{u a_0^{d-2}} \, \psi
\tag{2.6.7}
$$

$$
m_1^2 \;+\; m_2^2 \;+\; m_3^2 = 1
\tag{2.6.8}
$$

Substituting (2.6.5), (2.6.6) and (2.6.7) in (2.6.3), the action becomes [22]:

$$
\tilde{\mathcal{S}}_d = \frac{1}{2} \int d^d x \left((\partial_{\mathbf{x}} \psi)^2 + \frac{1 - u a_0^{d-2} \psi^2}{u a_0^{d-2}} (\partial_{\mathbf{x}} \gamma)^2 + \frac{u a_0^{d-2}}{1 - u a_0^{d-2} \psi^2} (\psi \partial_{\mathbf{x}} \psi) \right)
\tag{2.6.9}
$$

This expression can be further simplified expanding it in a Taylor series regarding the coupling constant u as small: that is precisely the limit one should take into consideration to have a semiclassical expansion. What we find, keeping terms up to the second order in u is [22]:

$$
\begin{aligned}
\tilde{\mathcal{S}}_d &= \frac{1}{2} \int d^d x \left((\partial_{\mathbf{x}} \psi)^2 + \frac{1}{u a_0^{d-2}} (\partial_{\mathbf{x}} \gamma)^2 - \psi^2 (\partial_{\mathbf{x}} \gamma)^2 + \right. \\
&\quad + \left. u a_0^{d-2} (\psi \partial_{\mathbf{x}} \psi)^2 + u^2 a_0^{2(d-2)} \psi^2 (\psi \partial_{\mathbf{x}} \psi)^2 \right)
\end{aligned}
\tag{2.6.10}
$$

Let us consider the superior cutoff κ for the momentum $|\mathbf{p}|$, which is of the order of the inverse of the space cutoff, $\kappa \sim \frac{1}{a_0}$. The fluctuations of this order of magnitude are precisely the one we want to integrate out of the partition function, in order to study the low-energy approximation: the idea is that phenomena at very different momentum scales do not interact strongly, so they can be considered separately. It is now possible to perform the path integral which express the averaging of these fluctuation in the partition function; it will be done only over a shell of values for the momenta, $\kappa b < |\mathbf{p}| < \kappa$, with $0 < b < 1$ [22]:

$$
\int_{\kappa b < |\mathbf{p}| < \kappa} D\psi(\mathbf{p}) e^{-\frac{1}{2} \int d^d x \left((\partial_{\mathbf{x}} \psi)^2 + \frac{1}{u a_0^{d-2}} (\partial_{\mathbf{x}} \gamma)^2 - \psi^2 (\partial_{\mathbf{x}} \gamma)^2 \right)}
\tag{2.6.11}
$$

We can now transport ψ and γ from the coordinate space to the momenta space through a Fourier transform; keeping in mind that we can regard γ as varying at a sufficiently small rate, in the limit $b \to 1$ - so that the Fourier transform of its gradient does not give momenta in the shell of values considered in the path integral -, (2.6.11) may be rewritten as:

$$
\int_{\kappa b < |\mathbf{p}| < \kappa} D\psi(\mathbf{p}) e^{-\frac{1}{2(2\pi)^d} \int d^d p |\psi(\mathbf{p})|^2 \mathbf{p}^2 + \frac{1}{2(2\pi)^d} \int d^d p |\psi(\mathbf{p})| (\partial_{\mathbf{x}} \gamma)^2} \sim
$$
$$
\sim e^{\frac{1}{2(2\pi^d)} \int_{\kappa b < |\mathbf{p}| < \kappa} d^d p \ln \left(\frac{2\pi}{\mathbf{p}^2} \right) + \frac{1}{2(2\pi)^d} (\partial_{\mathbf{x}} \gamma)^2 \int_{\kappa b < |\mathbf{p}| < \kappa} d^d p \frac{1}{\mathbf{p}^2}}
\tag{2.6.12}
$$

The previous formula can be found calculating naively the first integral as it was a usual gaussian integral and then exponentiating the result [22]. Substituting this result in the expression for the partition function, the effective d-dimensional Lagrangian density assumes the following form, ignoring all the terms from the first order in u:

$$
\mathcal{L}_d^{eff} = -\frac{1}{2(2\pi^d)} \int_{\kappa b < |\mathbf{p}| < \kappa} d^d p \ln \left(\frac{2\pi}{\mathbf{p}^2} \right) + \frac{1}{2} (\partial_{\mathbf{x}} \psi)^2 +
$$
$$
+ \frac{1}{2} \left(\frac{1}{u a_0^{d-2}} - \frac{1}{(2\pi)^d} \int_{\kappa b < |\mathbf{p}| < \kappa} d^d p \frac{1}{\mathbf{p}^2} \right) (\partial_{\mathbf{x}} \gamma)^2 - \frac{1}{2} \psi^2 (\partial_{\mathbf{x}} \gamma)^2
$$
$$
\tag{2.6.13}
$$

The form of the effective Lagrangian is the same as the one we started from, preceded by a shifting constant, and with a redefinition of the coupling parameter - exactly what we expected, having performed a Renormalization Group transformation -:

$$\frac{1}{u a_0^{d-2}} \rightarrow \left(\frac{1}{u a_0^{d-2}} - \frac{1}{(2\pi)^d} \int_{\kappa b < |\mathbf{p}| < \kappa} d^d p \, \frac{1}{\mathbf{p}^2} \right) \tag{2.6.14}$$

One more thing that is important to underline is that, having averaged all the quantum fluctuations with momenta in the shell $\kappa b < |\mathbf{p}| < \kappa$, the cutoff for the momentum has been changed by the transformation - and equivalently the spacial one:

$$\kappa' = b\kappa \tag{2.6.15}$$

$$a_0' = \frac{a_0}{b} \tag{2.6.16}$$

It is clear that to a decrease of the momentum cutoff (2.6.15) corresponds an increase in the spacial cutoff (2.6.16). (2.6.14) may now be expressed as [22]:

$$\begin{aligned} \frac{1}{u' a_0'^{d-2}} &= \frac{1}{u a_0^{d-2}} - \frac{1}{(2\pi)^d} \int_{\kappa b < |\mathbf{p}| < \kappa} d^d p \, \frac{1}{\mathbf{p}^2} \\ &= \frac{1}{u a_0^{d-2}} - \frac{\mathrm{S}_d}{(2\pi)^d} \frac{1}{d-2} (1 - b^{d-2}) \kappa^{d-2} \end{aligned} \tag{2.6.17}$$

In (2.6.17) the integral has been evaluated and S_d is the surface of the d-dimensional sphere. This expression may be expanded in a Taylor series of the coupling constant (we will keep only terms up to the second order), with the additional condition that the parameter $\varepsilon = d - 2$ should be regarded as small; in this way it is then possible to find the so called β-function [22]:

$$\beta(u) = \frac{du}{d \ln(a_0)} = -\varepsilon u + \frac{u^2}{2\pi} \tag{2.6.18}$$

The system we considered at the beginning has one spacial dimension and one "temporal" dimension, that is $d = 2$ ($\varepsilon = 0$). What we find is then:

$$\beta(u) = \frac{u^2}{2\pi} \tag{2.6.19}$$

The β-function for a two-dimensional system is always positive; it means that, to an increase of the spacial cutoff, an increase of the coupling parameter corresponds; it implies that, looking at an effective theory for lower energy modes, the effective coupling constant is increased respect to the one we started with. This result is

more striking if we remember that the coupling constant is linked to the spin S of the chain:

$$u \propto \frac{1}{S} \tag{2.6.20}$$

So, at lower energy, it is possible to define an effective spin, which turns out to decrease as the faster modes of the system are averaged and integrated out from the partition function.These results are the starting point for the so called Haldane conjecture about the behaviour of the Heisenberg Chain depending on whether the spin is an integer or a semi-integer number, which will be enunciated and motivated in the next section [22, 27].

2.7 The Haldane Conjecture

The main feature of the system is its correlation length ξ, which is inversely proportional to the mass of the system. If it is finite, then the model presents a gap in its energy spectrum: the first excited states must have a finite difference in energy respect to the ground state. If the correlation length diverges, it turns out that the spectrum is gapless: excitations from the ground state can be find with arbitrarily small variations of the ground state energy. In the first case, the system is massive, in the second one is massless, or critical. The Haldane Conjecture [27] states that half-integer Antiferromagnetic Heisenberg Spin Chains are massless, while the ones with integer S have a gap in the spectrum; the explanation we will give now is not a formal prove of this statement, but only a goodsense-based reasoning strongly supporting it - and that is why it is called "conjecture", even though there are many evidences, also from a numerical point of view, that it should be right. First of all, let us consider the correlation length ξ of the model, and let us study how it changes under a change of the coupling constant [22]. In general, since ξ is, dimensionally speaking, a length, it may be written as:

$$\xi = a_0 f(u) \tag{2.7.1}$$

In this formulation, a_0 is the spacial scale of the system and f is an adimensional function depending on u. Since ξ should be invariant under a Renormalization Group transformation, we can assume that:

$$\frac{d\xi}{d\ln(a_0)} = 0 \tag{2.7.2}$$

From this expression one can get the following differential equation, in which the β-function appears:

$$\beta(u)\frac{d\xi}{du}(u) + \xi(u) = 0 \tag{2.7.3}$$

Using (2.6.19) the solution can be easily calculated:

$$\xi(u_1) = \xi(u_2)e^{\frac{2\pi}{u_1} - \frac{2\pi}{u_2}} \qquad (2.7.4)$$

We are interested in the calculation of $\xi(u_0)$, with $u_0 = \frac{2}{g}$ - that's where we started -, supposing that u_2 is sufficiently large - at limit infinite - to make $e^{\frac{2\pi}{u_2}}$ negligible:

$$\xi(u_0) \sim \xi(u_2)e^{\pi S} \qquad (2.7.5)$$

If the spin is integer, the partition function (2.5.11) presents no topological term, so we have a "pure" Non Linear σ Model, with no influence from the topological phase. Since it is well known that the O(3) NLσM is massive, it can be reasonably inferred that the integer spin chain has a gap too; the correlation length may be evaluated from (2.7.5):

$$\xi(u_0) \sim a_0 e^{\pi S} \qquad (2.7.6)$$

In (2.7.6) the correlation length of the system with the usual coupling constant u_0 is estimated to be finite, supporting the thesis of the massiveness of the Heisenberg Antiferromagnetic model with integer spin [22, 27]. The same can not be said for the case of the half spin Heisenberg Chain, since the influence of the topological term is relevant and difficult to analyze. Anyway, it is a well known result of Bethe-Ansatz techniques [10] that in the $\frac{1}{2}$-spin case the model is massless. Since we are interested only in the low-energy limit, we should keep in mind the result we have found through the Renormalization Group transformation performed before: the effective coupling constant increases as the fastest modes are integrated out of the partition function in the semiclassical approximation we are considering. Since the consequence is that the effective spin decreases, we can suppose that the effective theory for a generic half-integer valued spin behaves roughly as the model with the lowest half-integer valued spin possible, that is $S = \frac{1}{2}$. As we know that this particular case is critical, it is possible to suppose that all the half-spin chain are gapless, though obviously not reproducing exactly the behaviour of the $\frac{1}{2}$-spin Antiferromagnetic Heisenberg Chain [22, 27].

Chapter 3

Theoretical and experimental approach to SU(n) systems

In the previous chapter we have seen how the SU(2) Heisenberg model can be treated theoretically. An extension of this model to SU(n) degrees of freedom has been object of research in the past years [1–3, 38, 39]; of course, one may ask why we should be interested in lattice models showing a SU(n) symmetry, since we usually use SU(2) degrees of freedom in order to describe spin systems.

SU(n) groups are well known in the literature since they constitute the gauge symmetry of many phenomena in high energy physics; one example is SU(3) which is the (non abelian) gauge group for Quantum Chromodynamics. In a SU(n) gauge theory, the idea is to describe a (non-abelian) vector potential, belonging to $\mathfrak{su}(n)$ algebra, in interaction with a set of fields which transform according to some representation of the SU(n) group.

Usually, lattice theories are mapped into field theories through semiclassical approximations, as the continuum limit examined for the SU(2) Heisenberg model in Chapter 2. In this way, it is possible to extrapolate information about the lattice model from the continuum theory - in the case analyzed for SU(2), we could estimate the presence or absence of a mass gap in the spectrum of the system depending on the value of the topological term. For gauge theories defined in a continuous space, it can be useful to do precisely the opposite thing, defining a (simplified) gauge theory on a lattice, which is formulated by means of SU(n) degrees of freedom; in this way, all the instruments and techniques of statistical mechanics can be applied also to gauge problems [31]. Numerical simulations can be realized and phase transitions can be examined from a different point of view. In this sense, the formulation of SU(n) models on a lattice constitutes a bridge between high energy physics and condensed matter systems.

This link has recently become even more important thanks to the experimental results obtained in the study of SU(n) systems on a lattice: indeed, the increas-

ing experimental ability in manipulating ultracold atoms trapped in an optical lattice has made it possible to realize experimentally SU(n) systems in a controlled framework, with the possibility to realize many different (effective) SU(n) Hamiltonians on a lattice by tuning the setting parameters of the experiment. In this sense, experimental settings involving ultracold atoms trapped into an optical lattice have all the potentiality to constitute a quantum simulator for SU(n) gauge theories [8, 24].

Since the focus of this work is on SU(3) symmetric 1-dimensional lattice models, an introduction to SU(n) lattice systems both from an experimental and from a theoretical point of view is due. Firstly, some insight on the experimental techniques used in this fields and on why this experimental method is so powerful is given; then, a brief description of how in the literature SU(n) lattice models has been theoretically studied, also from the point of view of semiclassical approximations - similar to the one described for the SU(2) case in the previous chapter - is provided.

3.1   Experimental approach to SU(n) models

Recently many researchers have focused their attention on the experimental implementation of SU(n) symmetric systems, like the ones we have introduced in the previous paragraph. Many experiments have been done using fermionic ultracold alkaline-earth atoms (usually some isotopes of Ytterbium or Strontium) trapped into an optical lattice realized in order to simulate systems whose effective Hamiltonian presents a SU(n) symmetry, making it possible to investigate from an experimental point of view gauge theories defined on a lattice, which, as said before, can be put in relation with many high energy physics phenomena. In this sense experiments with ultracold atoms in optical lattices constitute a powerful and promising quantum simulator for a wide variety of physical phenomena; also the possibility of simulating not only lattice theories with just gauge degrees of freedom, but also the interaction between matter and gauge fields is being investigated [8]. In recent times, the possibility to use Ytterbium atoms in order to study SU(6)-symmetric systems has been explored both from a theoretical [13] and an experimental point of view [44].

Let us now turn to a brief outline of the implementation of SU(n) systems with this promising experimental technique [24]. The ultracold atoms are confined into a lattice, which is created by a periodic potential generated by a set of laser beams. In this way, it is possible to reproduce lattices in various dimensions. Alkaline-earth atoms are the properest ones for this kind of experiments, due to their characteristic features: firstly, their electronic configuration presents an excited state ($|e\rangle$) and a ground state ($|g\rangle$) with total electron spin $\mathcal{J}$ equal to zero in

both cases; secondly, their nuclear spin degree of freedom is almost completely decoupled to the electron spin, given the constraint that the total wave function must be antisymmetric. Together, these two features make these atoms a good choice to simulate $SU(n)$ systems, though, of corse, both nuclear and electronic spin constitute a $SU(2)$ degree of freedom.

Let us now explain why it is so. Thanks to these characteristics, the effective strong-coupling Hamiltonian of these kind of systems can be formulated by means of a set of destruction (creation) operators $c_{j,\alpha,m}$ ($c^\dagger_{j,\alpha,m}$) which destruct (create) an atom at the j-th site of the lattice, in the electronic state α - which can be $|g\rangle$ or $|e\rangle$ - and, denoting with I the nuclear spin, I_z equal to m - which, of course, can vary in the set $(-I, -I+1, \ldots, I-1, I)$. Using these operators it is possible to define a further one, S_{mn}, which fulfills $\mathfrak{su}(n)$ algebra, with $n = 2I + 1$:

$$S_{mn} = \sum_{j,\alpha} c^\dagger_{j,\alpha,n} c_{j,\alpha,m} \tag{3.1.1}$$

$$[S_{mn}, S_{pq}] = \delta_{mq} S_{pn} - \delta_{pn} S_{mq} \tag{3.1.2}$$

It is now clear these are particularly suitable in order to represent $SU(n)$ models on a lattice. Moreover, due to the fact that the number of particles with a certain nuclear spin on the lattice is constant, S_{mm} is constant too for each value of m in $(-I, -I+1, \ldots, I-1, I)$; this implies that, by fixing S_{mm} to zero for some values of m, it is possible to reproduce a $SU(n)$ symmetry with $n < 2I + 1$.

This experimental technique is incredibly powerful. For example, depending on the number of particles on each site of the lattice, it is possible to fix the representation of the $SU(n)$ group on each site. Indeed, the number of particles at the j-th site of the lattice, n_j, ($n_j = \sum_{\alpha,m} c^\dagger_{j,\alpha,m} c_{j,\alpha,m}$) is equal to the sum of the heights of each column of the Young diagram corresponding to the representation of $SU(n)$ on that site (let's keep in mind that, due to the total antisymmetry of the wave function and to the restriction on the possible electron states, the maximum number of columns in such a tableaux is two).

3.2 Read's and Sachdev's approach to SU(n) systems

It has been shown in Chapter 2, in which the $SU(2)$-symmetric Heisenberg model has been studied, how in that case it is possible to get the underlying low-energy field theory from the lattice model through the continuum limit. It is important to remark, however, that this kind of limit is, of course, an approximation, since we are dealing with a semiclassical approach. An approach to this problem in the context of $SU(n)$ chains has been proposed by Sachdev and Read [38,39]; this

section is devoted to a review of their work. The model they are interested in is the SU(n)-symmetric generalization of the Antiferromagnetic Heisenberg model, which is defined substituting in the proper way SU(n) generators to the SU(2) ones of the usual formulation.

The aim of Read's and Sachdev's work is to study a semiclassical approximation for a SU(n) antiferromagnetic Heisenberg Chain, in case there are conjugate representations of the SU(n) group on even and odd sites.

3.2.1 The fermionic formulation of the SU(n) generators

The Hamiltonian Read's and Sachdev's are interested in is given by the following straightforward SU(n)-symmetric generalization of the antiferromagnetic Heisenberg model:

$$H = \frac{J}{n} \sum_i \sum_{\alpha\beta} S_{\alpha\beta}(i) S_{\beta\alpha}(i+1) \tag{3.2.1}$$

$S_{\alpha\beta}$ are the generators of the $\mathfrak{su}(n)$ algebra, in a chosen representation on the odd sites and in its conjugate representation on the even ones. If we label with n_c the number of columns and with m the number of rows of a rectangular tableau, we have that the conjugate of a SU(n) representation (m, n_c) is characterized by $(n - m, n_c)$. A particular case, on which we will focus in the next chapters of this work, is the one of fundamental and antifundamental representations of SU(3):

$$\{3\} \;=\; \Box \qquad\qquad (m = 1, n_c = 1) \tag{3.2.2}$$

$$\{\overline{3}\} \;=\; \begin{array}{c}\Box\\[-3pt]\Box\end{array} \qquad\qquad (m = 2, n_c = 1) \tag{3.2.3}$$

The generators of the $\mathfrak{su}(n)$ algebra can be redifined using fermionic operators. The idea is to describe the SU(n) degrees of freedom of a site by the presence (absence) of one or more fermions on that site, with n possible types of fermions, each one with n_c possible colours.

In order to do so, let us introduce the set of SU(n) operators:

$$\hat{S}_{\alpha\beta} = \sum_a c^\dagger_{a,\beta} c_{a,\alpha} - \delta_{\alpha\beta} \frac{n_c}{2} \tag{3.2.4}$$

The operators c_α ($c^\dagger_\alpha$) are fermionic destruction (creation) operators of tha α-th species, $\alpha \in \{1, \ldots, n\}$ in the a-th colour, $a \in \{1, \ldots, n_c\}$. It is easily verified that the operators so defined fulfill the $\mathfrak{su}(3)$ algebra:

$$\left[\hat{S}_{\alpha\beta}, \hat{S}_{\gamma\delta} \right] = \hat{S}_{\gamma\beta} \delta_{\alpha\delta} - \hat{S}_{\alpha\delta} \delta_{\beta\gamma} \tag{3.2.5}$$

The constraint on the number of fermions on odd $((m, n_c)$ representation) and even $((n - m, n_c)$ representation) sites is:

$$\sum_\alpha c^\dagger_{a,\alpha} c_{b,\alpha} = \delta_{ab} m \qquad \text{on odd sites} \qquad (3.2.6)$$

$$\sum_\alpha c^\dagger_{a,\alpha} c_{b,\alpha} = \delta_{ab}(n - m) \qquad \text{on even sites} \qquad (3.2.7)$$

Another equivalent picture for the even-sublattice representation is found performing a particle-hole transformation on the even sites. In that case, the generators acting upon odd sites are (3.2.4), while on the even sites the generators are defined as:

$$-\hat{S}_{\alpha\beta} = \sum_a d^\dagger_{a,\alpha} d_{a,\beta} - \delta_{\alpha\beta} \frac{n_c}{2} \qquad (3.2.8)$$

$d_{a,\alpha}$ and $d^\dagger_{a,\alpha}$ are new fermionic operators, and formally destroy and create holes on the even sites. The constraint on the number of holes on each (even) site is given by (3.2.6).

3.2.2   SU(n) coherent states

In order to write the partition function of the systems by means of a path integral, as described for the SU(2) case in Chapter 2, it is necessary to introduce coherent states for a SU(n) symmetry. There are many different definitions (see for example [35], or [25,32] for a study of SU(3) coherent states), but we will stick to the one provided by Read and Sachdev in [38,39], since it is the one best fitting their construction.

First of all, let us introduce the highest weight state for the (m, n_c) representation. It is defined as the state $|\Psi_0(m, n_c)\rangle$ which fulfills:

$$\hat{S}_{\alpha\alpha}|\Psi_0(m, n_c)\rangle = +\frac{n_c}{2} \qquad \alpha \in \{1, m\} \qquad (3.2.9)$$

$$\hat{S}_{\alpha\alpha}|\Psi_0(m, n_c)\rangle = -\frac{n_c}{2} \qquad \alpha \in \{m + 1, n\} \qquad (3.2.10)$$

On the even sublattice, the highest weight state is defined as the state $|\Psi_0(n - m, n_c)\rangle$ which fulfills:

$$\hat{S}_{\alpha\alpha}|\Psi_0(n - m, n_c)\rangle = -\frac{n_c}{2} \qquad \alpha \in \{1, m\} \qquad (3.2.11)$$

$$\hat{S}_{\alpha\alpha}|\Psi_0(n - m, n_c)\rangle = +\frac{n_c}{2} \qquad \alpha \in \{m + 1, n\} \qquad (3.2.12)$$

Coherent states for the representation (m, n_c) are found applying the exponential of the generators on the highest weight state; the explicit expression for a

coherent state is:

$$|q\rangle = \exp\left(q_{\lambda\mu}\hat{S}_{\mu\lambda} - q^*_{\lambda\mu}\hat{S}_{\lambda\mu}\right)|\Psi_0(m, n_c)\rangle \tag{3.2.13}$$

$q_{\lambda\mu}$ are complex fields. In the previous formula, $\lambda \in \{1, m\}$ and $\mu \in \{m+1, n\}$. In this way, the exponential in (3.2.13) does not take into account those generators which leave the highest weight state invariant. If we call U the matrix exponential of the generators in (3.2.13), what we get is:

$$|q\rangle = U|\Psi_0\rangle \tag{3.2.14}$$

$$U = \exp\left[\begin{pmatrix} 0 & q \\ -q^\dagger & 0 \end{pmatrix}\right] \tag{3.2.15}$$

With q we denote the complex fields $q_{\lambda\mu}$ disposed accordingly with the value of λ and μ.

Precisely the same construction holds for the conjugate representation on the even sites.

3.2.3 The path integral formulation of the partition function

The coherent states introduced in the previous paragraph are the starting point for Read's and Sachdev's formulation of the partition function Z through a path integral.

It is now possible to replicate all the calculation performed in Chapter 2 in order to evaluate the partition function with a path integral; the type of reasonment is precisely the same, but SU(3) coherent states are used instead of SU(2) ones. What Sachdev and Read get is:

$$Z = \int DQ(\tau)\exp\left(-\mathcal{S}\right) \tag{3.2.16}$$

$$\mathcal{S} = \int_0^\beta d\tau H(Q(\tau)) + \mathcal{S}_B \tag{3.2.17}$$

$$\mathcal{S}_B = -\int_0^\beta d\tau \langle q|\dot{q}\rangle \tag{3.2.18}$$

Analogously to the vector $\mathbf{\Omega}$ introduced in the SU(2) case (see section 2.2), Q is the tensor found calculating the expectation value of the SU(n) generators $\hat{S}_{\alpha\beta}$ on the coherent state. Also in this case, a Berry phase term, $\mathcal{S}_B$, is present, and is of fundamental importance in order to determine the behaviour of the system.

In order to perform the continuum limit, it is necessary to work in the semiclassical approximation $n_c \to \infty$; in this limit, Read and Sachdev find a continuous

non-linear sigma model in 2 dimensions with a topological term, as a function of a unitary hermitian tensor field $\Omega(x, \tau)$:

$$S = S_B + \frac{1}{2} \int_0^\beta d\tau dx \mathrm{Tr} \left[\frac{Jn_c^2}{4n} (\partial_x \Omega)^2 + \frac{n}{16Ja^2} (\partial_\tau \Omega)^2 \right] \tag{3.2.19}$$

With a we denote the lattice spacing of the chain. This action is of particular interest since it has a $\mathrm{U}(n)/(\mathrm{U}(m) \times \mathrm{U}(n - m))$, and so it is a so called grassmannian non-linar σ model [3]. In this sense, in the large-n_c limit, the system under study breaks the $\mathrm{SU}(n)$ symmetry into a smaller one.

A case of particular interest is the one with $m = 1$. In this case, after some calculus, Sachdev [39] finds the following explicit formulation for the continuum limit of S:

$$S = S_{CP^{n-1}} + S_B \tag{3.2.20}$$

$$S_{CP^{n-1}} = \frac{2}{g} \int dxd\tau \left(\partial_\mu \mathbf{z} \cdot \partial_\mu \mathbf{z}^* - (\mathbf{z}^* \cdot \partial_\mu \mathbf{z}) (\mathbf{z} \cdot \partial_\mu \mathbf{z}^*) \right) \tag{3.2.21}$$

$$S_B = \frac{n_c}{2} \int dxd\tau \epsilon_{\mu\nu} (\partial_\mu \mathbf{z}^*) (\partial_\nu \mathbf{z}) \tag{3.2.22}$$

In the previous formulæ, g is the rescaled coupling constant, $g = \frac{4a}{n_c}$. $\mathbf{z}$ is a complex vector field with n components, which are assumed to vary slowly. It fulfills the constraint:

$$\mathbf{z} \cdot \mathbf{z}^* = 1 \tag{3.2.23}$$

Action (3.2.21) is the action of the so called $CP^{(n-1)}$ model [37]; it depends on a complex n-dimensional vector field with the constraint expressed by (3.2.23) living in a two-dimensional space. CP^1 correspond to the O(3) non-linear σ model described in section 2.5. Let us now turn to a brief description of the properties of the CP^{n-1} model [37].

3.2.4 CP^{n-1} models

The Lagrangian of the CP^{n-1} model is [37]:

$$\mathcal{L}_{CP^{n-1}} = \partial_\mu \mathbf{z} \cdot \partial_\mu \mathbf{z}^* - (\mathbf{z}^* \cdot \partial_\mu \mathbf{z}) (\mathbf{z} \cdot \partial_\mu \mathbf{z}^*) \tag{3.2.24}$$

$\mathbf{z}$, as said before, is a n-dimensional complex vector field with norm equal to one:

$$\mathbf{z} = \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix} \qquad \mathbf{z} \cdot \mathbf{z}^* = 1 \tag{3.2.25}$$

It should be noticed that $\mathbf{z} \cdot \partial_\mu \mathbf{z}$ is a pure imaginary number, because, due to the constraint (3.2.25) it holds that:

$$\partial_\mu(\mathbf{z} \cdot \mathbf{z}^*) = \partial_\mu \mathbf{z} \cdot \mathbf{z}^* + \mathbf{z} \cdot \partial_\mu \mathbf{z}^* = 0 \Rightarrow \mathrm{Re}(\mathbf{z}^* \cdot \partial_\mu \mathbf{z}) = 0 \tag{3.2.26}$$

One important feature of the model is the presence of a $U(1)$ gauge invariance; the lagrangian $\mathcal{L}_{CP^{n-1}}$ is invariant under a transformation:

$$z_j(x, \tau) \rightarrow z_j(x, \tau)\mathrm{e}^{i\alpha(x,\tau)} \qquad j \in \{1, ..., n\} \tag{3.2.27}$$

Due to this symmetry, we can introduce an auxiliary gauge vector field A_μ, precisely as it is usually done in the context of QED. This field doesn't describe any physical degree of freedom, but expresses the gauge invariance of the system; indeed one can rewrite the Lagrangian as:

$$\mathcal{L}_{CP^{n-1}} = \partial_\mu \mathbf{z} \cdot \partial_\mu \mathbf{z}^* + A_\mu A_\mu - 2A_\mu(i\mathbf{z}^* \cdot \partial_\mu \mathbf{z}) \tag{3.2.28}$$
$$A_\mu = i\mathbf{z}^* \cdot \partial_\mu \mathbf{z} \tag{3.2.29}$$

With (3.2.29), which expresses the equation of motion of A_μ from Lagrangian (3.2.28), the two formulations of the CP^{n-1} Lagrangian (3.2.24) and (3.2.28) coincide. To continue our parallelism with QCD, we can formulate the Lagrangian once again using the covariant derivative:

$$\mathcal{L}_{CP^{n-1}} = (D_\mu \mathbf{z})^* \cdot (D_\mu \mathbf{z}) \tag{3.2.30}$$
$$D_\mu = \partial_\mu + iA_\mu \tag{3.2.31}$$

We can now find the equation of motion, which should also keep track of the constraint on the modulus of $\mathbf{z}$. In order to do so, we must extremize:

$$\mathcal{S}_{tot} = \int dx d\tau \left(\mathcal{L}_{CP^{n-1}} + \lambda(x, \tau)(\mathbf{z} \cdot \mathbf{z}^* - 1) \right) \tag{3.2.32}$$

The equation of motion we find, simplified by means of the constraint - which makes it possible to express $\lambda(x, \tau)$ in terms of $\mathbf{z}$ and the gauge field - is [37]:

$$D_\mu D_\mu \mathbf{z} - (\mathbf{z}^* \cdot D_\mu D_\mu \mathbf{z}) \mathbf{z} = 0 \tag{3.2.33}$$

It can be shown [37] that, in order to avoid divergencies of the action, the limit of the vector field $\mathbf{z}$ for $r = \sqrt{x^2 + \tau^2} \to \infty$ must fulfill:

$$\lim_{r \to \infty} \mathbf{z}(x, \tau) = \mathbf{z}_0 \mathrm{e}^{i\phi(\theta)} \tag{3.2.34}$$

θ is the angle which, with the radius r, describes in polar coordinates the two-dimensional (x, τ) physical space. $\mathbf{z}_0$ is fixed, while the phase angle ϕ can vary in

function of θ - so, it depends on the direction from which the limit is calculated. ϕ, being an angle, describes a one dimensional sphere (that is, a circumference), which we shall call S_1^{int}, since it describes the internal space of the fields at infinity, while the circumference formed by the possible values of by θ describe the physical space, so it is called S_1^{phys}. The boundary conditions in (3.2.34), in this sense, describe a mapping between two cirmuferences:

$$\phi(\theta) : S_1^{phys} \rightarrow S_1^{int} \tag{3.2.35}$$

As for the case of mappings between spheres S_2, also maps between S_1 spheres can be divided in homotopy classes, that is, classes of mappings which can be deformed with continuity one in the other. These homotopy classes form a group, $\pi_1(S_1)$, which is isomorphic to $\mathbb{Z}$; in this sense, each homotopy class can be labeled by an integer number called winding number, and denoted with $\mathcal{Q}$. It can be demonstrated [37] that in our case the explicit expression for $\mathcal{Q}$ is:

$$
\begin{aligned}
\mathcal{Q} &= -\frac{i}{2\pi} \int dx d\tau \epsilon_{\mu\nu} (D_\mu \mathbf{z})^* (D_\mu \mathbf{z}) \\
&= -\frac{i}{2\pi} \int dx d\tau \left(\epsilon_{\mu\nu} \, \partial_\mu \mathbf{z}^* \cdot \partial_\nu \mathbf{z} \right. + \\
&+ \left. \epsilon_{\mu\nu} \left(A_\mu A_\nu + i A_\mu \, \partial_\nu \mathbf{z}^* \cdot \mathbf{z} + i A_\nu \, \partial_\mu \mathbf{z}^* \cdot \mathbf{z} \right) \right) \\
&= -\frac{i}{2\pi} \int dx d\tau \epsilon_{\mu\nu} \, \partial_\mu \mathbf{z}^* \cdot \partial_\nu \mathbf{z} \tag{3.2.36}
\end{aligned}
$$

We can now go back to the partition function in the continuum limit for the $SU(n)$ Heisenberg model described before. The Berry phase (3.2.22) can be written in terms of the winding number $\mathcal{Q}$:

$$\mathcal{S}_B = i\pi n_c \mathcal{Q} \tag{3.2.37}$$

In order to take into consideration all the homotopy sectors - that is, all the possible paths for $\mathbf{z}$, the partition function we have is:

$$Z = \sum_{\mathcal{Q}} \int D\mathbf{z} D\mathbf{z}^* \delta(\mathbf{z} \cdot \mathbf{z}^* - 1) \mathrm{e}^{-S_{CP^{n-1}}} (-1)^{n_c \mathcal{Q}} \tag{3.2.38}$$

From the previous expression, it is clear that if n_c is even it does not influence the partition function while, if it is odd, the oscillating term in the partition function makes it much difficult to study the behaviour of the model through a path integral formulation. CP^{n-1} models have been investigated deeply both from a numerical [9] and a theoretical point of view [37], due to the fact that it has been argued that this class of model may be used in order to describe QCD.

3.3   Some remarks on the SU(3) chain

In this chapter, we have provided some known results about SU(n) systems on a lattice, with particular emphasis on the SU(n) Heisenberg model with alternate representations. Aim of this work is to study the SU(3) Antiferromagnetic Heisenberg model. The formulation with the fundamental and antifundamental representation of SU(3) alternated on even and odd sites of the chain can be regarded to be of particular interest, since, due to Sachdev's and Read's calculations discussed in the previous section, it can be linked to a model (CP^2) of particular interest in the study of high energy phenomena. It should be kept in mind, however, that the results discussed before hold only in a semiclassical approximation - that is, for $n_c \to \infty$ -. Since the fundamental and antifundamental representations - which both have $n_c = 1$ - are far from this limit, this result should be applied with particular attention to this peculiar case.

One other reason which makes this chain particularly interesting is the fact that SU(n) Heisenberg models of the type described by Read and Sachdev have been inferred [14] to be gapped with $n > n_{critical}$, and gapless with $n < n_{critical}$, with $n_{critical} = 3$; in this sense, the SU(3) Heisenberg chain with alternated representations constitutes a "transition point" for this class of Hamiltonians.

It is clear that the SU(3) Heisenberg chain is a system whose peculiar features are very interesting. In the next chapters, we will provide a map which allows us to write this chain and its "twin" one with the same representation on each site into spin-1 chains, whose behaviour is well known, and some new numerical results will be discussed. Moreover, due to the limitations highlighted before, an alternative approach to the path integral formulation of the partition function of these SU(3) systems is proposed, which may be applied to a wider class of Hamiltonians.

Chapter 4

SU(3) Antiferromagnetic Heisenberg Model

This chapter is devoted to the study of the SU(3) quantum Antiferromagnetic Heisenberg Hamiltonian, and to provide some new results about it. Firstly, the two possible non-equivalent formulations of a Heisenberg Hamiltonian showing a SU(3) symmetry are presented and discussed; the one we are more interested in is the one with alternated fundamental and antifundamental representations on odd and even sites. Secondly, an explicit mapping between SU(3) operators and SU(2) generators in its spin-1 representation is proposed, and the models we get mapping the Heisenberg SU(3) chains into spin-1 are introduced and described. Some new numerical results about the SU(3) Heisenberg chains with alternated representations are presented and compared with the known analytical predictions. Finally, we propose an alternative approach to the path integral formulation of the SU(3) lattice models which could be useful in a wide variety of cases.

4.1 Two non-equivalent Hamiltonians

The model we want to study in this work is the so called SU(3) Antiferromagnetic Heisenberg Model. Its Hamiltonian resembles the one of the SU(2) case (2.1.1), but the generators SU(2) are replaced with the ones of SU(3). Precisely as in the case of a SU(2) symmetry, one may ask which representation - the equivalent of the SU(2) spin - is used in the formulation of this quantum Hamiltonian. If we want to stick to the simplest ones, that is, the fundamental and antifundamental representations, the variety of Heisenberg-like models is wider than in the SU(2) case, due to the fact that for SU(2) fundamental and antifundamental representations coincide, while for SU(3) it is not so. The most straightforward Heisenberg

Hamiltonians with a SU(3) degree of freedom on each site are:

$$\hat{H} = J\sum_i \sum_{\alpha=1}^{8} \lambda_\alpha^{2i-1}\overline{\lambda}_\alpha^{2i} + J\sum_i \sum_{\alpha=1}^{8} \overline{\lambda}_\alpha^{2i}\lambda_\alpha^{2i+1} \tag{4.1.1}$$

$$\hat{H}' = J\sum_i \sum_{\alpha=1}^{8} \lambda_\alpha^{i}\lambda_\alpha^{i+1} \tag{4.1.2}$$

In (4.1.1) and (4.1.2) the site index is denoted in roman letters, while the greek letters label the matrices of the Gell Mann set (in the fundamental or antifundamental representation). The sign of J determines the (anti)ferromagnetic behaviour of these models; our main interest is on the antiferromagnetic case $(J > 0)$. Moreover, it is quite evident that we are considering only isotropic chains.

The main difference between these two systems is given by the SU(3) degrees of freedom that can be found on the sites of a chain: in the model described by $\hat{H}'$, the "particle" at each site can be described by means of SU(3) fundamental representation, while the Hamiltonian $\hat{H}$ describes a system with a SU(3) antifundamental representation on even site and fundamental representation on the odd ones. Hamiltonian $\hat{H}'$ has been studied in literature [2,5]; of particular importance is the possibility to map this system in a spin-1 model with Hamiltonian:

$$\hat{H}_{LS} = J\sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2\right) \tag{4.1.3}$$

This model is the well known Lai-Sutherland model, which is known to be critical [43]; this of course implies that also the model $\hat{H}'$ is critical, as confirmed by numerical results [5]. In particular, its central charge is $c = 2$, as the correspondent field theory is a SU(3) Wess Zumino Witten model of level $k = 1$. An explicit mapping between SU(3) systems and spin-1 models which can be applied also to this case is proposed in the next section. The quantum numbers of this system are:

$$\hat{X} = \sum_i X_i \tag{4.1.4}$$

$$\hat{Y} = \sum_i Y_i \tag{4.1.5}$$

Through this quantum numbers it is possible to catalogue all the states in the spectrum, which, of course, are organized according to SU(3) representations:

$$\{3\} \otimes \{3\} \otimes \ldots = \{\overline{3}\} \oplus \{6\} \ldots \tag{4.1.6}$$

$$\tag{4.1.7}$$

The hamiltonian $\hat{H}$ is of particular importance. It has not been investigated very much in its SU(3) formulation, but it is known to correspond to a pure biquadratic spin 1 chain [2, 14]:

$$H_{biq} = -J \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} \right)^2 \tag{4.1.8}$$

The mapping between SU(3) degrees of freedom and spin-1 ones proposed in the next chapter will make this correspondence clear. Since H_{biq} is known to be massive [29, 30], also our system has a non-null energy gap.

Just from the fact that one is massless and the other is massive, it is clear that the choice of the representations used in the formulation of a SU(3) Heisenberg model makes $\hat{H}'$ and $\hat{H}$ completely different from a physical point of view, though they seem so similar one to the other. It shouldn't arrive as a surprise, however: it is easy to see, after an explicit calculation of the $\overline{\lambda}_\alpha$ keeping in mind (1.3.11), that the Hamiltonian with alternated fundamental and antifundamental representations may be written as an anisotropic all-fundamental SU(3) Heisenberg spin-chain:

$$\hat{H} = J \sum_i \left(-\lambda_1^i \lambda_1^{i+1} + \lambda_2^i \lambda_2^{i+1} - \lambda_3^i \lambda_3^{i+1} - \lambda_4^i \lambda_4^{i+1} \right.$$
$$\left. + \lambda_5^i \lambda_5^{i+1} - \lambda_6^i \lambda_6^{i+1} + \lambda_7^i \lambda_7^{i+1} - \lambda_8^i \lambda_8^{i+1} \right) \tag{4.1.9}$$

As a basis for a single site with a fundamental representation, the canonical basis for $\mathbb{C}^3$ may be chosen, since it is formed by the common eigenvectors of X and Y (see equation (1.3.5)), which correspond to the $|1\rangle$, $|2\rangle$, $|3\rangle$ states (u, d, s respectively) represented in figure 1.2:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |d\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |s\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{4.1.10}$$

The quantum numbers for the antifundamental representation are provided by $\overline{X} = -X$, $\overline{Y} = -Y$; this means that, also in the case of the antifundamental representation, the canonical basis for $\mathbb{C}^3$ can be chosen as basis for the Hilbert space of a single site. The three vectors of the basis correspond to the $|\overline{1}\rangle$, $|\overline{2}\rangle$, $|\overline{3}\rangle$ states ($\overline{u}$, $\overline{d}$, $\overline{s}$) depicted in figure 1.3:

$$|\overline{u}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |\overline{d}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |\overline{s}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{4.1.11}$$

It is important to highlight that, though these basis are formally the same, from a physical point of view they describe very different entities, being related to

fundamental and antifundamental representation respectively (that is, to particles and antiparticles!). The hilbert space of the chain may also be described through the use of Young diagrams:

$$\{3\} \otimes \{\overline{3}\} \otimes \{3\} \otimes \{\overline{3}\} \otimes \ldots \ = \ \{1\} \oplus \{8\} \oplus \{1\} \oplus \ldots \qquad (4.1.12)$$

$$(4.1.13)$$

One of the quantum numbers of the chain is given, of course, by the sum of X on the odd site and $\overline{X}$ on the even sites; the other one is the sum of Y on the odd sites and $\overline{Y}$ on the even sites.

$$\tilde{X} \ = \ \sum_i (X_{2i-1} + \overline{X}_{2i}) = \sum_i (-1)^{i+1} X_i \qquad (4.1.14)$$

$$\tilde{Y} \ = \ \sum_i (Y_{2i-1} + \overline{Y}_{2i}) = \sum_i (-1)^{i+1} Y_i \qquad (4.1.15)$$

$\tilde{X}$ and $\tilde{Y}$ are used to label all states, and so divide the spectrum in "spin" sectors.

4.2   A mapping into a spin-1 chain

The Hamiltonians introduced in the previous section are defined through the use of 3×3 matrices; one may ask if they are related to some SU(2) invariant spin-1 chain, since also in the case of a spin-1 system the Hilbert space of a single site is $\mathbb{C}^3$. Indeed, we will show that this is the case. In order to do so, it is necessary to map a set of SU(3) operators into spin operators fulfilling the $\mathfrak{su}(2)$ algebra. A good choice, in our case, is provided by:

$$S_1 = \lambda_7 \qquad S_2 = -\lambda_5 \qquad S_3 = \lambda_2 \qquad (4.2.1)$$

These three operators fulfill the relations:

$$\begin{aligned}
[\lambda_7, -\lambda_5] &= i\lambda_2 \\
[\lambda_7, \lambda_2] &= -i\,(-\lambda_5) \\
[-\lambda_5, \lambda_2] &= i\lambda_7
\end{aligned} \qquad (4.2.2)$$

These reproduce the $\mathfrak{su}(2)$ algebra:

$$[S_i, S_j] = \epsilon_{ijk} S_k \qquad (4.2.3)$$

By multiplying the three spin components between themselves, we get all the other Gell-Mann matrices:

$$
\begin{aligned}
(S_1)^2 &= \frac{1}{2}\left(-\lambda_3 - \frac{1}{\sqrt{3}}\lambda_8 + \frac{4}{3}\mathbb{I}\right) \\
(S_2)^2 &= \frac{1}{2}\left(\lambda_3 - \frac{1}{\sqrt{3}}\lambda_8 + \frac{4}{3}\mathbb{I}\right) \\
(S_3)^2 &= \frac{1}{\sqrt{3}}\lambda_8 + \frac{2}{3}\mathbb{I} \\
S_1 S_2 &= -T \qquad\qquad S_2 S_1 = -T^\dagger \\
S_2 S_3 &= -U \qquad\qquad S_3 S_2 = -U^\dagger \\
S_3 S_1 &= -V \qquad\qquad S_1 S_3 = -V^\dagger
\end{aligned}
\tag{4.2.4}
$$

Of course, a mapping of this type implies a mapping between spin-1 states and SU(3) states. Due to the fact that for our purposes we will use the all-fundamental formulation of the Hamiltonian $\hat{H}$, the correspondence between SU(2) and SU(3) states is the same on even and odd sites of the chain. In this sense, a basis for the Hilbert space of a single site is found diagonalizing the third component of spin, that is the λ_2 Gell-Mann matrix. Its eigenvalues are $\{-1, 0, 1\}$, as expected for the operator S_3 of a SU(2) symmetry with spin equal to one. A choice for the respective eigenstates is provided by:

$$
\begin{aligned}
|-1\rangle &= \begin{pmatrix} \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \frac{i|u\rangle + |d\rangle}{\sqrt{2}} \\[2mm]
|0\rangle &= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = |s\rangle \\[2mm]
|1\rangle &= \begin{pmatrix} -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \frac{-i|u\rangle + |d\rangle}{\sqrt{2}}
\end{aligned}
\tag{4.2.5}
$$

It is clear that, in the mapping, the u and d states of the fundamental representation are mixed (summed and subtracted) in order to get the proper spin-1 eigenstates.

First of all, let us notice that the SU(2) Heisenberg model in this formulation assumes the form:

$$
H_{Heis} = J\sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1}\right) = J\sum_i \left(\lambda_2^i \lambda_2^{i+1} + \lambda_5^i \lambda_5^{i+1} + \lambda_7^i \lambda_7^{i+1}\right)
\tag{4.2.6}
$$

Of particular interest in our case is the SU(2) spin-1 biquadratic chain:

$$H_{biq} = -J \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \tag{4.2.7}$$

Indeed, we find that it corresponds to the SU(3) Antiferromagnetic Heisenberg Hamiltonian with alternate representations on the chain in the formulation (4.1.9), up to a multiplicative constant and an additive term whose only consequence is to shift the spectrum of the model:

$$
\begin{aligned}
H_{biq} &= \frac{J}{2} \sum_i \Big(-\lambda_1^i \lambda_1^{i+1} + \lambda_2^i \lambda_2^{i+1} - \lambda_3^i \lambda_3^{i+1} - \lambda_4^i \lambda_4^{i+1} \\
&\quad + \lambda_5^i \lambda_5^{i+1} - \lambda_6^i \lambda_6^{i+1} + \lambda_7^i \lambda_7^{i+1} - \lambda_8^i \lambda_8^{i+1} - \frac{8}{3} \Big) \\
&= \frac{1}{2} \hat{H} - \frac{4}{3} L \tag{4.2.8}
\end{aligned}
$$

The final additive term in (4.2.8) does not constitute a problem since it is linear respect to the size L of system, which means that it just shifts the energy density of the chain in the thermodynamic limit.

The general Hamiltonian which can be found combining (4.2.6) and (4.2.7) has been deeply investigated in literature. It can be formulated as:

$$
\begin{aligned}
H_{tot} &= J_1 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} - J_2 \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 = \\
&= J \left(\cos(\alpha) \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \sin(\alpha) \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right) \\
J_1 &= J \cos(\alpha) \\
J_2 &= J \sin(\alpha) \tag{4.2.9}
\end{aligned}
$$

In the previous expression we are assuming $J > 0$. It can be easily verified that, if we set $\alpha = -\frac{\pi}{4}$ in the previous expression, corresponding to the Lai-Sutherland chain, the explicit Hamiltonian we get in terms of SU(3) generators corresponds to Hamiltonian (4.1.2) describe in the previous section.

The physics of the system changes sensibly varying the angle α; the phase diagram as proposed by many works in literature (see, for example, [2, 6, 14, 21]) is represented in figure 4.1. Also its generalization to a higher dimensional lattice has been deeply investigated [45].

There are some points of the diagram, corresponding to particular values of the angle α, which enjoy a SU(3) symmetry. First of all the pure biquadratic chain with a negative coupling may be recovered for $\alpha = \frac{\pi}{2}$ (point F on the phase
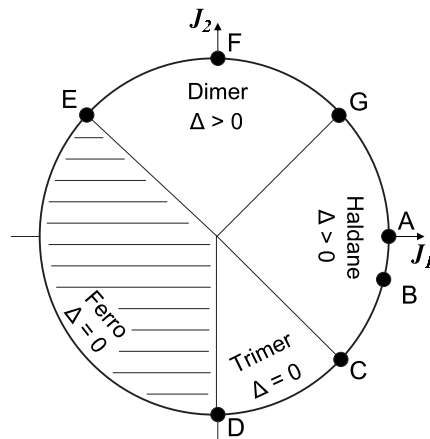
Figure 4.1: The phase diagram of the Hamiltonian (4.2.9) in function of α.
Figure taken from [6].

diagram); as seen before, it corresponds to the antiferromagnetic Heisenberg SU(3) model with alternated representations. It turns out to be exactly solvable and it is in a massive phase [29, 30]. The diametrically opposite point $\alpha = -\frac{\pi}{2}$ (D in figure 4.1) corresponds to the SU(3) ferromagnet with alternated representations on the sites (that is, we have just switched the sign of the coupling of the biquadratic chain); it is at the transition point between two massless phases [36]. Also point C $\left(\alpha = -\frac{\pi}{4}\right)$ is quite interesting: it is the well known Lai-Sutherland model, which, as pointed out before, can be mapped into a the SU(3) antiferromagnetic chain with the fundamental representation at each site. It is massless and its central charge is $c = 2$ (the underling field theory is a Weiss Zumino Witten model of level $k = 1$) [2, 5] . Changing the overall sign of the Hamiltonian, one turns to the equivalent of a SU(3) ferromagnetic chain with the same representation at every site (point E in figure, $\alpha = \frac{3}{4}\pi$).

4.2.1   The map applied to the quantum numbers

The mapping proposed in this Chapter is quite useful also because it makes much more explicit which are the quantum numbers in those points of the diagram 4.1 which have a SU(3) symmetry. Indeed, for the antiferromagnetic SU(3) Heisenberg model with the same representation all over the chain, the quantum

numbers are:

$$\hat{X} = \sum_i X_i$$

$$\hat{Y} = \sum_i Y_i \qquad (4.2.10)$$

Of course, they still are quantum numbers also in the case of a ferromagnetic coupling. Thanks to the map provided in (4.2.2) and (4.2.4), we may translate these quantum numbers in the spin-1 language; if we do so we obtain the quantum numbers for the Hamiltonian:

$$H_{LS} = J\left(\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2\right) \qquad (4.2.11)$$

As said before, depending on the type of coupling, it corresponds to the point C (Lai-Sutherland model, antiferromagnetic coupling) and E (ferromagnetic coupling) in the phase diagram in fig. 4.1. Its quantum numbers turn out to be (up to multiplicative and additive constants, which can be ignored):

$$\hat{X} = \sum_i (S_3^2)_i$$

$$\hat{Y} = \sum_i (S_2^2 - S_1^2)_i$$

$$(4.2.12)$$

Using the commutation relations of the $\mathfrak{su}(2)$ algebra it can be verified in a straightforward way that $\hat{X}$ and $\hat{Y}$ commute with H_{LS}, confirming in this way that they are good quantum numbers for the model.

Precisely the same thing happens for the point F and D in figure 4.1, which, as already noticed, correspond to the SU(3) antiferromagnet and ferromagnet respectively with alternate representations on odd and even sites. Since $\tilde{Y}$ and $\tilde{X}$ (see (4.1.14) and (4.1.15)) are quantum numbers for the SU(3) Hamiltonian $\hat{H}$, the correspondent SU(2) operators are quantum numbers of the spin-1 chain H_{biq} (4.2.7). In this sense, from (4.1.14), (4.1.15) and (4.2.4) we find that, up to multiplicative and additive factors, which do not influence the properties of commutation with the Hamiltonian, the biquadratic spin-1 chain has the following conserved quantities:

$$\tilde{X} = \sum_i (-1)^{i+1} \left(S_2^2 - S_1^2\right)_i$$

$$\tilde{Y} = \sum_i (-1)^{i+1} \left(S_3^2\right)_i \qquad (4.2.13)$$

It can be easily shown that these two operators commute with the Hamiltonian H_{biq}.

If an Hamiltonian has a SU(2) symmetry - as it is for the model (4.2.9) for any value of the angle α -, one of the spin components is chosen as quantum number in order to classify the spectrum. Usually $S_3^{tot} = \sum_i (S_3)_i$ is the chosen one, but of course also S_2^{tot} or S_1^{tot} would be fine (each of them commutes with a SU(2) Hamiltonian, but they do not commute between themselves). Of course, this reasoning may be translated into the SU(3) operator language. Due to the map (4.2.1), we could choose each one of λ_2, $-\lambda_5$ and λ_7 as quantum number; in order to keep the usual convention, we will choose $S_3^{tot} = \sum_i \lambda_2^i$. In this sense, it turns out to be a good quantum number for any value of α in the Hamiltonian (4.2.9), no matter if the corresponding model is SU(3) symmetric or not.

This fact becomes much more interesting for those values of α for which the Hamiltonian is SU(3) symmetric, since it makes explicit a non-obvious quantum number (λ_2 is not diagonal in the defining representation, so usually it is not used in order to classify the spectrum of a SU(3) Hamiltonian). Let us consider the Heisenberg Hamiltonian with fundamental representation on each site ($\alpha = -\frac{1}{4}\pi$ for the antiferromagnet, $\alpha = \frac{3}{4}\pi$ for the ferromagnet); we have:

$$S_3^{tot} = \sum_i \lambda_2^i \qquad (4.2.14)$$

For the one with alternated representations ($\alpha = \frac{\pi}{2}$ for the antiferromagnet, $\alpha = -\frac{\pi}{2}$ for the antiferromagnet) we have:

$$S_3^{tot} = \sum_i \left(\lambda_2^{2i-1} + \overline{\lambda}_2^{2i} \right) = \sum_i \lambda_2^i \qquad (4.2.15)$$

The last relation is due to the fact that $\lambda_2 = \overline{\lambda}_2$. We have found that these two models, which are symmetric under SU(3) transformations in different ways, due to the different structures of the representations on the chain, share a common quantum number.

Let us now have some considerations about the relation between spectrum and quantum numbers for these two chains. Of course, the spectrum of an Hamiltonian with just a SU(2) symmetry will be split into different SU(2) representations (that is, different spin sectors); states into each sectors are labeled through S_3^{tot} eigenvalues. In the case of a SU(3) symmetry, precisely the same things happens, but two quantum numbers ($\tilde{X}$ and $\tilde{Y}$, or $\hat{X}$ and $\hat{Y}$ depending on the "type" of SU(3) symmetry) are needed to classify the states of the various SU(3) representations. Since the SU(3) Heisenberg Hamiltonians enjoy not only the SU(3) symmetry, but also a SU(2) one - which we may expect, since SU(2) is a subgroup of SU(3) - we may split the spectrum both respect to SU(3) and to SU(2) representations. Of

course, the two ways of cataloguing the spectrum are equivalent, but it is convenient to choose one of the two depending on whether we want to study the system as SU(3) Heisenberg model or as SU(2) quadratic chain. Obviously, the two ways of dividing the spectrum must be coherent one with the other, keeping in mind that states of a same representation are degenerate.

4.3   Numerical results

In this section we provide some results known in literature, and use them as a comparison with the results of our DMRG simulations. The Hamiltonian analyzed is the one of the Antiferromagnetic SU(3) Heisenberg model with alternated representations on even and odd sites. Let us recall its explicit formulation:

$$H = J \sum_i \sum_{\alpha=1}^{8} \overline{\lambda}_\alpha^{2i-1} \lambda_\alpha^{2i} + J \sum_i \sum_{\alpha=1}^{8} \lambda_\alpha^{2i} \overline{\lambda}_\alpha^{2i+1} \tag{4.3.1}$$

As shown in the previous section through our mapping, it turns out to be equivalent to the SU(2) Hamiltonian (which, due to this equivalence, has also a SU(3) symmetry):

$$
\begin{aligned}
H_{biq} &= -J \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} \right)^2 \\
&= \frac{1}{2} H - \frac{4}{3} L
\end{aligned} \tag{4.3.2}
$$

The mapping presented in the previous section is of great importance, since it allows us to use all the known results about this SU(2) chain in the study of our SU(3) system. Indeed, the biquadratic SU(2) Hamiltonian has been object of intense study in literature, since it turns out to be exactly solvable. Many analytical and numerical works can be found about this subject; in particular, Klümper [29, 30] showed that this theory is massive, and was able to provide an analytical computation for the ground-state energy density in the thermodynamic limit ($\varepsilon_0 = -2.796863\dots$ in units of the coupling constant J), for the gap with the first excited state ($\Delta = 0.1731788\dots$ in units of the coupling constant J) and for the correlation length ($\xi = 21.0728505\dots$ in units of the lattice space). Since the two Hamiltonians are not precisely the same through our mapping, but there are some multiplicative and additive constant factors in this corrispondence, the gap and the ground-state energy density must be rescaled in order to have the proper

ones for our SU(3) system, so that we find:

$$\varepsilon_0 = -2.927059\ldots$$

(in units of the coupling constant J rescaled to get (4.1.9))

$$\Delta = 0.3463576\ldots$$

(in units of the coupling constant J rescaled to get (4.1.9))

It has been argued [4, 14] that the biquadratic chain (4.2.7) corresponds to a SU(3) symmetric system with alternated representations on the sites; our mapping realizes explicitly this correspondence, allowing us to consider the two hamiltonians (4.2.7) and (4.1.1) equivalent. Moreover, it has also been argued [4, 14] that the first two states of the Hamiltonian are SU(3) singlets which become degenerate in the thermodynamic limit: this is due to the so called dimerization. Dimerization happens when the symmetry under translation of one site is broken, and so there are two degenerate ground-states which are respectively even and odd under translation of one site. Of course, these two states are not degenerate in a finite length chain, and for a finite system one of them corresponds to an excited state.

In terms of the SU(3) chain, we see from the exact diagonalization of the Hamiltonian (4.1.1) with periodic boundary conditions and a number of sites $L = 4, 6$ that effectively the first two SU(3) singlet appearing in the spectrum are respectively even (the ground state one) and odd (the excited one) under translation of one site; it should be noticed that for so short a chain the ground state is given by a representation $\{1\}$ of SU(3), but the antisymmetric singlet becomes the first excited state only for longer chains ($L \geq 8$ as can be seen from DMRG simulations with PBC): there is a crossover phenomenon between a set of degenerate eigenstates forming a representation $\{8\}$ and the singlet (see fig 4.2). The problem of crossover has been mentioned in [11, 42].

From what we said before, it is clear that the correlation length of the system is very large (or equivalently, the gap is very small); it means that, of course, our system is not critical, but it is not so far from criticality. This implies that numerical results must be interpreted carefully since, especially with periodic boundary conditions, the system seems to be somehow critical, which has always made numerical work on this system - or, more properly, on its equivalent SU(2) chain - trickier [11, 42].

Let us now turn to the discussion of the results of our DMRG simulations. The Hamiltonian under exam is (4.1.9), with $J = 1$. In the following graphics, the number of states we keep in the DMRG truncation of the reduced density matrix is denoted with M.

The code used in this work is the one used by the Group IV of the section of Bologna of the INFN in order to study fermionic, bosonic and spin systems. It has been written by F. Ortolani, and it is the same used for numerical research
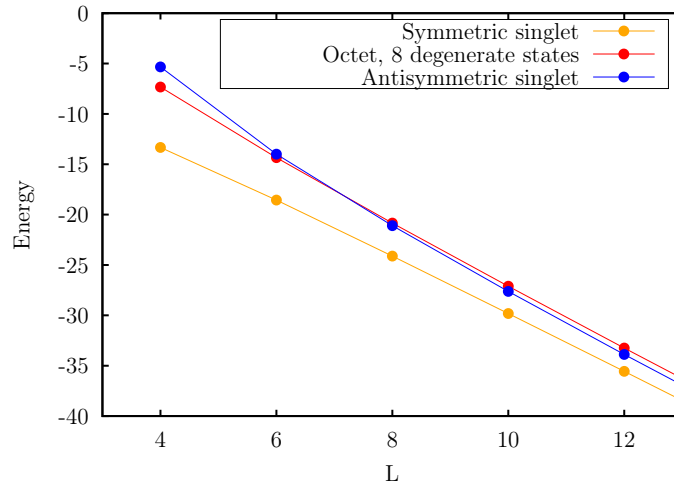
Figure 4.2: The first three states of the energy spectrum from numerical simulations with PBC. The coloured lines have been drawn as a guide for the eye.

about the SU(3) antiferromagnetic Heisenberg Hamiltonian with the fundamental representation at each site in [5]. For a description of the potentialities of the algorithm and of the code in the study of phase transition and critical systems with particular emphasis on spin-1 chains see [18]

4.3.1 Numerical results for the Von Neumann Entropy

Firstly, let us consider the behaviour of the Entropy for the ground-state of the Hamiltonian (4.3.1). Due to the problem pointed out above, under PBC, DMRG data for the Entanglement Entropy of a partition of size l of a chain of length L seems to be fitted quite well by the Cardy-Calabrese formula (see Appendix C) [12] for critical systems:

$$S(l) = \frac{c}{3} \log \left(\frac{L}{a} \sin \left(\frac{\pi l}{L} \right) \right) \tag{4.3.3}$$

DMRG results for $S(l)$ with PBC and for different fixed values of L are presented in figure 4.3. Entropy is calculated using a base-2 logarithm, and (4.3.3) is rescaled consequently in order to estimate a (fictious) value of the central charge c. Also the fit curve representing (4.3.3) is shown. Indeed, the Cardy-Calabrese formula seems to hold, though there is a hint that the model is not really massless: the estimated value of c undergoes huge variations depending on the length L of the chain, from $c \sim 1.405$ for $L = 20$ to $c \sim 1.215$ for $L = 52$.

This problem is solved if we consider open boundary conditions. For a massive system, the entropy of a partition of the system into two halves as a function of
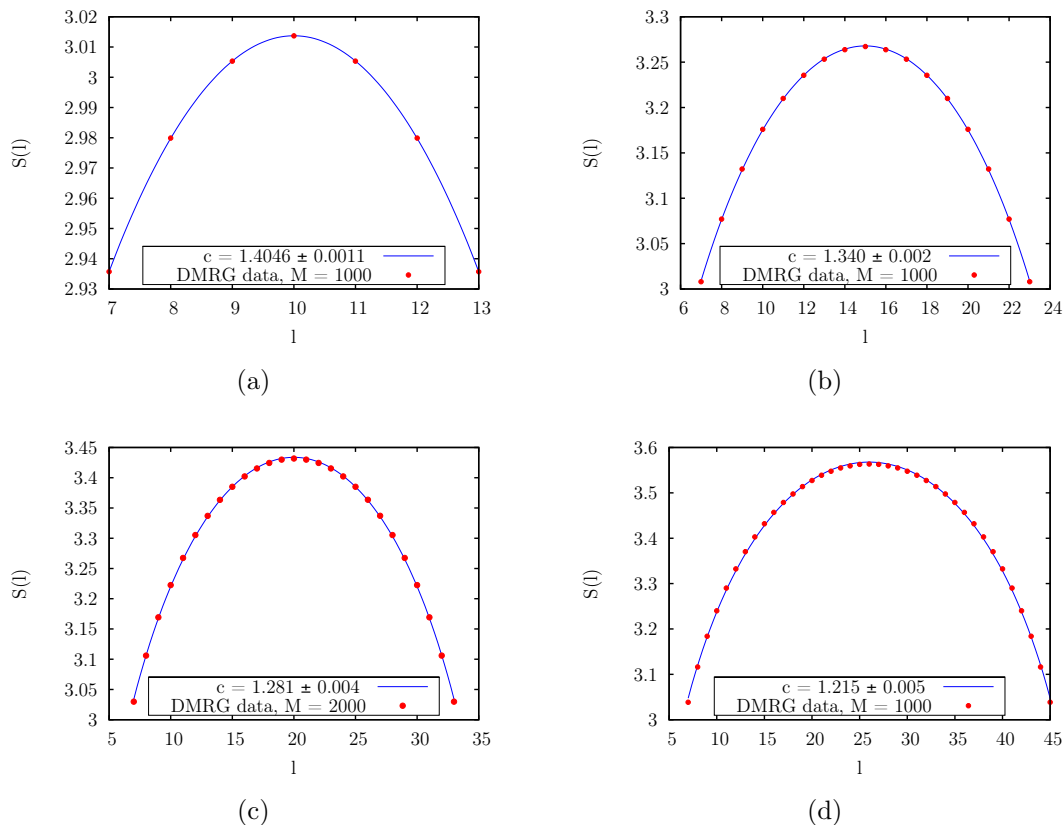
Figure 4.3: DMRG with PBC results for Entanglement Entropies for finite length chains, as a function of the size of the partition considered l. (a) Entropy for $L = 20$. (b) Entropy for $L = 30$. (c) Entropy for $L = 40$. (d) Entropy for $L = 52$

L is expected to saturate to a constant, while for a massless one, as can be easily recovered from (4.3.3) it scales as the logarithm of L. It is well known [12] that for a massive theory in the thermodynamic limit (with $L \gg \xi$), it holds that the entanglement entropy of a part A of a bipartited chain is:

$$S_A \propto \log\left(\frac{\xi}{a}\right) \tag{4.3.4}$$

It is clear that S_A is constant, no matter the length of the chain or the size of the partition. The behaviour of the entanglement entropy in our DMRG simulations with OBC confirms that the system is massive: in figure 4.4 the entropy for a partition of length $\frac{L}{2}$ is shown as function of the size of the chain. For a sufficiently long chain, it clearly saturates to a constant value, as expected.

We can conclude that the estimate of the Entropy for the ground-state through numerical simulations with periodic boundary conditions is not conclusive in order
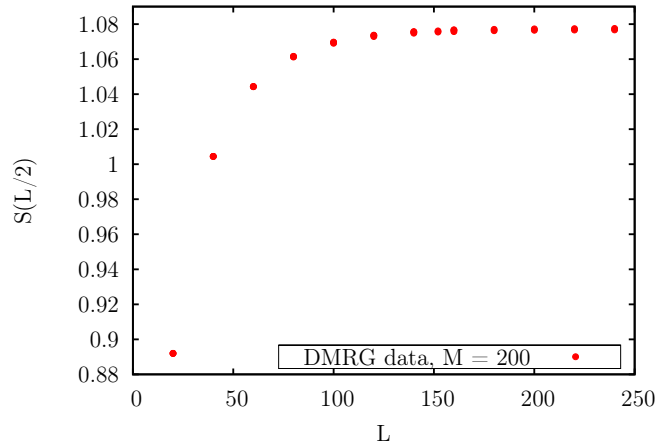
Figure 4.4: Entropy of the bipartited chain as a function of L, using OBC.

to highlight the non-criticality of the system; on the other hand, the massiveness of the theory becomes evident looking at DMRG results for the Entanglement Entropy obtained with open boundary conditions.

4.3.2 Numerical results for the energy spectrum

Also the spectrum of the Hamiltonian has been investigated by means of DMRG simulations; in this way we could estimate the ground-state energy density ϵ_0 in the thermodynamic limit and the gap Δ. The results we will show are obtained targeting only states with $\tilde{X} = 0$ and $\tilde{Y} = 0$: the singlets of the ground state (representation $\{1\}$) have these quantum numbers and the first excited energy level (representation$\{8\}$, so formed by 8 degenerate states) has two states belonging to this "spin" sector.

Before giving the numerical results obtained, it is necessary to stress the difference between OBC and PBC in the study of the structure of the spectrum. With PBC, the two dimerized singlets described at the beginning of the section form the first two states of the spectrum; simulations with periodic boundary conditions make apparent how the two states become degenerate in the thermodynamic limit. In this sense, in order to evaluate Δ from this kind of simulations we should not look at the difference in energy between the first two states (which are degenerate for a chain of infinite length), but at the gap between these states and the third one (which belongs to a representation $\{8\}$). In DMRG simulations with OBC, the situation is completely different: due to the fact that the two boundaries of the chain are not linked by the Hamiltonian with open boundary conditions, we can not see the broken symmetry of translation of one site. These simulations show
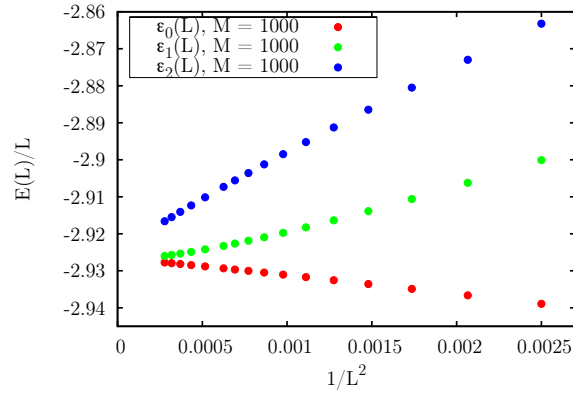
(a)
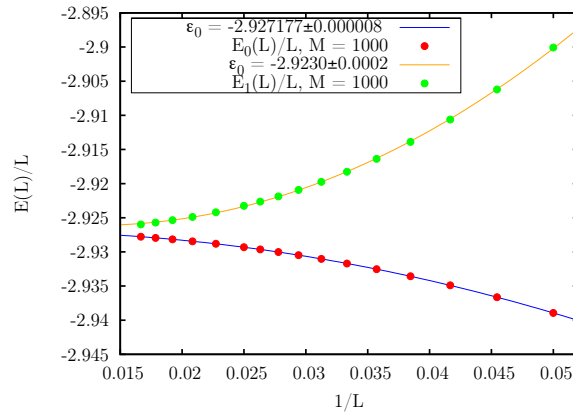
(b)

(c)

Figure 4.5: DMRG results for the energy of the system with periodic boundary conditions. (a) Energy density of the first three states of the spectrum as a function of $\frac{1}{L^2}$. (b) Energy density of the first two states as a function of $\frac{1}{L}$ and estimates of ϵ_0. (c) Difference of energy between the state of the octet and the two singlets as a function of $\frac{1}{L}$, and estimates of the gap Δ.

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us just one singlet as ground state, and the first excited level is formed by the {8} representation.

In figure 4.5 we show the numerical results for the study of the spectrum with periodic boundary conditions. All the fit curves are obtained interpolating the DMRG data with a second-degree polynomial of $\frac{1}{L}$. Both the singlets - which become degenerate in the thermodynamic limit - appear, labeled respectively with E_0 and E_1 since they are not degenerate for a finite length chain. E_2 is the energy of one of the two $\tilde{X} = \tilde{Y} = 0$ states of the octet. From figure 4.5(a), it is clear how the energy densities of the two singlets become more and more similar at the enlarging of the chain; in figure 4.5(b) the estimates for ϵ_0 are reported. The values we get for ϵ_0 (so, the asymptotic value of $E_0(L)/L$ and $E_1(L)/L$ for $L \to \infty$, or $1/L \to 0$) are $\epsilon_0 \sim -2.927$ (if we use the lower-lying singlet) and $\epsilon_0 \sim -2.923$ (if we use the "excited" one). Both this estimates coincide in a good degree of approximation with the theoretical value $\epsilon_0 = -2.927059$. The evaluation of the gap Δ (the difference in energy between the states of the octet and the two singlets, supposed to be degenerate in the thermodynamic limit) changes very much if we use the lower or the higher singlet in order to estimate it, as can bee seen in figure 4.5(c). The values of Δ (as asymptotic value for ΔE in the limit $L \to \infty$, or $1/L \to 0$) we get are $\Delta \sim 0.237$ if we use the lower-lying singlet state, and $\Delta \sim 0.347$ if we consider the higher one. While the first estimate is not so accurate, the second one is highly consistent with the theoretical value $\Delta = 0.3463576$.

In figure 4.6 some numerical results obtained by DMRG simulations using open boundary conditions are presented . Also in this case, all the fit curves are obtained interpolating the DMRG data with a second-degree polynomial of $\frac{1}{L}$. As explained before, in this case there is just one singlet present (whose energy is labeled with E_0). The first excited state in the sector $\tilde{X} = 0, \tilde{Y} = 0$ belongs to the degenerate octet. In figure 4.6(a) data for the energy density of both the ground state and the excited one are presented: the presence of a gap, due to the non-criticality of the model, is evident. From the numerical data shown in figure 4.6(b) we could extrapolate the value of ϵ_0 (that is, the value of $E_0(L)/L$ in the limit $1/L \to 0$): our estimate, $\epsilon_0 \sim -2.927$ is in good agreement with the theoretical one. Not so good is the precision of the value of the gap Δ obtained by a fit of the DMRG data in figure 4.6(c). Indeed, we find an estimate $\Delta \sim 0.299$ which is consistent with the expected value $\Delta = 0.3463576$, though with a certain degree of approximation.

To conclude, we can affirm that energy values obtained with DMRG simulations, both with periodic and open boundary conditions, are coherent with the theoretical prediction of non-criticality of the SU(3) antiferromagnetic Hamiltonian with alternated representations on even and odd sites of the chain. The estimates of the ground-state energy density and of the gap are consistent with the theoretical ones.
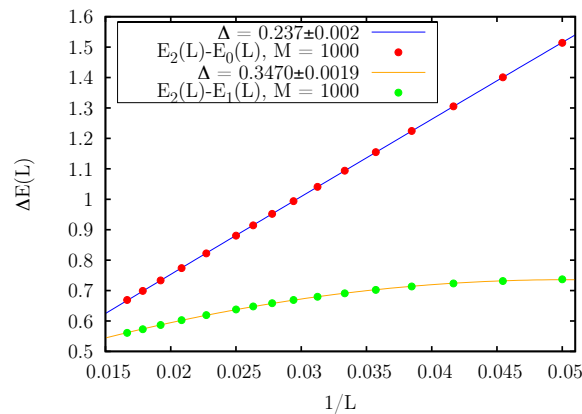
(a)
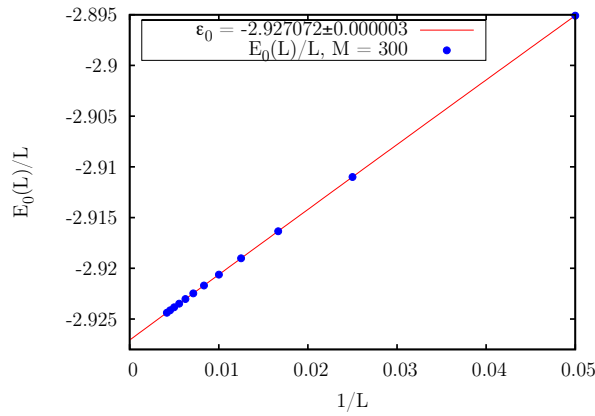
(b)
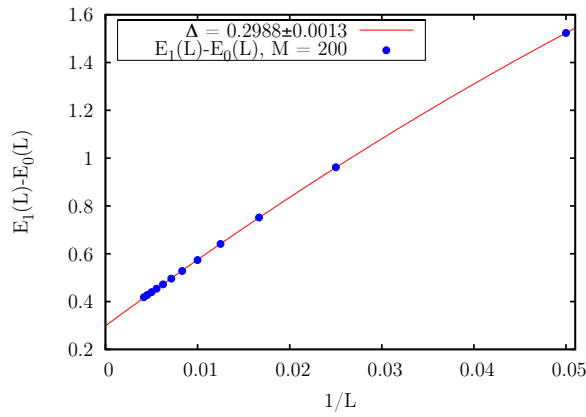
(c)

Figure 4.6: DMRG results for the energy of the system with open boundary conditions. (a) Energy density of the first two states of the spectrum as a function of $\frac{1}{L^2}$. (b) Energy density of the first state as a function of $\frac{1}{L}$ and estimate of ϵ_0. (c) Difference of energy between the state of the octet and the singlet as a function of $\frac{1}{L}$, and estimate of the gap Δ.

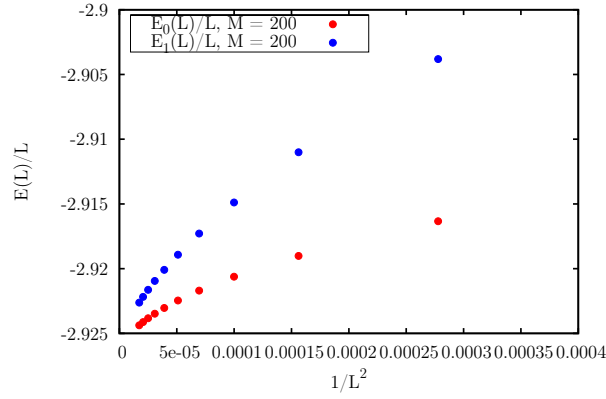# 4.4 Approach to a path integral formulation of the bilinear-biquadratic chain

In this section our aim is to propose a formulation of the path integral for the bilinear-biquadratic chain introduce in the previous chapter by means of SU(3) coherent states. First of all, such coherent states [25] are introduced and their explicit formulation is discussed for both fundamental and antifundamental representations. Then, we calculate the expectation value of the spin-1 Hamiltonian under exam, formulated in terms of SU(3) operators, on the chosen basis of coherent states; this calculation can be considered the first step in order to calculate the continuum limit for the chain at any value of the parameter α.

4.4.1 Coherent states for SU(3)

In this section we present the explicit formulation for SU(3) coherent states in both fundamental and antifundamental representation, basing our reasoning on [25]; this construction resembles the one used by Read and Sachdev in [38,39], but the coherent states we study here are built *ad hoc* for SU(3) fundamental and antifundamental representations.

Coherent states for the fundamental representation

As generators of SU(3) in the fundamental representation, let us choose:

$$\hat{S}_{ij} = |i\rangle\langle j| \qquad (4.4.1)$$

The base states are given, of course, by the canonical base for $\mathbb{C}^3$:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad (4.4.2)$$

It is easy to verify that it holds that:

$$\hat{S} = \begin{pmatrix} \frac{1}{2}\lambda_3 + \frac{1}{2\sqrt{3}}\lambda_8 + \frac{\mathbb{I}}{3} & T^\dagger & V \\ T & -\frac{1}{2}\lambda_3 + \frac{1}{2\sqrt{3}}\lambda_8 + \frac{1}{3}\mathbb{I} & U^\dagger \\ V^\dagger & U & -\frac{1}{\sqrt{3}}\lambda_8 + \frac{1}{3}\mathbb{I} \end{pmatrix} \qquad (4.4.3)$$

We will refer to operators $\hat{S}_{ij}$ as lowering operators if $j < i$ and as raising operators if $i < j$. It should be noticed that in this formulation we are, formally, considering the whole U(3) group, since we are considering also the identity operator among the generators.

The highest weight state is the state $|\Psi_1\rangle$ which fulfills:

$$\hat{S}_{ij}|\Psi_1\rangle = 0 \qquad \forall\, i < j \tag{4.4.4}$$

It can be easily shown that:

$$|\Psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{4.4.5}$$

In order to define the coherent state, we use a triplet of indipendent complex fields, $(\gamma_1, \gamma_2, \gamma_3)$; the coherent state $|\gamma'\rangle$ is found applying the exponential of the lowering operators to the highest weigh state:

$$|\gamma'\rangle = \mathrm{e}^{\gamma_3 \hat{S}_{31}} \mathrm{e}^{\gamma_1 \hat{S}_{21}} \mathrm{e}^{\gamma_2 \hat{S}_{32}} |\Psi_1\rangle = \begin{pmatrix} 1 \\ \gamma_1 \\ \gamma_3 \end{pmatrix} \tag{4.4.6}$$

It should be noticed that our state $|\gamma'\rangle$ does not depend upon γ_2; this doesn't come as a surprise, however, since $|\Psi_1\rangle$ is invariant under the action of $\mathrm{e}^{\gamma_2 S_{32}}$. Moreover, it is necessary to normalize the state $|\gamma'\rangle$, in order to find the normalized coherent state:

$$|\gamma\rangle = \frac{1}{\sqrt{f_1}}|\gamma'\rangle \qquad f_1 = 1 + |\gamma_1|^2 + |\gamma_3|^2 \tag{4.4.7}$$

Thanks to this explicit formulation of SU(3) coherent states in the fundamental representation, it is now possible to find the expectation values of the generators $\hat{S}_{ij}$ calculated on the state $|\gamma\rangle$:

$$\langle \hat{S} \rangle = \frac{1}{f_1} \begin{pmatrix} 1 & \gamma_1 & \gamma_3 \\ \gamma_1^* & |\gamma_1|^2 & \gamma_1^*\gamma_3 \\ \gamma_3^* & \gamma_1\gamma_3^* & |\gamma_3|^2 \end{pmatrix} \tag{4.4.8}$$

Coherent states for the antifundamental representation

The construction of the coherent states for the antifundamental representation is analogue to the one described before for the fundamental representation. We start from the generators of this representation, which are:

$$\hat{\bar{S}}_{ij} = -|i\rangle\langle j| \tag{4.4.9}$$

The basis of states chosen is the same of the fundamental representation case (4.4.2). The explicit formulation of the generators is:

$$\hat{\bar{S}} = \begin{pmatrix} \frac{1}{2}\overline{\lambda}_3 + \frac{1}{2\sqrt{3}}\overline{\lambda}_8 + \frac{\mathbb{I}}{3} & \overline{T}^{\dagger} & \overline{V} \\ \overline{T} & -\frac{1}{2}\overline{\lambda}_3 + \frac{1}{2\sqrt{3}}\overline{\lambda}_8 + \frac{1}{3}\mathbb{I} & \overline{U}^{\dagger} \\ \overline{V}^{\dagger} & \overline{U} & -\frac{1}{\sqrt{3}}\overline{\lambda}_8 + \frac{1}{3}\mathbb{I} \end{pmatrix} \tag{4.4.10}$$

It is evident that the previous expression is analogue to the one of the fundamental representation case, with the operators of one representation exchanged with the one of the other. Also in this case we will refer to operators $\hat{\overline{S}}_{ij}$ as lowering operators if $j < i$ and as rising operators if $i < j$.

The highest weigh state is defined as the state $|\Psi_2\rangle$ which fulfills:

$$\hat{\overline{S}}_{ij}|\Psi_2\rangle = 0 \qquad \forall\, i < j \tag{4.4.11}$$

It is easily verified that:

$$|\Psi_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{4.4.12}$$

Precisely as we have done before, we can define the coherent state for the antifundamental representation using the same triplet of complex fields $(\gamma_1, \gamma_2, \gamma_3)$:

$$|\overline{\gamma}'\rangle = e^{\gamma_3 \hat{\overline{S}}_{31}} e^{\gamma_1 \hat{\overline{S}}_{21}} e^{\gamma_2 \hat{\overline{S}}_{32}} |\Psi_2\rangle = \begin{pmatrix} \gamma_1\gamma_2 - \gamma_3 \\ -\gamma_2 \\ 1 \end{pmatrix} \tag{4.4.13}$$

We are allowed to put $\gamma_1 = 0$ for the antifundamental representation, since $|\Psi_2\rangle$ is invariant under the action of $e^{\gamma_1 \hat{\overline{S}}_{21}}$. The properly normalized coherent state for this representation is:

$$|\overline{\gamma}\rangle = \frac{1}{\sqrt{f_2}}|\overline{\gamma}'\rangle \qquad f_2 = 1 + |\gamma_2|^2 + |\gamma_3|^2 \tag{4.4.14}$$

The expectation values of the generators $\hat{\overline{S}}_{ij}$ calculated respect to this state are:

$$\langle\hat{\overline{S}}\rangle = \frac{1}{f_2}\begin{pmatrix} -|\gamma_3|^2 & -\gamma_2^*\gamma_3 & \gamma_3 \\ -\gamma_2\gamma_3^* & -|\gamma_2|^2 & \gamma_2 \\ \gamma_3^* & \gamma_2^* & 1 \end{pmatrix} \tag{4.4.15}$$

4.5 The expectation value of the Hamiltonian

The Hamiltonian we are interested in is the bilinear-biquadratic spin-1 chain we have described in the previous section:

$$H_{tot} = J\left(\cos(\alpha)\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \sin(\alpha)\sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2\right) \tag{4.5.1}$$

In terms of SU(3) matrices, through the mapping introduced in the previous sections, it can be written as:

$$H_{tot} = J\left(\cos(\alpha) \sum_i \left(\lambda_2^i \lambda_2^{i+1} + \lambda_5^i \lambda_5^{i+1} + \lambda_7^i \lambda_7^{i+1} \right) \right)$$

$$+ \frac{1}{2} \sin(\alpha) \sum_i \left(-\lambda_1^i \lambda_1^{i+1} + \lambda_2^i \lambda_2^{i+1} - \lambda_3^i \lambda_3^{i+1} - \lambda_4^i \lambda_4^{i+1} \right.$$

$$\left. + \lambda_5^i \lambda_5^{i+1} - \lambda_6^i \lambda_6^{i+1} + \lambda_7^i \lambda_7^{i+1} - \lambda_8^i \lambda_8^{i+1} + const. \right) \right) \qquad (4.5.2)$$

We have chosen to use the same representation (the fundamental one) on the various sites, but of course we may also formulate it using fundamental representation on the odd sites and the antifundamental one on the even ones, expressing the operators in the proper way. In this way, it is made much more evident that the term preceded by $\sin(\alpha)$ corresponds - up to multiplicative and additive constants - to the Heisenberg SU(3) Hamiltonian with alternated representations. The formulation of the bilinear-biquadratic spin-1 Hamiltonian becomes then:

$$H_{tot} = \sum_i H_{2i-1,2i} + \sum_i H_{2i,2i+1}$$

$$H_{2i-1,2i} = J\left(\cos(\alpha) \left(\lambda_2^{2i-1} \overline{\lambda}_2^{2i} + \lambda_5^{2i-1} \overline{\lambda}_5^{2i} + \lambda_7^{2i-1} \overline{\lambda}_7^{2i} \right) \right.$$

$$+ \frac{1}{2} \sin(\alpha) \left(\sum_{\alpha=1}^{8} \lambda_\alpha^{2i-1} \overline{\lambda}_\alpha^{2i} + const. \right) \right)$$

$$H_{2i,2i+1} = J\left(\cos(\alpha) \left(\overline{\lambda}_2^{2i} \lambda_2^{2i+1} + \overline{\lambda}_5^{2i} \lambda_5^{2i+1} + \overline{\lambda}_7^{2i} \lambda_7^{2i+1} \right) \right.$$

$$+ \frac{1}{2} \sin(\alpha) \left(\sum_{\alpha=1}^{8} \overline{\lambda}_\alpha^{2i} \lambda_\alpha^{2i+1} + const. \right) \right) \qquad (4.5.3)$$

The additive constants in the previous formula do not change the behaviour of the system, since their only effect is to shift the energy of the model.

Our purpose now is to evaluate the expectation value of H_{tot}, calculated on a total state constituted by coherent states of fundamental and antifundamental representations on odd and even sites respectively. Since this calculation constitutes the main result of this section, let us introduce the context in which we are doing it. It is well known, as we have seen both in Chapters 2 and 3, much information on a quantum theory on a lattice may be extrapolated from the path integral formulation of the partition function of the model and the subsequent

continuum limit through a semiclassical approximation. In this chapter, it has been shown that the bilinear-biquadratic spin-1 Hamiltonian (4.5.1) has a very rich phase diagram with both massive and massless phases, and in some peculiar points of this diagram presents a SU(3) symmetry. It would be very interesting to study in which way this symmetry appears and disappears throughout the phase diagram, analyzing the continuum limit for the general Hamiltonian H_{tot}, in order to see how the low-energy effective field theory changes throughout the phase diagram. To do so, it is necessary, as has been done in Chapters 2 and 3, to introduce a basis of coherent states to use in order to define the path integral of the model. The partition function would be of this kind:

$$
\begin{aligned}
Z &= \int D\boldsymbol{\gamma}\, \mathrm{e}^{-\mathcal{S}} \\
\mathcal{S} &= \int_0^\beta d\tau \langle H_{tot}(\tau)\rangle + \mathcal{S}_{\mathcal{B}} \\
\mathcal{S}_B &= -\int d\tau \langle \boldsymbol{\gamma}|\dot{\boldsymbol{\gamma}}\rangle
\end{aligned}
\qquad (4.5.4)
$$

In this work, we will not estimate the Berry phase $\mathcal{S}_B$, but only the expectation value of the Hamiltonian on a total state formed by alternated fundamental and antifundamental coherent states. In this way, we introduce three complex fields $(\gamma_1, \gamma_2, \gamma_3)$, which in the continuum limit should describe the effective field theory of the model. When the value of the parameter α is such that the system is not in a SU(3)-symmetric phase, we expect that some of these degrees of freedom would turn out to be redundant, since the residual symmetry is SU(2), which is a subgroup of SU(3). In this work, we present the preliminary calculation of $\langle H_{tot}(\tau)\rangle$ with the formalism of coherent states described in this section. In the following, the dipendence on the Wick-rotated "time" τ will be omitted for the sake of simplicity.

Let us now turn to the explicit calculation. First of all, it is useful to remark how the Hamiltonian (4.5.3) may be formulated by means of $\hat{S}$ and $\hat{\bar{S}}$. Firstly, in order to do so, it is useful to formulate it thorugh the ladders operators for the

two representations:

$$H_{tot} = \sum_i H_{2i-1,2i} + \sum_i H_{2i,2i+1}$$

$$
\begin{aligned}
H_{2i-1,2i} = J\bigg(& \cos(\alpha)\left(-T^\dagger_{2i-1}\overline{T}^\dagger_{2i} + T^\dagger_{2i-1}\overline{T}_{2i} - U^\dagger_{2i-1}\overline{U}^\dagger_{2i} + U^\dagger_{2i-1}\overline{U}_{2i}\right. \\
- \ & \left. V^\dagger_{2i-1}\overline{V}^\dagger_{2i} + V^\dagger_{2i-1}\overline{V}_{2i} + h.c.\right) + \sin(\alpha)\left(T^\dagger_{2i-1}\overline{T}_{2i} + U^\dagger_{2i-1}\overline{U}_{2i}\right. \\
+ \ & \left.V^\dagger_{2i-1}\overline{V}_{2i} + h.c + \frac{1}{2}\lambda^{2i-1}_3\overline{\lambda}^{2i}_3 + \frac{1}{2}\lambda^{2i-1}_8\overline{\lambda}^{2i}_8 + const.\right)\bigg)
\end{aligned}
$$

$$
\begin{aligned}
H_{2i-1,2i} = J\bigg(& \cos(\alpha)\left(-\overline{T}^\dagger_{2i}T^\dagger_{2i+1} + \overline{T}_{2i}T^\dagger_{2i+1} - \overline{U}^\dagger_{2i}U^\dagger_{2i+1} + \overline{U}_{2i}U^\dagger_{2i+1}+\right. \\
- \ & \left. \overline{V}^\dagger_{2i}V^\dagger_{2i+1} + \overline{V}_{2i}V^\dagger_{2i+1} + h.c.\right) + \sin(\alpha)\left(\overline{T}_{2i}T^\dagger_{2i+1} + \overline{U}_{2i}U^\dagger_{2i+1}\right. \\
+ \ & \left.\overline{V}_{2i}V^\dagger_{2i+1} + h.c. + \frac{1}{2}\overline{\lambda}^{2i}_3\lambda^{2i+1}_3 + \frac{1}{2}\overline{\lambda}^{2i}_8\lambda^{2i+1}_8 + const.\right)\bigg) \quad (4.5.5)
\end{aligned}
$$

This Hamiltonian can be formulated in a much simpler way through (4.4.3) and (4.4.10) as:

$$
\begin{aligned}
H_{2i-1,2i} = J\bigg(& \frac{1}{2}\cos(\alpha)(\hat{S} - \hat{S}^T)^{2i-1}_{\alpha\beta}(\hat{\overline{S}} - \hat{\overline{S}}{}^T)^{2i}_{\beta\alpha} \\
+ \ & \sin(\alpha)\left(\hat{S}^{2i-1}_{\alpha\beta}\hat{\overline{S}}{}^{2i}_{\beta\alpha} + const.\right)\bigg)
\end{aligned}
$$

$$
\begin{aligned}
H_{2i,2i+1} = J\bigg(& \frac{1}{2}\cos(\alpha)(\hat{\overline{S}} - \hat{\overline{S}}{}^T)^{2i}_{\beta\alpha}(\hat{S} - \hat{S}^T)^{2i+1}_{\alpha\beta} \\
+ \ & \sin(\alpha)\left(\hat{\overline{S}}{}^{2i}_{\alpha\beta}\hat{S}^{2i+1}_{\beta\alpha} + const.\right)\bigg) \quad (4.5.6)
\end{aligned}
$$

In the previous expression the sum over repeated greek letter is implied. The expectation value of the Hamiltonian can then be simply evaluated as:

$$
\begin{aligned}
\langle H_{2i-1,2i}\rangle = J\bigg(& \frac{1}{2}\cos(\alpha)\mathrm{Tr}\left[\langle\hat{S} - \hat{S}^T\rangle^{2i-1}\langle\hat{\overline{S}} - \hat{\overline{S}}{}^T\rangle^{2i}\right] \\
+ \ & \sin(\alpha)\mathrm{Tr}\left[\langle\hat{S}\rangle^{2i-1}\langle\hat{\overline{S}}\rangle^{2i}\right]\bigg) \quad (4.5.7)
\end{aligned}
$$

$$
\begin{aligned}
\langle H_{2i,2i+1}\rangle = \bigg(& \frac{1}{2}\cos(\alpha)\mathrm{Tr}\left[\langle\hat{\overline{S}} - \hat{\overline{S}}{}^T\rangle^{2i}\langle\hat{S} - \hat{S}^T\rangle^{2i+1}\right] \\
+ \ & \sin(\alpha)\mathrm{Tr}\left[\langle\hat{\overline{S}}\rangle^{2i}\langle\hat{S}\rangle^{2i+1}\right]\bigg) \quad (4.5.8)
\end{aligned}
$$

This expectation value can, of course, be expressed in terms of the complex quantities $(\gamma_1, \gamma_2, \gamma_3)$ defined on each site. Using (4.4.8) and (4.4.15) we find:

$$\langle H_{tot} \rangle = \sum_i \langle H_{2i-1,2i} \rangle + \sum_i \langle H_{2i,2i+1} \rangle \tag{4.5.9}$$

$$
\begin{aligned}
\langle H_{2i-1,2i} \rangle &= \frac{J}{f_1^{2i-1} f_2^{2i}} \Bigg(\cos(\alpha) \left[\gamma_1^{2i-1} (\gamma_2^* \gamma_3 - \gamma_2 \gamma_3^*)^{2i} \right. \\
&+ \gamma_1^{*\,2i-1} (\gamma_2 \gamma_3^* - \gamma_2^* \gamma_3)^{2i} \\
&+ \gamma_3^{2i-1} (\gamma_3^* - \gamma_3)^{2i} + \gamma_3^{*\,2i-1} (\gamma_3 - \gamma_3^*)^{2i} \\
&+ (\gamma_1 \gamma_3^*)^{2i-1} (\gamma_2 - \gamma_2^*)^{2i} + (\gamma_1^* \gamma_3)^{2i-1} (\gamma_2^* - \gamma_2)^{2i} \Big] \\
&+ \sin(\alpha) \left[-\gamma_1^{2i-1} (\gamma_2 \gamma_3^*)^{2i} + \gamma_3^{2i-1} \gamma_3^{*\,2i} \right. \\
&- \gamma_1^{*\,2i-1} (\gamma_2^* \gamma_3)^{2i} - |\gamma_1|^{2\,2i-1} |\gamma_2|^{2\,2i} + (\gamma_1^* \gamma_3)^{2i-1} \gamma_2^{*\,2i} \\
&+ \gamma_3^{*\,2i-1} \gamma_3^{2i} + (\gamma_1 \gamma_3^*)^{2i-1} \gamma_2^{2i} + |\gamma_3|^{2\,2i-1} - |\gamma_3|^{2\,2i} \Big] \Bigg)
\end{aligned}
\tag{4.5.10}
$$

$$
\begin{aligned}
\langle H_{2i,2i+1} \rangle &= \frac{J}{f_2^{2i} f_1^{2i+1}} \Bigg(\cos(\alpha) \left[(\gamma_2^* \gamma_3 - \gamma_2 \gamma_3^*)^{2i} \gamma_1^{2i+1} \right. \\
&+ l\, (\gamma_2 \gamma_3^* - \gamma_2^* \gamma_3)^{2i} \gamma_1^{*\,2i+1} \\
&+ (\gamma_3^* - \gamma_3)^{2i} \gamma_3^{2i+1} + (\gamma_3 - \gamma_3^*)^{2i} \gamma_3^{*\,2i+1} \\
&+ (\gamma_2 - \gamma_2^*)^{2i} (\gamma_1 \gamma_3^*)^{2i+1} + (\gamma_2^* - \gamma_2)^{2i} (\gamma_1^* \gamma_3)^{2i+1} \Big] \\
&+ \sin(\alpha) \left[-(\gamma_2 \gamma_3^*)^{2i} \gamma_1^{2i+1} + \gamma_3^{*\,2i} \gamma_3^{2i+1} \right. \\
&- (\gamma_2^* \gamma_3)^{2i} \gamma_1^{*\,2i+1} - |\gamma_2|^{2\,2i} |\gamma_1|^{2\,2i+1} + \gamma_2^{*\,2i} (\gamma_1^* \gamma_3)^{2i+1} \\
&+ \gamma_3^{2i} \gamma_3^{*\,2i+1} + \gamma_2^{2i} (\gamma_1 \gamma_3^*)^{2i+1} + |\gamma_3|^{2\,2i+1} - |\gamma_3|^{2\,2i} \Big] \Bigg)
\end{aligned}
\tag{4.5.11}
$$

In this way, we have seen how the expectation value of the Hamiltonian on the basis of coherent states can be written in terms of three complex fields, which, in the continuum limit, would describe the effective field theory for this lattice model. The next steps should be the evaluation of the Berry phase and the proper mapping into a continuum theory, which we do not discuss here. It is clear, however, that this method can turn out to be very useful in a unified description of the bilinear-biquadratic spin-1 chain in each point of its phase diagram (that is, for any value of the angle α). In this way, we may have an analytical tool to study how the symmetries of the model change throughout its phase diagram.

Conclusions

In this work we have focused on SU(n)-symmetric systems defined on a lattice, with particular emphasis on the SU(3) Heisenberg model. This field of research is of great interest both theoretically and experimentally: SU(n) lattice models can be regarded as simplified models on a discretized space for many high energy phenomena. SU(3) models are of particular interest since SU(3) constitutes the gauge symmetry of QCD. Experimentally, the ability to manipulate in laboratories cold atoms in a optical lattice has become recently so advanced that through this experimental technique it is possible to simulate many different quantum Hamiltonians showing a SU(n) symmetry.

After reviewing the main topics on this field of research, both from an experimental and a theoretical point of view, we have presented a study of the link between spin-1 chains and SU(3) symmetric models. The class of spin-1 Hamiltonians we find shows SU(3)-symmetry in particular points of its phase diagram, which is quite rich, presenting various phase transitions and both massive and massless phases. The link between this class of SU(2)-symmetric chains and SU(3) ones is given by an explicit mapping of SU(3) degrees of freedom into SU(2) ones; this mapping turns out to be very useful, since it makes evident the symmetries of the Hamiltonian.

We presented also some new numerical results about the SU(3) Antiferromagnetic Heisenberg model; these results, obtained by means of the DMRG algorithm, are completely consistent with the ones predicted theoretically on the basis of the behaviour of the spin-1 chain our SU(3) model can be mapped to.

Finally, we have proposed an approach to the path integral for the partition function of SU(3)-symmetric systems through the use of coherent states of the fundamental and antifundamental representations of the SU(3) group. This approach may be applied to the whole class of spin-1 chains mentioned above, in order to understand how the extended SU(3) symmetry emerges at special points of the phase diagram of the SU(2) chain.

Appendix A

An outline of Group Theory

Both in Physics and Mathematics Group Theory is of fundamental importance; in particular, the invariance of a physical system under the action of certain groups gives us many information about the properties and the behaviour of that system. Aim of this Appendix is to provide some basic notions in Group Theory and Representation Theory [15, 26, 41]. Lie algebras and Lie groups will be defined and their properties quickly reviewed [15, 26, 41]. The link between group theory and physics will be described and stressed [26].

A.1   Groups and representations

A group G is defined as a collection of elements characterized by a set of properties:

- A law of composition (which will be denoted by the symbol '$\cdot$') exists between elements of the group. If a and b are elements of the group, then

$$a \cdot b = c$$

  is an element of the group.

- The law of composition is associative:

$$a \cdot (b \cdot c) = (a \cdot b) \cdot c \qquad a, b, c \in G$$

- An element e belonging to the group exists characterized by the property:

$$e \cdot g = g \cdot e = g \qquad g \in G$$

  There is just one element which fulfills this requirement and it is called identity.

- For each element g of the group, another element g^{-1} exists, such that:

$$g \cdot g^{-1} = g^{-1} \cdot g = e \qquad\qquad g^{-1} \in G$$

g^{-1} is called inverse, or reciprocal, of g.

A particular class of group is the one of abelian groups; G is called abelian (or commutative) if

$$g \cdot h = h \cdot g \qquad\qquad \forall g, h \in G \qquad\qquad (A.1.1)$$

It is clear that this definition is very general, and that groups of really different nature exist. Two basic examples of group are the sets $\mathbb{R}$ of real numbers, which may be considered a group with the ordinary sum as composition law, and $\mathbb{R} \setminus \{0\}$ with the ordinary product as composition law. Another trivial example is given by $\mathbb{Z}_2 = \{1, -1\}$ with the product as composition law. One group we will be very interested in is SU(3), which is formed by all 3×3 unitary matrices with determinant equal to one (so called 'special'); it will be studied thoroughly in the following.

One of the most interesting and important area of Group Theory is Representation Theory. Representations give us the chance to materialize such an abstract definition as the one of group through the use of matrices. A d-dimensional representation of a group G is defined as a group of $d \times d$ non-singular matrices with the matrix product as composition law, which is in a homomorphic relation with G itself; we will denote an element of the representation related to $g \in G$ as $\Gamma(g)$. If the homomorphic mapping between G and one of its representations is an isomorphism, the representation is called faithful. If all the elements of a representation are unitary matrices, the representation is called unitary. Two representations $\Gamma(g)$ and $\Gamma'(g)$ are called conjugate one of the other if

$$\Gamma'(g) = \Gamma(g)^*$$
$$\Gamma(g) = \Gamma'(g)^* \qquad\qquad (A.1.2)$$

Given two d-dimensional representations $\Gamma_1(g)$ and $\Gamma_2(g)$, these two are called equivalent if the matrices of the two representations are linked by a similarity transformation which does not depend on the element of the group g:

$$\Gamma_2(g) = S^{-1}\Gamma_1(g)S \qquad\qquad \forall g \in G \qquad\qquad (A.1.3)$$

In (A.1.3) S is a $d \times d$ non singular matrix.

Moreover, a representation may be reducible or irreducible. $\Gamma(g)$, acting on a vector space M, is reducible if it exists a (nontrivial) subspace $N \subseteq M$ so that:

$$\Gamma(g)n \in N \qquad\qquad \forall n \in N \subseteq M \qquad\qquad (A.1.4)$$

N is called invariant subspace. Equivalently, a d-dimensional representation $\Gamma(g)$ may be defined reducible if it can be written - up to a similarity transformation - in the following form:

$$\Gamma(g) = \begin{pmatrix} \Gamma_{11}(g) & \Gamma_{12}(g) \\ \mathbf{0}_{21} & \Gamma_{22}(g) \end{pmatrix} \tag{A.1.5}$$

The matrix $\Gamma(g)$ has been expressed through some matrices $\Gamma_{11}(g)$, $\Gamma_{12}(g)$, $\Gamma_{22}(g)$, which are $d_1 \times d_1$, $d_1 \times d_2$, $d_2 \times d_2$ matrices respectively, for some integer numbers d_1 and d_2 not depending on g with $d_1 + d_2 = d$. With $\mathbf{0}_{21}$ we denote the null matrix $d_2 \times d_1$. It can be proved that $\Gamma_{11}(g)$ and $\Gamma_{22}(g)$ are d_1-dimensional and d-2 dimensional representations of the same group G [15]; in this sense, when $\Gamma(g)$ is reducible, it means that it can be written by means of other 'smaller' representations.

A representation is called irreducible if it is not reducible. Irreducible representations are enough to characterize all unitary representations: it can be proved [15] that every (reducible) unitary representation $\Gamma(g)$, acting on a vector space M may be expressed as the direct sum of irreducible unitary ones $\Gamma_i(g)$, each one acting on a different ortogonal subspace N_i, so that:

$$M = \bigoplus_i N_i \qquad\qquad N_i \subset M\ \forall i \qquad\qquad N_i \perp N_j,\ i \neq j$$

$$\Gamma(g) = \bigoplus_i \Gamma_i \qquad\qquad \Gamma_i(g) : N_i \to N_i \tag{A.1.6}$$

Representations may also be multiplied one with another, and not only summed. The type of product needed to define a product operation between representations is the direct product. Given a $p \times p$ matrix A and a $q \times q$ matrix B, their direct product is defined as:

$$(A \otimes B)_{ijkl} = A_{ij} B_{kl} \qquad\qquad i, j \in \{1, \ldots, p\}, \qquad k, l \in \{1, \ldots, q\} \tag{A.1.7}$$

From (A.1.7) it is straightforward to define a product between representations, since each representation is given by a set of square matrices. Given a d_1-dimensional representation $\Gamma_1(g)$ of the group G acting on the space M_1 and a d_2-dimensional representation $\Gamma_2(g)$ of the same group, acting on the space M_2 , a new $d_1 d_2$-dimensional representation $\Gamma(g)$ may be defined by the direct product:

$$\Gamma(g) = \Gamma_1(g) \otimes \Gamma_2(g) \qquad\qquad \Gamma(g) : M_1 \otimes M_2 \to M_1 \otimes M_2 \tag{A.1.8}$$

Of course definition (A.1.8) may be generalized to any arbitrary number of representations. It is important to underline that, even if the $\Gamma_i(g)$ we are multiplying through the direct product are irreducible, $\Gamma(g)$ is a reducible representation: the direct product doesn't allow us to discover new irreducible representations of a

given group. The result of a direct product between unitary representations is still a unitary representation, and may be expanded as a sum of irreducible unitary ones, according to (A.1.6); this expansion is called Clebsch-Gordan series. The number of times each irreducible representation appears in a Clebsch-Gordan series is called Clebsch-Gordan coefficient.

A.2   Lie groups and Lie algebras

A class of groups which is of particular relevance in physics is the class of Lie groups. Lie groups have a richer structure than ordinary groups, because they have some additional properties. First of all, they are continuous groups; a continuous group G not only fulfills all the requirements of groups, but it is also a topological space, in the sense that a set of neighborhoods U_g may be defined for each element $g \in G$. The structure of topological space must be coherent with group properties and the group composition law. The concept of neighborhood makes it straightforward to define continuity upon such a group. Lie groups form a particular class of continuous groups, fulfilling these additional requirements:

- For any given neighborhood $U \subseteq G$ of the identity element e, each element $g \in U$ can be parametrized through a set of real numbers $(q_1, \ldots, q_n)$. e is parametrized by the set $(0, \ldots, 0)$.

- For any given neighborhood $U \subseteq G$ of the identity element e, the correspondence between elements of the group and the n-ples we use for the parametrization is continuous and $1 - 1$.

- The composition of two elements of the group $g_1(q_1, \ldots, q_n)$ and $g_2(q_1', \ldots, q_n')$ is given by $g_1(q_1, \ldots, q_n) \cdot g_2(q_1', \ldots, q_n') = g(p_1, \ldots, p_n)$; the real variables $(p_1, \ldots, p_n)$ are analytic functions of $(q_1, \ldots, q_n; q_1', \ldots q_n')$.

If a continuous group G has all these properties, then it is called a Lie group of dimension n [15, 41].

Let us now consider a d-dimensional representation of the Lie group G, $\Gamma(q_1, \ldots, q_n)$. If it is analytic respect to $(q_1, \ldots, q_n)$, we can define a set of n $d \times d$ matrices which are called generators of the group:

$$I_j = \frac{\partial \Gamma}{\partial q_j}(q_1 = \cdots = q_n = 0) \qquad\qquad j \in \{1, \ldots, n\} \qquad\qquad (A.2.1)$$

It is clear that the number of the generators does not depend on the representation we have chosen, and that it is equal to the dimension of the Lie group itself.

The concept of Lie group is deeply connected to the concept of Lie algebra [15, 41]. A (real) Lie algebra $\mathcal{L}$ is defined as a vector space V, upon which a inner

product - the 'commutator', which we will denote with the symbol '[...]' - is defined, which has the following properties:

- The commutator of two elements of the space V belongs to V:

$$[x, y] \in V \qquad\qquad x, y \in V$$

- The commutator is antisymmetric under exchange of the two variables:

$$[x, y] = -[y, x] \qquad\qquad x, y \in V$$

- The commutator is linear respect to the first variable:

$$[\alpha x + \beta y, z] = \alpha[x, z] + \beta[y, z] \qquad x, y, z \in V \qquad \alpha, \beta \in \mathbb{R}$$

- The commutator fulfills Jacobi's identity:

$$[x, [y, z]] + [z, [x, y]] + [y, [z, x]] = 0 \qquad\qquad x, y, z \in V$$

It is worth noticing that the second and the third properties listed above together imply that the commutator is linear also respect to the second variable. A particular case of Lie algebra is the one in which V is a space of matrices, and the commutator is indeed what we usually call commutator:

$$[A, B] = AB - BA \qquad\qquad A, B \in V \qquad\qquad (A.2.2)$$

Given a basis x_k for the space V, which we will assume to be n-dimensional, the commutator is univocally defined by its action upon the basis, that is:

$$[x_a, x_b] = \sum_{c=1}^{n} C_{abc} x_c \qquad\qquad (A.2.3)$$

The constants C_{abc} appearing in (A.2.3) are called structure constants of the Lie algebra $\mathcal{L}$, and, due to the antisymmetry of the commutator, are antisymmetric under the exchange of the firs two indices; moreover, as a consequence of the properties of the commutator, they fulfill Jacobi's identity too:

$$C_{abe} C_{ecd} + C_{bce} C_{ead} + C_{cae} C_{ebd} = 0 \qquad\qquad (A.2.4)$$

It is evident that the structure constants are everything we need to know to have a complete knowledge of the commutator itself. It is important to underline that, although the algebra is formed only by real linear combinations of its basis elements, there is no need for the elements themselves to be real. The concept of

representation may be applied to Lie algebra quite in the same way we have done with groups: a d-dimensional representation of a Lie algebra $\mathcal{L}$ is given by a set of $d \times d$ matrices $\Gamma(x)$ so that:

$$
\begin{aligned}
\Gamma(\alpha x + \beta y) &= \alpha \Gamma(x) + \beta \Gamma(y) & x, y \in \mathcal{L} & \qquad \alpha, \beta \in \mathbb{R} \\
\Gamma([x, y]) &= [\Gamma(x), \Gamma(y)] & x, y \in \mathcal{L} &
\end{aligned}
$$

It is clear that $\Gamma(x)$ form a Lie algebra themselves, with the same structure constants, and, if x_k provide a basis for $\mathcal{L}$, $\Gamma(x_k)$ are a basis for the representation. As in the case of groups, $\mathcal{L}$ and its representations stand in a homomorphic relation. Many concepts, as equivalence between representations or reducibility of a representation are precisely the same we have defined in the context of group theory.

We now come to the problem of the relation between Lie algebras and Lie groups. It can be proved that for every Lie group G a Lie algebra $\mathcal{L}$ exists; the number of generators I_j of the group is equal to the dimension of $\mathcal{L}$, and I_j provide a basis for $\mathcal{L}$ [15, 41]. This means that for every Lie group, we can specify some commutation relations between the generators and evaluate the structure constants, thanks to the associate Lie algebra. The commutation relations and the structure constants may help us to recognize different representations of the same Lie group: it may be shown that if a set of matrices acting on a certain space fulfills the relations of the Lie algebra $\mathcal{L}$ (and of its representations) associated to a certain Lie group G, then they provide a set of generators for a representation of G [15, 41].

The correspondence between Lie algebras and Lie groups gives us another powerful method to describe the representations of G: the exponential representation. Given a basis for the Lie algebra $\mathcal{L}$, I_j, and a neighborhood $U \subseteq G$ of the identity element of the group, e, for each element of the neighborhood $g \in U$ there is a n-ple $(q_1, \ldots, q_n)$ (the canonical coordinates), so that:

$$
g = \mathrm{e}^{q_1 I_1 + \cdots + q_n I_n} \tag{A.2.5}
$$

Precisely the same relation holds if we do not consider the group and the algebra themselves but their representations: given a n-dimensional Lie group and its Lie algebra, for every d-dimensional representation of the algebra with basis I_k, a d-dimensional representation of the Lie group exists with a choice of the generators provided by the set I_k itself, so that we can write:

$$
\Gamma(g) = \mathrm{e}^{q_1 I_1 + \cdots + q_n I_N} \qquad (q_1, \ldots, q_n) \in \mathbb{R}^n \tag{A.2.6}
$$

A.2.1 Simple Lie groups and Casimir operators

Given a Lie group G, a subgroup $A \subseteq G$ is called invariant if:

$$gag^{-1} \in A \qquad \forall g \in G, \ \forall a \in A \qquad (A.2.7)$$

A Lie group is called simple if there is no abelian (see (A.1.1)) continuous invariant subgroup for it; a less strong condition applies to the so called semisimple Lie groups, which do not possess continuous abelian invariant subgroups (but may have continuous non abelian ones).

It is called invariant operator, or Casimir operator of a Lie group G (in a certain representation) an operator K which commutes with all the generators I_j of the group:

$$[I_j, K] = 0 \qquad \forall j \in \{1, \ldots, \dim(G)\} \qquad (A.2.8)$$

Semisimple groups have a peculiar feature, described by Racah's theorem: every semisimple Lie group is provided with a number of Casimir operators equal to the largest number of generators of the group commuting with each other (that is, the so called rank of the group). Moreover, each Casimir operator may be expressed in terms of the generators of the group [26]. The importance of Casimir operators and of this theorem in physical applications will be made clear in the following.

A.3 Groups and symmetries in physics

Group theory in physics is of fundamental importance, because the transformations acting upon physical systems can usually be expressed in terms of representations of certain groups; in particular, if the action functional of a system is invariant under the action of a group - more precisely, of one of its representations - that group is said to constitute a symmetry group for the system. Lie groups are of particular relevance in the study of symmetries in physics, due to Nöther theorem; it states that for every continuous symmetry of the system, an integral of motion exists - that is, a quantity whose value doesn't change in time [41]. One basic example is energy: if the system is invariant under translations in time, energy is one of the integrals of motion. We will suppose that this assumption holds for the systems we will study. In the quantum case, conservation of energy allows us to catalogue the states depending on their energy, that is on the eigenvalue of the Hamiltonian. If other symmetries exist, the generators of each group commute with the Hamiltonian: the hamiltonian and the generators can be diagonalized at the same time, and states can be labeled by means of the eigenvalues of the proper number of generators of each group - depending on the rank of the group itself - and of the Hamiltonian. Every eigenvalue used to label the states is called quantum number of the system [26].

In physics, an invariant subspace (see (A.1.4)) for a certain representation of a Lie symmetry group G of the system is called a multiplet. It is quite straightforward to show that, due to the fact that the Hamiltonian and the generators of the group commute and to the Lie structure of the group, the elements of each multiplet have the same energy, that is they are degenerate [26]. Since both the Hamiltonian and the Casimir operators commute with the generators of the group, the invariant operators commute with the Hamiltonian too; moreover, different Casimir operators commute with each other. This means that the Hamiltonian and each of the Casimir operators may be diagonalized at the same time, and consequently that the multiplets are also degenerate eigenstates of the invariant operators: the eigenvalue of the Casimir operators is enough to define the multiplet completely. It is evident how powerful this idea is: it gives us the chance to catalogue uniquely all the possible eigenstates of an Hamiltonian - the states of our system - in terms of the eigenvalues of a limited set of operators. It should be noticed, however, that these considerations hold only if the symmetry group is semisimple, thanks to Racah's theorem.

Appendix B

An outline of DMRG

Density Matrix Renormalization Group (DMRG) is an algorithm that, from the '90s to nowadays, has been one of the most used and appreciated in the field of condensed matter numerical simulations. It has been introduced in 1992 by S.R. White [46, 47], and it allows to have very good estimates for the spectrum and the expectation values of a number of observables. This numerical method has been used in this work in order to study the SU(3) Antiferromagnetic Heisenberg model; in this sense, an introduction to the algorithm and to the main quantities analyzed with it are due.

In this chapter the DMRG algorithm is described [16, 40, 46, 47]; since it is necessary to be aware of the notion of density matrix and reduced density matrix in order to catch the main features of the algorithm, a brief introduction to these operators in physics is given [17, 33]. Moreover, since not only the spectrum but also the entropy of the system under study is analyzed through this numerical method, a qualitative introduction to Entanglement and Entanglement Entropy is provided [17].

B.1 The density matrix

B.1.1 Some general features

Let us suppose to study a quantum system; if it is in a certain (normalized) quantum state $|\psi\rangle$ it is possible to define its density matrix as:

$$\varrho = |\psi\rangle\langle\psi| \tag{B.1.1}$$

If (B.1.1) holds, then the system is said to be in a pure state, that is, its state is precisely defined as a unique quantum state. That is not always the case: it is possible to define also the so called mixed state. A mixed state can be written as

a statistical combination of pure states, that is:

$$\varrho = \sum_k p_k |\psi_k\rangle\langle\psi_k| \tag{B.1.2}$$

$$0 \leq p_k \leq 1 \tag{B.1.3}$$

$$\sum_k p_k = 1 \tag{B.1.4}$$

It is quite important to stress that a mixed state does not correspond to the system being in a quantum state which is a combination of the $|\psi_k\rangle$ appearing in (B.1.2) (which, on the contrary would give a pure state, since a superposition of quantum states is just another precisely determined quantum state): a mixed state is, on the contrary, a classical combination of pure states. Moreover, it is not necessary that the states $|\psi_k\rangle$ are orthogonal one to the other, though they should be normalized to one. In general, some properties hold for a density matrix ϱ [17]:

- ϱ is selfadjoint.

- ϱ is of trace class.

- ϱ is bounded:
$$\||\varrho|\psi\rangle\| \leq \||\psi\rangle\| \quad \rightarrow \quad \|\varrho\| \leq 1 \tag{B.1.5}$$

- ϱ is semipositive:
$$\langle\psi|\varrho|\psi\rangle \geq 0 \qquad \forall\,|\psi\rangle \tag{B.1.6}$$

B.1.2   Reduced density matrix and Schmidt decomposition

Let us suppose that the quantum system under examination is in a pure state (B.1.1). Of course, it is possible to divide it into two subsystems A and B; for each of them is possible to define its own density matrix, which can be found eliminating (tracing out) all the degrees of freedom of the other subsystem from the original density matrix ϱ. ϱ_A and ϱ_B obtained this way are called reduced density matrices [17]. More explicitly, let us start from the state of the total system:

$$|\Psi\rangle \;=\; \sum_{i,j} c_{ij} |i\rangle_A |j\rangle_B = \sum_i |i\rangle_A |\tilde{i}\rangle_B \tag{B.1.7}$$

$$|\tilde{i}\rangle_B \;=\; \sum_j c_{ij} |j\rangle_B \tag{B.1.8}$$

The density matrix can then be written as:

$$\varrho = |\Psi\rangle\langle\Psi| = \sum_{i,k} |i\rangle_A |\tilde{i}\rangle_B \,_A\langle k|_B \langle\tilde{k}| \tag{B.1.9}$$

We can suppose to have chosen the states $|i\rangle_A$ properly, so that it holds:

$$\varrho_A = \sum_i p_i |i\rangle_A {}_A\langle i| \tag{B.1.10}$$

The (reduced) density matrix for the subsystem A can then be evaluated:

$$
\begin{aligned}
\varrho_A = \mathrm{Tr}_B[\varrho] &= \sum_{i,k,j} {}_B\langle j| \left(|i\rangle_A |\tilde{i}\rangle_B {}_A\langle k|_B\langle \tilde{k}| \right) |j\rangle_B \\
&= \sum_{i,k} |i\rangle_A {}_A\langle k| \sum_j \left({}_B\langle \tilde{k}|j\rangle_B {}_B\langle j|\tilde{i}\rangle_B \right) \\
&= \sum_i p_i |i\rangle_A {}_A\langle i| \tag{B.1.11} \\
{}_B\langle \tilde{k}|\tilde{i}\rangle_B &= p_i \delta_{i,k} \tag{B.1.12}
\end{aligned}
$$

(B.1.12) not only tells us that the basis $|\tilde{i}\rangle_B$ we have chosen for the subsystem B is an orthonormal one, but also gives us the chance to have an explicit expression for the reduced density matrix ϱ_A. Moreover, it is quite easy to find also a formulation for $|\Psi\rangle$ and ϱ_B, after the suitable rescaling $|i'\rangle_B = \frac{1}{\sqrt{p_i}}|\tilde{i}\rangle_B$:

$$|\Psi\rangle = \sum_i \sqrt{p_i} |i\rangle_A |i'\rangle_B \tag{B.1.13}$$

$$\varrho_B = \sum_i p_i |i'\rangle_B {}_B\langle i'| \tag{B.1.14}$$

(B.1.13) is called Schmidt decomposition. It is very important to notice that due to (B.1.11), (B.1.13) and (B.1.14), the density matrices ϱ_A and ϱ_B have precisely the same number of non zero weights; this number is called Schmidt number. If it is equal to one, the state of the system is called separable, since it is possible to decompose $|\Psi\rangle$ in two states for the two subsystems, which are not correlated one with the other. On the other hand, if the Schmidt number is greater than one, then the state of the system is called entangled, since it is not possible to decompose $|\Psi\rangle$ in two uncorrelated states of the subsystems and the two subsystem are actually entangled. In the case of a separable state, ϱ_A and ϱ_B represent a pure state each, while, if entanglement is present, they both are mixed states. One particular case of entangled state is the one usually called maximally entangled; in this case ϱ_A has all its weights different from zero, and is, in a certain sense, "as mixed as possible".

B.2 Entanglement and Entropy

From a thermodynamical point of view, if we consider our global system as a canonical ensemble, the definition for its density matrix is [33]:

$$\varrho_{\mathrm{c}} = \frac{1}{Z}\mathrm{e}^{-\beta H} \tag{B.2.1}$$

$$Z = \mathrm{Tr}[\mathrm{e}^{-\beta H}] \tag{B.2.2}$$

To define the thermodynamical entropy, it is useful to remind the definition of free energy:

$$F = -\frac{1}{\beta}\ln(Z) \tag{B.2.3}$$

Entropy can then be expressed with the usual formulation:

$$\mathscr{S} = -\left(\frac{\partial F}{\partial T}\right) \tag{B.2.4}$$

After some calculation, it is straightforward to find [33]:

$$\mathscr{S} = -\langle\ln\left(\varrho_{\mathrm{c}}\right)\rangle = -\mathrm{Tr}\left[\varrho_{\mathrm{c}}\ln\left(\varrho_{\mathrm{c}}\right)\right] \tag{B.2.5}$$

(B.2.5) is a particular case (that is, restricted to the canonical ensemble) of the so called Von Neumann Entropy. It can be defined in a more general way for the density matrix of an arbitrary system as:

$$\mathscr{S} = -\mathrm{Tr}\left[\varrho\ln(\varrho)\right] \tag{B.2.6}$$

If we consider the reduced density matrix ϱ_A defined previously (B.1.10) relatively to the partition of the system under study into two subsystems A and B, the entropy becomes:

$$\mathscr{S}_A = -\sum_k p_k \log(p_k) \tag{B.2.7}$$

This is the explicit expression for the entropy of the subsystem A; since the weights p_k are the same for both the reduced density matrices ϱ_A and ϱ_B, $\mathscr{S}_A$ and $\mathscr{S}_B$ are precisely the same.

Von Neumann Entropy is a good measurement of Entanglement in a bipartite pure state as the one we have seen in the previous paragraph for a series of reasons [17]. In fact, it has a set of features which are usually required for an observable to be interpreted as an estimate of Entanglement:

- $\mathscr{S}(\varrho)$ is equal to zero if calculated using a pure state - so, if the two subsystems A and B seen before are not entangled their Entropy is null.

- The value of $\mathscr{S}(\varrho)$ does not vary under unitary global transformation (precisely as we expect from a local observable as the Entanglement).

- If ϱ is a $d \times d$ density matrix (and we calculate the logarithm in (B.2.6) in base d) it fulfills the relation:

$$\mathscr{S}(\varrho) \leq \ln(d) \tag{B.2.8}$$

  The relation with the identity sign is true only if the state is equipartited (that is, ϱ is a diagonal matrix with d diagonal elements each one equal to $\frac{1}{d}$).

- If ϱ is the density matrix of a system (possibly in a mixed state, due to quantum or thermic interactions with the environment) then, given its subsystems A and B, it holds that:

$$\mathscr{S}(\varrho) \leq \mathscr{S}(\varrho_A) + \mathscr{S}(\varrho_B) \tag{B.2.9}$$

  The equality holds only if the state is not entangled respect to the partition into the two subsystems A and B. Anyway, the entropy of the total system is always minor than the sum of the entropies of its components.

- $\mathscr{S}(\varrho)$ is a convex function:

$$\mathscr{S}(\alpha_1 \varrho_1 + \alpha_2 \varrho_2) \geq \alpha_1 \mathscr{S}(\varrho_1) + \alpha_2 \mathscr{S}(\varrho_2) \quad \alpha_1, \alpha_2 \geq 0 \quad \alpha_1 + \alpha_2 = 1 \tag{B.2.10}$$

B.3 The DMRG algorithm

DMRG stands for Density Matrix Renormalization Group. This algorithm has been incredibly successful in the study of a number of quantum many body systems, like the Heisenberg or the Hubbard model. The main idea is to keep only a certain number of degrees of freedom in the description of the Hamiltionian, which should catch the physics of the system and simplify the evaluation of the observables enough to have approximated but faithful estimates of their expectation values.

The first try in this sense was the Real Space Renormalization Group (RSRG) algorithm, ideated by K. G. Wilson in the '70s [48]. The idea of this algorithm is to use energy as criterion for deciding which states to keep in the approximation. A system with ℓ sites, Hilbert space of dimension M and described by the Hamiltonian $\hat{H}$, is put in interaction with another system equal to itself; the total system will have 2ℓ sites, a M^2-dimensional Hilbert space and will be described by the sum of the Hamiltonians of the two blocks plus an interaction term (which will

replicate the interaction between sites present in the original Hamiltonian). This Hamiltonian can be diagonalized; only the first M states with the lowest energy eigenvalues are kept as approximated basis for the 2ℓ chain, which becomes the starting system for the next iteration of the algorithm. This procedure is repeated until the desired length for the chain is reached. This algorithm seems reliable but it presents a physical problem of fundamental importance: its assumption is that the low energy states of a system are formed by the union of the low energy states of its subsystems. Rarely it is so: if we think at the typical example of a system formed by a free particle in a 1-dimensional box of finite length, its ground state wave function does not present any node wherever, while, if we put together the ground state wave functions for smaller boxes juxtaposed, the global wave function presents nodes at the "junctions" of the boxes [40].

DMRG overcomes the problems typical of the RSRG algorithm, selecting the degrees of freedom to be kept in the approximation procedure in a completely different way, introducing a cutoff on the eigenvalues of the density matrix of the system, and not on the energy spectrum. It has become one of the privileged algorithm for computation and numerical simulation in the field of many body quantum systems.

B.3.1 The infinite-system algorithm

Let us now analyze the first part of this algorithm, the so called infinite-system DMRG [16,40,46,47]. The starting point is a chain of length ℓ (in the program we use, it is equal to four), with an M-dimensional Hilbert space and Hamiltonian $\hat{H}_\ell$. The dimension of the Hilbert space is an input parameter of the code and, at the first iterations of the algorithm, due to the small length of the chain, may be larger than the real one (which is equal to d^ℓ, with d the dimension of the Hilbert space of a single site). What one would like to do now is to expand the chain in a proper way, in order to reach the needed length for the total system; in order to do so, the starting block is expanded by one site (and so described by a Hamiltonian $\hat{H}_{\ell+1}$, with a Md-dimensional Hilbert space) , and then reflected as in a mirror in order to get a second block (this second block is often referred to as environment (E), while the first ($\ell + 1$)-long block is simply called system (S)). The two blocks are then put in interaction through an interacting term (reproducing the interaction between sites in the original Hamiltonian). The result is a so-called superblock with $2\ell + 2$ sites and Hamiltonian $\hat{H}_{2\ell+2}$. As in the RSRG procedure, some kind of approximation is needed, in order to reduce the effective degrees of freedom under examination; $\hat{H}_{2\ell+2}$ is diagonalized and the ground state $|\psi\rangle$ found. It is then possible to define the density matrix for the total system in the usual way $\varrho = |\psi\rangle\langle\psi|$. It is possible to evaluate the reduced density matrix for the block S, tracing out the degrees of freedom of the block E: $\varrho_S = \text{Tr}_E[\varrho]$. Once it is

diagonalized, we choose to keep just the M eigenstates of ϱ_S corresponding to the highest eigenvalues of the reduced density matrix as (approximated) basis for the Hilbert space of the block S; of course, more states we keep, better is the approximation but longer is the computation time. What we have at this point is then a block S with a certain Hilbert space and of length $\ell + 1$, which is the starting block for the next iteration of the algorithm exactly as just described. Its (effective) hamiltonian is found as $\hat{H}_{\ell+1}^{eff} = T^\dagger \hat{H}_{\ell+1} T$, with T is the $(Md) \times M$ matrix having as column the states kept to generate the Hilbert space of the $\ell + 1$ chain. The procedure is repeated until the desired length for the chain is reached.

It should be noticed that the algorithm formulated this way works well in case the chain under consideration has open boundary condition; if the boundary conditions are periodic, during each step the two blocks S and E interact on the boundary, making the numerical analysis much more complicated. It is possible to overcome this difficulty through a small change in the algorithm. If we denote with $\mathcal{B}$ the initial block and p a single site, the construction of the superblock for the open boundary conditions may be summarized as "$\mathcal{B}pp\mathcal{B}$"; in order to take into account the periodic boundary conditions, it is enough to build the superblock as "$\mathcal{B}p\mathcal{B}p$".

B.3.2 The finite-system algorithm

After the necessary number of iterations of the infinite-system algorithm has been performed, we have an approximated set of states describing the system and an effective Hamiltonian, which keeps track of the eliminated degrees of freedom. It is then possible to improve the approximation of the Hilbert space of the system with another procedure, called finite-system algorithm [16, 40, 46, 47]. If we denote with L the size of the chain we want to reach, at the end of the procedure described in the above paragraph we have two blocks of length $\left(\frac{L}{2} - 1\right)$ and two sites between them (or an alternate disposition of blocks and sites if we are dealing with PBC; from now on we will consider only the case of OBC, keeping in mind that the algorithm can be properly modified for periodic boundary conditions). Keeping fixed the total length of the chain (L), the block on the left is step by step enlarged (precisely in the same way it happen for the infinite-system algorithm, with a proper choice of the states to keep in the Hilbert space) and the one on the right becomes smaller, always having two free sites in the middle. The basis for the second block - necessary to evaluate a basis for the Hilbert space of the first block - is recovered from memory: it is necessary to store it during the first part of the DMRG simulation. When the block on the left is of a size such that the block on the right can be exactly diagonalized using M states the role of the right and the left block are exchanged: the right block becomes bigger, and the approximation for its states is improved, while the states for the left block - whose length is decreased

step by step - are recovered from memory. This procedure comes to an end when all the chain has been examinated. This procedure is called sweep, and usually two or three sweeps are enough to have a convenient degree of approximation.

So far, it has always been said that the density matrix used to truncate the Hilbert space is the one related to the ground state; it should be noticed, however, that is possible also to® "target" different states (for example excited ones, or with certain specified quantum numbers), getting more data about excited states.

Appendix C

An outline of Conformal Field Theory

A brief introduction to some concepts of Conformal Field Theory (CFT) is provided in this chapter. First of all, conformal transformations are introduced and defined [20,34]; conformal dimensions and primary fields are then introduced, and the central charge is defined through the use of the so called Operator Product Expansion on the stress-energy tensor of the theory [20, 34]. The mapping of a theory living on a cylinder into a theory on a complex plane is described and some insight on the generators of the conformal transformations is given [20]. Finally, some well known results which turn out to be useful both in the analytical and the numerical study of conformal theories are provided [12, 20]

C.1   Conformal transformations in a 2-dimensional space

A system is said to be conformal if it is invariant under a local scale transformation (which is called conformal transformation) [34]:

$$x \rightarrow \lambda(x)x \tag{C.1.1}$$

Is a known result of CFT that every system which is invariant under global scale transformations, rotations and translations is also conformal; this statement turns out to be very useful in the analysis of conformal models [20]. Let us consider a d-dimensional space; under transformation (C.1.1) the metric tensor $g_{\mu\nu}$ of the space undergoes the following transformation:

$$g'_{\mu\nu}(x') = \Lambda(x)g_{\mu\nu}(x) \tag{C.1.2}$$

If we consider an infinitesimal transformation of kind (C.1.1) we find:

$$x'^{\mu} = x^{\mu} + \epsilon^{\mu}(x) \tag{C.1.3}$$

$$g'_{\mu\nu}(x') = g_{\mu\nu}(x) + \partial_{\mu}\epsilon_{\nu}(x) + \partial_{\nu}\epsilon_{\mu}(x) \tag{C.1.4}$$

If the system is conformal, of course it holds that $g'_{\mu\nu}(x') = g_{\mu\nu}(x)$. In this case it is quite easy to find that [20, 34]:

$$\partial_{\mu}\epsilon_{\nu}(x) + \partial_{\nu}\epsilon_{\mu}(x) = g_{\mu\nu}(x)\frac{2}{d}\partial \cdot \epsilon \tag{C.1.5}$$

From now on we will restrict our analysis to the case of a 2-dimensional euclidean space ($g_{\mu\nu}(x) = \delta_{\mu\nu}$). In this particular case, (C.1.5) can be substituted by this set of requirements:

$$\partial_1\epsilon_1(x) = \partial_2\epsilon_2(x) \tag{C.1.6}$$

$$\partial_1\epsilon_2(x) = -\partial_2\epsilon_1(x) \tag{C.1.7}$$

These requirements make it possible to move from the real space to the complex space. Indeed we can introduce the following complex quantities:

$$z = x_1 + ix_2 \tag{C.1.8}$$

$$\overline{z} = x_1 - ix_2 \tag{C.1.9}$$

$$\epsilon = \epsilon_1 + i\epsilon_2 \tag{C.1.10}$$

$$\overline{\epsilon} = \epsilon_1 - i\epsilon_2 \tag{C.1.11}$$

$$\partial_z = \frac{1}{2}(\partial_1 - i\partial_2) \tag{C.1.12}$$

$$\partial_{\overline{z}} = \frac{1}{2}(\partial_1 + i\partial_2) \tag{C.1.13}$$

These identities, together with (C.1.6) and (C.1.7), tell us that $\epsilon(z)$ and $\overline{\epsilon}(\overline{z})$ are respectively holomorphic and antiholomorphic functions. Though of course z and $\overline{z}$ are dipendent one to the other (we are using two complex variables - that is, four real parameters - to describe a 2-dimensional space!), they are usually treated as indipendent, as we would have done if x_1 and x_2 were continuously extended from $\mathbb{R}$ to $\mathbb{C}$. The metric tensor gets the form:

$$g_{\mu\nu} = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} \qquad \mu, \nu \in \{z, \overline{z}\} \tag{C.1.14}$$

An object which is always of great interest in the study of a theory is the stress-energy tensor $T_{\mu\nu}$; in the usual coordintes (x_1, x_2), it is the Noether Current found when applying a conformal transformation to the action of the model:

$$\delta\mathcal{S} = \frac{1}{2\pi}\int d^2x\, T_{\mu\nu}(x)\partial^{\mu}\epsilon^{\nu}(x) \tag{C.1.15}$$

Due to conformal symmetry (which, as we said, may be regarded as formed by translational, rotational and global scaling symmetries), this tensor has some features of great importance:

$$\partial_\mu T^{\mu\nu}(x) = 0 \qquad T^{\mu\nu}(x) = T^{\nu\mu}(x) \qquad T^\mu_\mu(x) = 0 \qquad (C.1.16)$$

These properties may be translated into the complex language: the new stress-energy tensor can be found through a proper transformation, and properties (C.1.16) change consequentely. The (renormalized) diagonal elements (T and $\overline{T}$) of the new energy tensor are [28] :

$$T = T_{11} - T_{22} - 2iT_{12} \qquad (C.1.17)$$
$$\overline{T} = T_{11} - T_{22} + 2iT_{12} \qquad (C.1.18)$$

From (C.1.16) the following relations hold:

$$\partial_{\overline{z}} T(z, \overline{z}) = \partial_z \overline{T}(z, \overline{z}) = 0 \qquad (C.1.19)$$

This means that T and $\overline{T}$ depend only on z and $\overline{z}$ respectively.

C.2   Primary fields and Operator Product Expansion

Let us now turn to a conformal 2-dimensional field theory. A field φ of the model is called primary if under a conformal transformation ($z' = f(z)$, $\overline{z}' = \overline{f}(\overline{z})$) it transforms as:

$$\varphi'(z', \overline{z}') = \left(\frac{df(z)}{dz}\right)^{-h} \left(\frac{d\overline{f}(\overline{z})}{d\overline{z}}\right)^{-\overline{h}} \varphi(z, \overline{z}) \qquad (C.2.1)$$

The parameters h and $\overline{h}$ are real ones, and are called conformal dimensions of the field. Primary fields constitute a generalization of the so called quasi-primary fields, which transform as C.2.1 only under the action of a certain set of global conformal transformations, and not of a general local conformal transformation.

When studying a model, one is usually interested in the study of the correlation functions of the fields of the theory. In the context of CFT, correlation functions are usually expressed as Operator Product Expansion (OPE); for two given fields A and B, their OPE is defined as:

$$A(z)B(w) = \sum_k \frac{\alpha_k(w)}{(z-w)^k} \qquad (C.2.2)$$

This notation works in the following way: this relation holds only if the lefthand side of the identity belongs to a correlator, the fields α_k are regular when evaluated in w, and terms which are regular in w are omitted from the sum. One clarifying example is the so called Ward Identity; if we define X as a product of n primary fields $(X = \varphi_1(z_1, \overline{z}_1) \ldots \varphi_n(z_n \overline{z}_n))$ with conformal dimensions $(h_i, \overline{h}_i)$, the Ward Identities for the holomorphic and antiholomorphic parts of the stress-energy tensor reads [20]:

$$\langle T(z) X(w_1, \overline{w}_1, \ldots, w_n, \overline{w}_n) \rangle = \sum_{i=1}^{n} \left(\frac{h_i}{(z - w_i)^2} + \frac{1}{z - w_i} \partial_i \right) \langle X(w_1, \overline{w}_1, \ldots, w_n, \overline{w}_n) \rangle \tag{C.2.3}$$

$$\langle \overline{T}(\overline{z}) X(w_1, \overline{w}_1, \ldots, w_n, \overline{w}_n) \rangle = \sum_{i=1}^{n} \left(\frac{\overline{h}_i}{(\overline{z} - \overline{w}_i)^2} + \frac{1}{\overline{z} - \overline{w}_i} \overline{\partial}_i \right) \langle X(w_1, \overline{w}_1, \ldots, w_n, \overline{w}_n) \rangle \tag{C.2.4}$$

In the notation of OPE, the Ward Identities for a single field may be written as:

$$T(z) \varphi(w, \overline{w}) \sim \frac{h}{(z - w)^2} \varphi(w, \overline{w}) + \frac{1}{z - w} \partial_w \varphi(w, \overline{w}) \tag{C.2.5}$$

$$\overline{T}(\overline{z}) \varphi(w, \overline{w}) \sim \frac{\overline{h}}{(\overline{z} - \overline{w})^2} \varphi(w, \overline{w}) + \frac{1}{\overline{z} - \overline{w}} \partial_{\overline{w}} \varphi(w, \overline{w}) \tag{C.2.6}$$

For the correlation function of the stress-energy tensor evaluated in two different points, it holds that [20]:

$$T(z) T(w) \sim \frac{c/2}{(z - w)^4} + \frac{2T(w)}{(z - w)^2} + \frac{\partial T(w)}{(z - w)} \tag{C.2.7}$$

From the comparison between (C.2.5) and (C.2.7) it is clear that the stress-energy tensor is a quasi-primary field with conformal dimension $h = 2$. The constant c appearing in (C.2.7) is a fundamental quantity in CFT, and it is called central charge; its value depends on the degrees of freedom of the system under consideration. In general, models with the same central charge belong to a so called universality class, that is, an ensemble of systems which behave substantially in the same way and can be regarded as equivalent after a proper mapping; in this sense, once the central charge of a conformal system is known, it is possible to extrapolate information about its behaviour from the behaviour of the other systems of the same class.

C.3 Radial Quantization and the Virasoro Algebra

In the context of conformal field theory, the usual method of quantization is the so called radial quantization [20]. First of all, let us consider a 1+1 dimensional model defined on an infinite cylinder: its height (which goes from $-\infty$ to $+\infty$) is the time coordinate t, while the space coordinate x, belonging to the interval $(0, L)$, describes the circumferences which form the cylinder, and has periodic boundary conditions (the space time point $(0, t)$ is identified with (L, t)). It is possible to map this cylinder into the complex plane with complex coordinate z, using the following transformation:

$$z = e^{\frac{2\pi\xi}{L}} \tag{C.3.1}$$

$$\xi = t + ix \tag{C.3.2}$$

In this picture, each space-time position is described by a complex point on the plane; points with the same modulus (that is, at the same distance from the origin of the plane) describe the same time moment, but in different spacial positions. In this sense, it is clear that the origin of the plane corresponds to $t = -\infty$ and, if the complex plane is compactified into an S^2 sphere, $t = +\infty$ is described by the northern pole of this sphere.

This construction is needed in order to have a well defined Hilbert space. As first step, it is necessary to define a vacuum state for the theory ($|0\rangle$) upon which the proper creation operators may be applied in order to get all the possible states; this vacuum has to be invariant under conformal transformations. Usually, in QFT, the fields of an interacting theory are regarded as free in the limit $t \to \pm\infty$; the fields obtained in this limit are called asymptotic fields, and from the action of an asymptotic field upon the vacuum one gets a so-called asymptotic state. The same procedure can be followed also in the case of a CFT with radial quantization; let us consider the asymptotic "in" field, defined at $t = -\infty$, which in the formalism of radial quantization can be recast as:

$$\varphi_{in} = \lim_{z, \overline{z} \to 0} \varphi(z, \overline{z}) \tag{C.3.3}$$

The asymptotic "in" state assumes the form:

$$|\varphi_{in}\rangle = \varphi_{in}|0\rangle = \lim_{z, \overline{z} \to 0} \varphi(z, \overline{z})|0\rangle \tag{C.3.4}$$

Let us now suppose that $\varphi(z, \overline{z})$ is a (quasi)primary field with conformal dimensions h and $\overline{h}$. Of course, it is possible to perform a Taylor expansion of the field in

order to get [20]:

$$\varphi(z,\overline{z}) \;=\; \sum_{m,n \in \mathbb{Z}} z^{-m-h}\overline{z}^{-n-\overline{h}}\varphi_{m,n} \tag{C.3.5}$$

$$\varphi_{m,n} \;=\; \frac{1}{2\pi i}\oint dw\, w^{m+h-1}\frac{1}{2\pi i}\oint d\overline{w}\,\overline{w}^{n+\overline{h}-1}\varphi(w,\overline{w}) \tag{C.3.6}$$

Looking carefully at (C.3.4), (C.3.5), (C.3.6), it is clear that for (C.3.4) to hold it is necessary that:

$$\varphi_{m,n}|0\rangle = 0 \qquad m > -h,\; n > -\overline{h} \tag{C.3.7}$$

This kind of expansion can be applied to the stress-energy tensor in a quite straightforward way: keeping in mind that for $T(z)$, the conformal dimension h is equal to 2, (C.3.5) and (C.3.6) become:

$$T(z) \;=\; \sum_{n \in \mathbf{Z}} z^{-n-2}L_n \tag{C.3.8}$$

$$L_n \;=\; \frac{1}{2\pi i}\oint dw\, w^{n+1}T(w) \tag{C.3.9}$$

In a quite analogous way, one can find, for the antiholomorphic stress-energy tensor:

$$\overline{T}(\overline{z}) \;=\; \sum_{n \in \mathbf{Z}} \overline{z}^{-n-2}\overline{L}_n \tag{C.3.10}$$

$$\overline{L}_n \;=\; \frac{1}{2\pi i}\oint d\overline{w}\,\overline{w}^{n+1}\overline{T}(\overline{w}) \tag{C.3.11}$$

L_n and $\overline{L}_n$ constitute the set of generators of the conformal transformations on the Hilbert space defined before. They form the Virasoro Algebra, which is characterized by the following commutation relations:

$$[L_n, L_m] \;=\; (n-m)L_{n+m} + \frac{c}{12}n(n^2-1)\delta_{n+m,0} \tag{C.3.12}$$

$$\left[L_n, \overline{L}_m\right] \;=\; 0 \tag{C.3.13}$$

$$\left[\overline{L}_n, \overline{L}_m\right] \;=\; (n-m)\overline{L}_{n+m} + \frac{c}{12}n(n^2-1)\delta_{n+m,0} \tag{C.3.14}$$

The operators L_0 and L_0 are peculiar, since they generate dilatations in the complex plane, corresponding to time translation in the radial quantization formalism; keeping in mind that energy is the conserved charge related to time-translation invariance, this implies that the Hamiltonian must be proportional to the sum of

these two generators. Indeed, the Hamiltonian of a conformal theory on a cylinder may be formulated as [20]:

$$H = \frac{2\pi}{L}(L_0 + \overline{L}_0) - \frac{c\pi}{6L} \tag{C.3.15}$$

This Hamiltonian constitutes the evolution operator of the system. This kind of Hamiltonian is often found as continuum limit of (critical) Hamiltonians defined on a lattice. When performing this limit from the discrete space of the lattice to a continuum space coordinate, the resulting Hamiltonian usually differs by a multiplying constant v from the expression C.3.15. Though this doesn't affect the physics of the model at all, it is important because it constitutes a characteristic velocity of the model. In the following we will keep this constant explicit when needed. L_1, $\overline{L}_1$, L_{-1} and $\overline{L}_{-1}$ generate all the other global conformal transformations; the vacuum has to be invariant under the action of these generators plus the two generators of time-translations:

$$L_n|0\rangle = 0 \qquad n \in \{0, 1, -1\} \tag{C.3.16}$$
$$\overline{L}_n|0\rangle = 0 \qquad n \in \{0, 1, -1\} \tag{C.3.17}$$

It is possible to generate new states through the action of an asymptotic field of conformal dimensions $(h, \overline{h})$ on the conformal vacuum:

$$|h, \overline{h}\rangle = \varphi(0,0)|0\rangle \tag{C.3.18}$$

These asymptotic states are labeled through the conformal dimensions of the field because the following relations hold:

$$L_0|h, \overline{h}\rangle = h|h, \overline{h}\rangle \tag{C.3.19}$$
$$\overline{L}_0|h, \overline{h}\rangle = \overline{h}|h, \overline{h}\rangle \tag{C.3.20}$$

Due to (C.3.15), conformal states defined this way are eigenstates of the hamiltonian; moreover, since in the case we are interested in (that is, in unitary theories) the conformal dimensions are positive, the conformal vacuum turns out to be the ground state of the system.

Starting from an asymptotic state it is possible to build a tower of conformal states, through the action of the Virasoro operators upon it:

$$L_n|h, \overline{h}\rangle = 0 \qquad n > 0 \tag{C.3.21}$$
$$\overline{L}_n|h, \overline{h}\rangle = 0 \qquad n > 0 \tag{C.3.22}$$
$$L_{-n}|h, \overline{h}\rangle = |h+n, \overline{h}\rangle \qquad n > 0 \tag{C.3.23}$$
$$\overline{L}_{-n}|h, \overline{h}\rangle = |h, \overline{h}+n\rangle \qquad n > 0 \tag{C.3.24}$$

C.4 Some useful relations

At the beginning of the previous section, our starting point was a conformal theory defined on a cylinder (and so, with a finite spacial length L), which was then mapped into a complex plane. All the comments and definitions that followed did not keep track of the finite length of the system, but only of the lucky case of having transferred the theory to the complex plane. In physics, we are usually interested in studying systems with infinite length (that is, in the thermodynamic limit) though often - for example, through the use of numerical methods - only finite length systems can be properly studied in every detail. In this sense, it is of great importance to understand what happens to some physical observables, like energy or Entropy, when the system under study is of finite or infinite size.

The fact is that, if we study a theory living on a cylinder, we should keep in mind that in some way we are introducing a boundary, though the manifold under consideration is infinite: a finite correlation length (ξ) exists, due to the presence of a characteristic length scale L, though in a conformal theory we expect $\xi = \infty$. Every problem disappears in the limit $L \to \infty$. This is exactly what happens when studying the so called critical systems. When a system (for example, defined on a linear lattice) is at a critical point (respect to some coupling parameters), it is expected to have an infinite correlation length - that is, to be massless.

Let us consider a theory on the cylinder. It is possible to define the free energy of the system (F) per unit of (physical) length (as before, let us call it L), and to evaluate it. This result is well known and derives from (C.3.15); it states that [20]:

$$\frac{F}{L} = f_0 - \frac{\pi c v}{6L^2} \tag{C.4.1}$$

Moreover, from the definition of the excited states in a Verma module and of the Hamiltonian, it is possible to estimate the energy gap between the ground state and an excited state with conformal dimensions $\left(h + N, \overline{h} + \overline{N}\right)$ (h and $\overline{h}$ are the conformal dimensions of the asymptotic state and N and $\overline{N}$ give us the shift of the conformal dimensions of the excited state from the ones of the asymptotic state) [20, 28]:

$$\delta E = \frac{2\pi \left(h + \overline{h} + N + \overline{N}\right) v}{L} \tag{C.4.2}$$

Of course, the gap closes as the size of the system becomes bigger, as expected for a critical system.

Another quantity that gives us a huge amount of information about the system is the Entanglement Entropy. About it a well known result exists, which can be very useful not only from an analytical point of view, but also in the context of numerical simulations. Let us consider a theory defined on a finite chain of length

L with lattice spacing a; moreover, let us assume that the correlation length of the chain, ξ - which is non infintite because of the finiteness of the system - is much bigger than a. The chain can be divided into a subsystem of size ℓ (let's call it A) and a subsystem of size $L - \ell$ (labelled with B). Given the density matrix ϱ of the system, it is possible to estimate the entanglement entropy of the partition:

$$\varrho_A = \mathrm{Tr}_B\left[\varrho\right] \tag{C.4.3}$$

$$S_A = -\mathrm{Tr}_A\left[\varrho_A \ln \varrho_A\right] \tag{C.4.4}$$

Through the path integral formulation of the partition function and of the density matrix, Calabrese and Cardy [12] studied the entropy of a bipartited system of this kind, under the hypothesis it is conformal in the thermodynamic limit; they were able to provide the celebrated Cardy-Calabrese formula, which, for a system with periodic boundary conditions, reads:

$$S_A = \frac{c}{3}\ln\left(\frac{L}{\pi a}\sin\left(\frac{\pi \ell}{L}\right)\right) + b \tag{C.4.5}$$

b is a non universal constant. It is important to stress that this formula relates the Entanglement Entropy with the central charge, which gives us a powerful tool for the estimate of c through numerical data, also due to the fact that equation (C.4.5) does not have any dependence on the characteristic velocity v (while (C.4.1) and (C.4.2) do); moreover, precisely as one should expect, S_A has its maximum when $\ell = \frac{L}{2}$.

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