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Non-local order parameters in one-dimensional spin systems

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Abstract

Per molti anni si è creduto che la teoria di Landau sulla rottura spontanea di simmetria esaurisse la descrizione di tutte le fasi in cui è possibile osservare la materia. Ogni transizione di fase si riteneva dunque dover essere sempre accompagnata da un cambiamento della simmetria del sistema. È da diversi decenni ormai che però siamo consapevoli dell'esistenza di fasi della materia distinte che posseggono esattamente la stessa simmetria. A queste fasi è stato dato il nome di fasi topologiche, e chiaramente non possono essere descritte e previste dalla teoria di Landau. In sistemi unidimensionali è possibile osservare fasi topologicamente non banali in presenza di alcune simmetrie. L'esempio più importante in questo contesto è fornito dalla fase in cui si trova la catena di Heisenberg di spin 1 antiferromagnetica, la cosiddetta fase di Haldane. Essa risulta una dei primi esempi di fase topologica, e presenta già diverse caratteristiche proprie di queste fasi, come la presenza di stati di bordo e di ordini di stringa nascosti. Infatti una delle peculiarità delle fasi topologiche è quella di essere rilevate da parametri d'ordine non locali, che a differenza dai comuni parametri d'ordine che caratterizzano le diverse fasi associate a rotture spontanee di simmetria, sono forniti da valori di aspettazione di operatori non locali. In questa tesi vengono introdotti nuovi parametri d'ordine non locali, diversi rispetto a quelli comunemente utilizzati, ma ugualmente efficaci nella rilevazione delle diverse fasi massive in cui è possibile trovare il nostro modello di spin 1 di riferimento, ovvero il cosiddetto modello bilineare-biquadratico. Questi parametri d'ordine non locali sono stati valutati sia numericamente che analiticamente laddove fosse disponibile una rappresentazione esatta dello stato fondamentale del sistema.

Contents

To my parents

Introduction

Physicists have shown interest in one-dimensional spin systems since the first decades of the twentieth century, but for a long time they erroneously assumed that the properties of these systems were all alike. Specifically it was thought that the most studied model of the time, i.e. the antiferromagnetic $s = 1/2$ Heisenberg chain for which an exact solution was available, could qualitatively describe also higher spin models in one dimension, which were then thought to be all gapless. Moreover, according to spin waves theory, also higher dimensional spin systems display gapless excitations. Therefore there was some skepticism when in 1982 Duncan Haldane predicted that integer spin chains have a finite energy gap in the excitation spectrum by mapping the antiferromagnetic Heisenberg models onto a well known field theory, the so-called O(3) non-linear sigma model. Such a prediction was difficult to prove due to the lack of exact solutions for higher spin systems, nevertheless several numerical studies have shown unambiguously the validity of this conjecture in the following years.

Haldane's argument relied on the assumption that the spin was large, so to have a semi-classical behavior, but it was expected that its conclusions could be extended also to lower spins, down to $s = 1$. Thus I. Affleck, T. Kennedy, E. Lieb and H.Tasaki proposed a solvable spin-1 toy model, the so-called AKLT model, to show analytically the existence of the Haldane gap in lower integer spin systems. This model, despite its simplicity, shows some other characteristic features, such as the presence of low-lying edge modes, which actually characterize the whole massive phase the AKLT and the spin-1 Heisenberg models belong to, that is the Haldane phase.

This phase was particularly interesting as it could not be classified in the familiar scheme of Landau's theory of symmetry breaking. Indeed, for a long time, it was believed that the different phases of matter could only be distinguished by their symmetries. A paradigmatic example may be given by the two-dimensional $\mathbb{Z}_2$-symmetric classical Ising model $H = -J\sum_{ij}\sigma_i^z\sigma_j^z$. This well known system has two different phases, i.e. a symmetric (disordered) phase at high temperatures which retains the $\mathbb{Z}_2$ symmetry of the Hamiltonian, and a symmetry-broken (ordered) phase at low temperatures which has no longer the original symmetry and is doubly degenerate. Similarly if we consider the quantum Ising model with a transverse field $H = -J\sum_{ij}\sigma_i^z\sigma_j^z - h\sum_i\sigma_i^x$ we found two phases with two different symmetries in the limit $J \to \infty$ and $h \to \infty$ respectively. Indeed when $J \ll h$ the ground state is $\otimes_i(|\uparrow_z\rangle_i + |\downarrow_z\rangle_i)$ and it has the same symmetry of the Hamiltonian, while when $h \ll J$ the two degenerate ground states are $\otimes_i |\uparrow_z\rangle_i$ and $\otimes_i |\downarrow_z\rangle_i$, which clearly break the $\mathbb{Z}_2$ symmetry. On the other hand if we consider the following spin-1 class of Hamiltonians $H = J\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + D\sum_i (S_i^z)^2$ we

found two distinct phases in the limits $D \to 0$ and $D \to \infty$, but this time *both* phases have the *same unbroken symmetry*. The Haldane phase $(D \to 0)$ represents indeed an instance of a new kind of order, called *topological order*, which was unknown before and utterly undetected by Landau's theory.

Nevertheless symmetries play an important role in the context of these new topological phases. First of all, more specifically, the Haldane phase is a so-called *symmetry protected topological* phase, meaning that it remains intact even if we add small but symmetry-preserving perturbations. The symmetries which need to be preserved are said to *protect* this topological phase, given that if those are explicitly broken then the phase disappears and becomes *topological trivial*. On the other hand it has been shown, using the Matrix Product State representation of quantum states, that all symmetry protected topological phases can be classified by the second cohomology group $\mathbb{H}^2(G, \mathbb{C})$ of the corresponding symmetry group G, i.e. by the projective representations of the latter.

These topological phases, like the Haldane phase, are massive and have short-range order, that is exponentially decaying correlation functions and consequently the conventional *order parameters* which were widely used to detect and distinguish different symmetry-breaking orders are insensitive to this new kind of topological order. Nevertheless it was noticed that the Haldane phase have a hidden *string order* detected by a different type of order parameters, i.e. *non-local order parameters*, given by the expectation value of some non-local operator. These non-local order parameters can distinguish the various topological phases or signal the presence of trivial topological order. They are intimately related to the local symmetries of the system, and once the connection between these two was revealed it was clear how to suitably define new non-local order parameters which could characterize the different phases.

In this thesis we will mainly focus on a particular SU(2)-symmetric class of spin-1 models, that is the *bilinear-biquadratic* model:

$$H = \sum_i J_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right] \tag{1}$$

which is of particular interest given that it provides for two massive phases, i.e. the topological Haldane phase and the trivial dimer phase. Moreover for particular values of the parameter β we find both the Heisenberg and the AKLT models, and SU(3)-symmetric systems as well. We will use here the matrix product state representation of the AKLT state, as representative of the Haldane phase, and of the dimer state, as representative of the dimer phase, in order to analytically evaluate new non-local order parameters which can characterize and detect the two massive phases of the bilinear-biquadratic model, as it will be then shown in numerical simulations using the DMRG algorithm. Specifically:

1. in chapter 1 we will introduce the Heisenberg model and its mapping

onto the non-linear sigma model, showing how the Haldane's conjecture emerges;

2. in chapter 2 we will review the bilinear-biquadratic model and its phases, focusing in particular on the AKLT state and its characteristic features, which it shares with the Haldane phase, such as the hidden string order and the presence of edge states of spin-$1/2$;

3. in chapter 3 we will give a more extensive introduction to phase transitions, topological phases and the role of symmetries in the classification of the latter, and how those symmetries can be exploited in order to define generalized non-local order parameters. In this chapter we will widely use the Matrix Product States (MPS), thus a substantial section will be reserved to this topic;

4. in chapter 4 we will finally find the MPS representation of the AKLT and dimer states, and we will analytically evaluate new non-local order parameters using these representative states and show, also numerically, how they correctly detect the two massive phases of the model in exam. In the last section of the chapter we will eventually discuss some field theoretical predictions for the SU(N) Heisenberg models with bond alternation, focusing on the cases of interest $N = 2, 3$.

Chapter 1

Quantum Heisenberg spin chains and the Haldane conjecture

One of the simplest model that can describe quantum mechanically a magnetic system is the Heisenberg Model in which the interactions favor parallel alignment of adjacent spins in case of ferromagnets or antiparallel alignment in case of antiferromagnets. Classically, in frustration-free systems, both cases can be treated on an equal footing: indeed a transformation which flips all spins in a sublattice maps one model into the other. Obviously there will be a clear physical difference between the two. For example in the ground states the magnetization, which will have a definite value in a ferromagnet, vanishes in an antiferromagnet. In the latter case there is still long-range order as signaled by the staggered magnetization, i.e. the proper order parameter for antiferromagnets but when we take into account the quantum counterparts, only the ferromagnetic order parameter benefits from a conservation law and as a result the zero-point fluctuations may alter the antiferromagnetic classic order. In case that these fluctuations are small enough, both ferromagnets and antiferromagnets still have ordered ground states which break the continuous rotational symmetry of the system and therefore gapless excitations know as spin waves emerge in the spectrum. But if the quantum fluctuations are strong enough to destroy the antiferromagnetic order we may have a completely different behavior. This is indeed what happens in one dimensional spin systems. Here, surprisingly, a gap appears only if the spin is integer as conjectured by Haldane [16, 18]. This result was far from obvious given that in addition to the higher dimensional systems also the well known and exact solutions of the spin-½ Heisenberg chain provide for gapless excitations.

The main goal of this chapter is to introduce the Heisenberg model and to show how the Haldane conjecture results from the study of its continuum limit using a path-integral approach. In § 1.1 the model is defined, in § 1.2 we show how the spin wave theory fails in one dimension, giving us a clue of the different behavior of quantum spin chains compared to spin systems in higher dimensions. In § 1.3 the spin coherent states are defined and used to construct the path integral which will lead in § 1.4 to the field theory that describes the continuum limit of the quantum antiferromagnetic chain: the Non Linear Sigma Model with a topological term. In § 1.5 and § 1.6 we will take a closer look to this field theory and explain how the topological term accounts for the different behavior of integer and half-integer spin chains. Eventually

in § 1.7 it will be presented a generalization of the preceding results to the quasi one dimensional case of spin ladders.

1.1 The SU(2) Heisenberg Model

Let us consider quantum spin operators $\mathbf{S}_i$ localized on the sites of a d-dimensional bipartite square lattice, i.e. a lattice made up of two sublattices such that every spin on a sublattice interacts only with the nearest neighboring spins on the other sublattice as follows:

$$H = \frac{J}{2} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{1.1}$$

where $\langle ij \rangle$ denotes summation over nearest neighbor indexes only. In this chapter we will always assume periodic boundary conditions. Here the quantum spins are some irreducible representations of the $su(2)$ algebra and obey the corresponding commutation relations ($\hbar = 1$):

$$[S_i^a, S_j^b] = i\delta_{ij}\epsilon_{abc}S_i^c \tag{1.2}$$

Given an irreducible representation, the Hilbert space of the quantum spin is $\mathbb{C}^{2s+1}$ where s is the "value" of the spin given by:

$$\mathbf{S}_i^2 = s(s+1)\mathbb{I} \tag{1.3}$$

The Hilbert space of the many-spin system then is just the tensor product of the Hilbert space of each of the N quantum spins of the lattice $(\mathbb{C}^{2s+1})^{\otimes N}$.
Defining the total spin operator:

$$\mathbf{S} = \sum_i \mathbf{S}_i \tag{1.4}$$

it is easy to check that the Hamiltonian (1.1) commutes with this operator and then it is SU(2) symmetric.
The Heisenberg model is indeed the simplest example of SU(2)-symmetric spin Hamiltonian, and it describes *ferromagnets* ($J < 0$) and *antiferromagnets* ($J > 0$) according to the sign of the *coupling constant* J.
Our aim is to know more about the ground state of this model and whether or not there is a long-range order. Classically the ground state of the Heisenberg model[1] is easily found to be the *ordered* state with all spins antiparallel (parallel) for the antiferromagnetic (ferromagnetic) case. The antiferromagnetic state in this classical configuration is called the *Néel state*. The quantum counterpart of these classical ground states would be written as:

$$|\Psi_0\rangle = \bigotimes_i |s, \eta_i s\rangle_i \tag{1.5}$$

[1]The classical Heisenberg Model is defined by (1.1) where the spins are classical vectors of fixed length.

where

$$\eta_i = \begin{cases} 1 & \textit{ferromagnetic case} \\ (-1)^i & \textit{antiferromagnetic case} \end{cases} \tag{1.6}$$

and

$$\begin{aligned} S_i^z \left|s, \eta_i s\right\rangle_i &= \eta_i s \left|s, s\right\rangle_i \\ \mathbf{S}_i^2 \left|s, \eta_i s\right\rangle_i &= s(s+1) \left|s, \eta_i s\right\rangle_i . \end{aligned} \tag{1.7}$$

In order to see if these states are actually the ground states of the quantum model we rewrite the Hamiltonian (1.1) in terms of raising and lowering operators:

$$S_i^{\pm} = S_i^x \pm S_i^y \tag{1.8}$$

as

$$H = \frac{J}{2} \sum_{\langle ij \rangle} \left[\frac{1}{2} (S_i^+ S_j^- + S_j^+ S_i^-) + S_i^z S_j^z \right]. \tag{1.9}$$

The ferromagnetic state is still the ground state for the quantum ferromagnet, but the same is not true for the Néel state. Acting with the Hamiltonian operator on this state gives a different state in which pairs of neighboring spins have been raised and lowered by the operators (1.8). In other words the Néel state is not an eigenstate of the antiferromagnetic Heisenberg Hamiltonian and therefore quantum antiferromagnets should be treated quite differently from the corresponding ferromagnets conversely to what happens classically.

1.2 Spin waves theory

We would like to get some knowledge about the quantum antiferromagnetic ground state starting from the fact that the Néel state becomes an exact ground state of the model in the classical limit, i.e. in the limit $s \to \infty$. When s is large it is natural to expect only small fluctuations of S_i^z about $\pm s$, so it will be convenient to introduce the Holstein-Primakoff boson operator a in order to find corrections in powers of $1/s$ to the Néel state. In terms of these bosons the spin operators can be expressed as [1, 6]:

$$\begin{aligned} S_i^z &= s - a_i^\dagger a_i; \quad S_i^- = \sqrt{2s} a_i^\dagger \left(1 - \frac{a_i^\dagger a_i}{2s}\right)^{\frac{1}{2}}; \quad S_i^+ = \sqrt{2s} \left(1 - \frac{a_i^\dagger a_i}{2s}\right)^{\frac{1}{2}} a_i \\ S_j^z &= -s + a_j^\dagger a_j; \quad S_j^- = \sqrt{2s} \left(1 - \frac{a_j^\dagger a_j}{2s}\right)^{\frac{1}{2}} a_j; \quad S_j^+ = \sqrt{2s} a_j^\dagger \left(1 - \frac{a_j^\dagger a_j}{2s}\right)^{\frac{1}{2}} \end{aligned}$$

where i is a site belonging to a sublattice and j to the other. Using $[a_i, a_j^\dagger] = \delta_{ij}$ it can be easily checked that the commutation relations (1.2) are still obeyed. We have redefined the spin operators in this fashion such that the Néel state corresponds to the state with no bosons at all. Bosons are created or destroyed, dependently on the sublattice considered, by S^+ and S^-. In any case in this semiclassical limit we should expect that the number of bosons

will always be small compared to $2s$. When $s \gg 1$ the square roots can be expanded in powers of $1/s$:

$$\left(1 - \frac{a_i^\dagger a_i}{2s}\right)^{\frac{1}{2}} = 1 - \frac{1}{2}\frac{a_i^\dagger a_i}{2s} - \frac{1}{8}\left(\frac{a_i^\dagger a_i}{2s}\right)^2 + \cdots \tag{1.10}$$

and keeping only the lowest order in the expansion the corresponding expressions for the spin operators greatly simplify:

$$S_i^- \approx \sqrt{2s}a_i^\dagger; \quad S_i^+ \approx \sqrt{2s}a_i; \quad S_j^- \approx \sqrt{2s}a_j; \quad S_j^+ \approx \sqrt{2s}a_j^\dagger. \tag{1.11}$$

Inserting (1.11) in (1.9) and keeping terms up to the quadratic order we get:

$$H \approx -\frac{Jzs^2N}{2} + \frac{Js}{2}\sum_{\langle ij\rangle}\left(a_i a_j + a_i^\dagger a_j^\dagger + a_i^\dagger a_i + a_j^\dagger a_j\right) \tag{1.12}$$

where z and N are the *coordination number* and the total number of sites of the lattice respectively. In terms of the Fourier components of the bosons:

$$a_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\cdot\mathbf{j}}a_j \tag{1.13}$$

we can express the Hamiltonian in momentum space (see appendix A):

$$H \approx -\frac{Jzs^2N}{2} + Jsz\sum_{\mathbf{k}}\left[a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{\gamma_{\mathbf{k}}}{2}\left(a_{\mathbf{k}}a_{-\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger\right)\right] \tag{1.14}$$

where

$$\gamma_{\mathbf{k}} = \gamma_{-\mathbf{k}} = \frac{1}{z}\sum_{\boldsymbol{\eta}} e^{i\mathbf{k}\cdot\boldsymbol{\eta}}, \tag{1.15}$$

$\boldsymbol{\eta}$ is a vector joining a site to its nearest neighbors and $\mathbf{k}$ belongs to the cubic Brillouin zone:

$$|k_\alpha| \leq \pi \qquad \alpha = 1, 2, ...d \tag{1.16}$$

Defining the spin wave operators $\alpha_{\mathbf{k}}$ by a *Boguliubov* transformation we can now diagonalize H:

$$\begin{aligned} \alpha_{\mathbf{k}} &= \cosh(\theta_{\mathbf{k}})a_{\mathbf{k}} - \sinh(\theta_{\mathbf{k}})a_{-\mathbf{k}}^\dagger \\ \alpha_{-\mathbf{k}}^\dagger &= -\sinh(\theta_{\mathbf{k}})a_{\mathbf{k}} + \cosh(\theta_{\mathbf{k}})a_{-\mathbf{k}}^\dagger \end{aligned} \tag{1.17}$$

where $\theta_{\mathbf{k}}$ is given by:

$$\tanh(2\theta_{\mathbf{k}}) = -\gamma_{\mathbf{k}}. \tag{1.18}$$

We eventually find the diagonalized quadratic Hamiltonian in terms of the new spin wave operators $\alpha_{\mathbf{k}}$:

$$H \approx -\frac{JNz}{2}s(s+1) + \sum_{\mathbf{k}}\left(\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} + \frac{1}{2}\right)\omega_{\mathbf{k}} \tag{1.19}$$

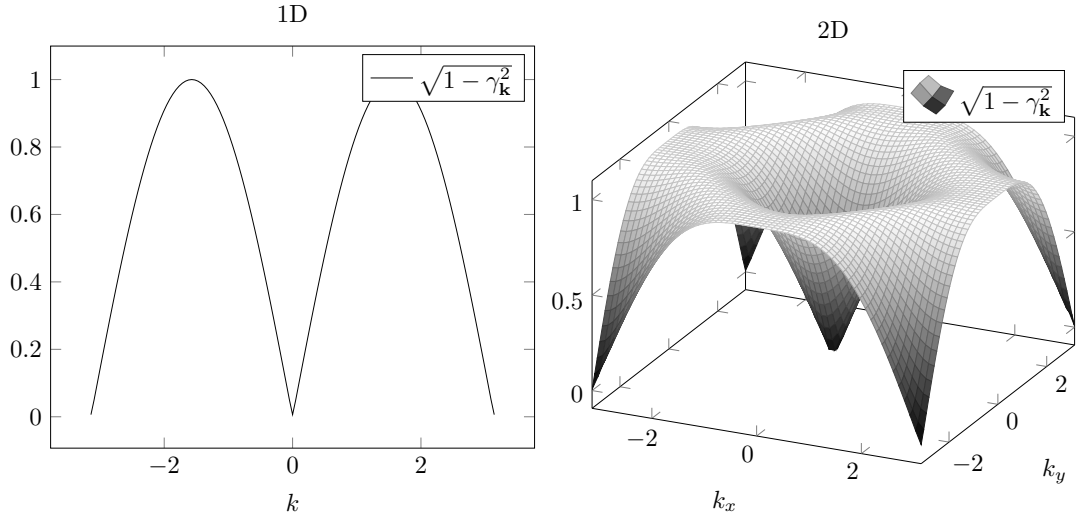


FIGURE 1.1: Plot of the function $\sqrt{1-\gamma_{\mathbf{k}}^2}$ for a one dimensional chain (left) and a two dimensional square lattice (right).

where

$$\omega_{\mathbf{k}} = Jsz\sqrt{1-\gamma_{\mathbf{k}}{}^2}. \tag{1.20}$$

In this approximation the ground state of the quantum antiferromagnet is the state with no $\alpha_{\mathbf{k}}$-bosons present and its energy is lower than the energy of the classical Néel state, as can be seen from (1.19):

$$\Delta E = \frac{Jzs}{2}\sum_{\mathbf{k}}(\omega_{\mathbf{k}} - 1) \leq 0. \tag{1.21}$$

Deviations of the spins away from the ground state are created then by the spin wave operators $\alpha_{\mathbf{k}}^\dagger$. The energy of these excitations vanishes linearly near $\mathbf{k} = \mathbf{0}$ and $\mathbf{k} = \boldsymbol{\pi} = (\pi, \pi, \dots)$ (see Fig.1.1):

$$\omega_{\mathbf{k}} \sim \begin{cases} Js\sqrt{2z}|\mathbf{k}| & \mathbf{k} \approx \mathbf{0} \\ Js\sqrt{2z}|\mathbf{k} - \boldsymbol{\pi}| & \mathbf{k} \approx \boldsymbol{\pi} \end{cases} \tag{1.22}$$

We are even more interested in the corrections to the staggered magnetization defined as follows:

$$m^s = \frac{1}{N}\left(\sum_i S_i^z - \sum_j S_j^z\right) \tag{1.23}$$

where i belongs to a sublattice and j to the other. The correction to this order parameter is given by the expectation value:

$$\Delta m^s = \langle m^s - s\rangle = -\frac{1}{N}\langle\sum_i a_i^\dagger a_i\rangle = -\frac{1}{N}\langle\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\rangle \tag{1.24}$$

evaluated using the antiferromagnetic ground state and (1.17):

$$\Delta m^s = -\frac{1}{2N}\sum_{\mathbf{k}}\left(\frac{1}{\sqrt{1-{\gamma_{\mathbf{k}}}^2}}-1\right). \tag{1.25}$$

While this correction should be small in higher dimensions and for large s [1], it has an infrared divergence for $d = 1$, meaning that the order of the Néel state is destroyed by the quantum fluctuations independently of the value of s. Then a quantum antiferromagnetic spin chain cannot be described, even approximately, by a spin wave theory. We have to find another path in order to get practical information about the ground state of a quantum antiferromagnet, its spectrum and its long range properties in one dimension. Note that the spectrum of quantum antiferromagnets in higher dimensions is always gapless, no matter the exact value of the spin. We can then understand the surprise that accompanied the discovery that in one dimension the behavior of spin chains could be totally different.

1.3 The Spin Path Integral

We have found that the spin wave theory fails in one dimension but works fine in higher dimensions, provided s is large enough. Our basic assumption was that we could select a classical ordered ground state (the Néel state) and treat the quantum effects as small fluctuations around it. In order to select such a state we assumed that the SU(2) symmetry of the model was spontaneously broken. But according to Mermin and Wagner's Theorem [6] there cannot be such a thing in one dimension, even at zero temperature, so our assumptions were wrong a priori in $d = 1$.
In this section we will show how the path integral approach makes possible to use the semiclassical approximation without assuming a spontaneously broken symmetry. Our starting point will be the partition function of the model $Z = \mathrm{Tr}\left[e^{-\beta H}\right]$ to be expressed as a path integral. In order to fulfill this task we have to define an important family of states: the *spin coherent states*.

1.3.1 Spin Coherent States

A spin coherent state is essentially created rotating a maximally polarized state in the basis where S^z is diagonal. This rotation is an element $\mathcal{R}$ of the SU(2) group of transformations which is parametrized by three Euler angles ϕ, θ, χ [6]:

$$\mathcal{R}(\phi,\theta,\chi) = e^{-i\phi S^z}e^{-i\theta S^y}e^{-i\chi S^z} \tag{1.26}$$

where the spin operators are generators of the group. So we define a spin coherent state $|\mathbf{\Omega}\rangle$ applying this rotation operator to $|s,s\rangle$ (defined in 1.7):

$$|\mathbf{\Omega}\rangle = \mathcal{R}(\phi,\theta,\chi)\,|s,s\rangle\,. \tag{1.27}$$

The spin coherent state is parametrized by the unit vector $\mathbf{\Omega}$:

$$\mathbf{\Omega} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{1.28}$$

that does not depend on χ, which can be chosen arbitrarily since it would just redefine the phase of the state. This set of states is not orthogonal as can be shown [6]:

$$\langle \mathbf{\Omega} | \mathbf{\Omega}' \rangle = \left(\frac{1 + \mathbf{\Omega} \cdot \mathbf{\Omega}'}{2} \right)^s e^{is\psi} \tag{1.29}$$

where

$$\psi = 2\arctan\left[\tan\left(\frac{\phi - \phi'}{2} \right) \frac{\cos\left[\frac{1}{2}(\theta + \theta')\right]}{\cos\left[\frac{1}{2}(\theta - \theta')\right]} \right] + \chi - \chi', \tag{1.30}$$

but it provides the following *resolution of the identity*:

$$\mathbb{I} = \frac{2s+1}{4\pi} \int d\mathbf{\Omega} \, |\mathbf{\Omega}\rangle \langle \mathbf{\Omega}| \tag{1.31}$$

This is thus an *overcomplete basis*.
We can define many spin coherent states just as product of single spin states:

$$|\mathbf{\Omega}\rangle = \bigotimes_{i=1}^{N} |\mathbf{\Omega}_i\rangle \,. \tag{1.32}$$

The relations (1.29) and (1.31) can be easily extended to the case of many spins:

$$\langle \mathbf{\Omega} | \mathbf{\Omega}' \rangle = \prod_i \left(\frac{1 + \mathbf{\Omega}_i \cdot \mathbf{\Omega}_i'}{2} \right)^s e^{is \sum_i \psi[\mathbf{\Omega}_i, \mathbf{\Omega}_i']} \tag{1.33}$$

$$\int \prod_i \left(\frac{2s+1}{4\pi} d\mathbf{\Omega}_i \right) |\mathbf{\Omega}\rangle \langle \mathbf{\Omega}| = \mathbb{I}. \tag{1.34}$$

The trace of any operator can be evaluated using spin coherent states:

$$\mathrm{Tr}\, \mathcal{O} = \frac{2s+1}{4\pi} \int d\mathbf{\Omega} \, \langle \mathbf{\Omega}| \, \mathcal{O} \, |\mathbf{\Omega}\rangle \tag{1.35}$$

This family of states resemble classical spin vectors. This analogy becomes more and more accurate as we consider larger value of s. Indeed according to (1.29), as $s \to \infty$, these states become orthogonal. Thus the quantum nature of spin variables is encoded in their *nonorthogonality*.
Another useful property is that $|\mathbf{\Omega}\rangle$ is an eigenstate of the spin component in the $\mathbf{\Omega}$ direction [6, 15]:

$$\mathbf{\Omega} \cdot \mathbf{S} \, |\mathbf{\Omega}\rangle = s \, |\mathbf{\Omega}\rangle \tag{1.36}$$

which can be used to express the Heisenberg Hamiltonian in this spin representation:

$$H[\mathbf{\Omega}] = \langle \mathbf{\Omega} | \, H \, | \mathbf{\Omega} \rangle = \frac{J}{2} s^2 \sum_{\langle ij \rangle} \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j \tag{1.37}$$

This is nothing but a classical Heisenberg Hamiltonian with coupling constant Js^2.

1.3.2 Path integrals for spin systems

Now we are ready to write down the path integral for the partition function:

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right]. \tag{1.38}$$

Here β is treated as an imaginary time interval to be split into N_ϵ steps of lenght ϵ such that $N_\epsilon \to +\infty$ and $\epsilon \to 0$ but $N_\epsilon \epsilon = \beta$, so:

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] = \mathrm{Tr}\left[\lim_{\substack{N_\epsilon \to +\infty \\ \epsilon \to 0}} \left(e^{-\epsilon H}\right)^{N_\epsilon}\right]. \tag{1.39}$$

This trace has to be evaluated using spin coherent states (1.35), and their identity resolution (1.34) (neglecting unimportant factors):

$$\begin{aligned} Z = \mathrm{Tr}\left[e^{-\beta H}\right] &= \lim_{\substack{N_\epsilon \to +\infty \\ \epsilon \to 0}} \int d\mathbf{\Omega}(\beta) \, \langle \mathbf{\Omega}(\beta) | \underbrace{e^{-\epsilon H} \cdot \mathbb{I} \cdot e^{-\epsilon H} \ldots \mathbb{I} \cdot e^{-\epsilon H}}_{N_\epsilon \text{ times}} | \mathbf{\Omega}(\beta) \rangle \\ &= \lim_{\substack{N_\epsilon \to +\infty \\ \epsilon \to 0}} \int \left(\prod_{j=1}^{N_\epsilon} d\mathbf{\Omega}(\tau_j) \right) \prod_{j=1}^{N_\epsilon} \langle \mathbf{\Omega}(\tau_{j+1}) | \, e^{-\epsilon H} \, | \mathbf{\Omega}(\tau_j) \rangle \end{aligned} \tag{1.40}$$

where $\{\tau_j\}$ is a set of intermediate times in the interval $[0, \beta]$. So $|\mathbf{\Omega}(\tau_1)\rangle = |\mathbf{\Omega}(0)\rangle$ and $|\mathbf{\Omega}(\tau_{N_\epsilon+1})\rangle = |\mathbf{\Omega}(\beta)\rangle = |\mathbf{\Omega}(0)\rangle$. Here $|\mathbf{\Omega}\rangle$ is a many spin coherent state as defined in (1.32).
If ϵ is small enough we can approximate the integrand as follows:

$$\begin{aligned} \langle \mathbf{\Omega}(\tau_{j+1}) | \, e^{-\epsilon H} \, | \mathbf{\Omega}(\tau_j) \rangle &\approx \langle \mathbf{\Omega}(\tau_{j+1}) | \, (1 - \epsilon H) \, | \mathbf{\Omega}(\tau_j) \rangle \\ &= \langle \mathbf{\Omega}(\tau_{j+1}) | \mathbf{\Omega}(\tau_j) \rangle - \epsilon \, \langle \mathbf{\Omega}(\tau_{j+1}) | \, H \, | \mathbf{\Omega}(\tau_j) \rangle \\ &= \langle \mathbf{\Omega}(\tau_{j+1}) | \mathbf{\Omega}(\tau_j) \rangle \left(1 - \epsilon \frac{\langle \mathbf{\Omega}(\tau_{j+1}) | \, H \, | \mathbf{\Omega}(\tau_j) \rangle}{\langle \mathbf{\Omega}(\tau_{j+1}) | \mathbf{\Omega}(\tau_j) \rangle} \right). \end{aligned} \tag{1.41}$$

In the limit $N_\epsilon \to \infty$ we can treat $\mathbf{\Omega}(\tau)$ as a continuous and differentiable function and substitute differences by derivatives:

$$\frac{\mathbf{\Omega}(\tau_{j+1}) - \mathbf{\Omega}(\tau_j)}{\epsilon} = \dot{\mathbf{\Omega}}(\tau_j) + \mathcal{O}(\epsilon). \tag{1.42}$$

So we obtain to leading order in ϵ [6]:

$$\left\langle \mathbf{\Omega}(\tau_{j+1})\middle|\mathbf{\Omega}(\tau_j)\right\rangle = 1 + \epsilon \left\langle \dot{\mathbf{\Omega}}(\tau_j)\middle|\mathbf{\Omega}(\tau_j)\right\rangle = \exp\left\{ is\epsilon \sum_i \dot{\phi}_i \cos\left[\theta_i(\tau_j)\right] + \dot{\chi}_i \right\}. \tag{1.43}$$

With a suitable choice for $\chi_i(\tau)$ we can set $\dot{\chi}_i = 0$. The second term we have to evaluate is the expectation value of the Hamiltonian:

$$H(\tau_j) = \frac{\left\langle \mathbf{\Omega}(\tau_{j+1})\right| H \left|\mathbf{\Omega}(\tau_j)\right\rangle}{\left\langle \mathbf{\Omega}(\tau_{j+1})\middle|\mathbf{\Omega}(\tau_j)\right\rangle} \tag{1.44}$$

which can be evaluated at equal times in our approximation, since it already multiplies ϵ in (1.41):

$$\frac{\left\langle \mathbf{\Omega}(\tau_{j+1})\right| H \left|\mathbf{\Omega}(\tau_j)\right\rangle}{\left\langle \mathbf{\Omega}(\tau_{j+1})\middle|\mathbf{\Omega}(\tau_j)\right\rangle} \approx \left\langle \mathbf{\Omega}(\tau_j)\right| H \left|\mathbf{\Omega}(\tau_j)\right\rangle. \tag{1.45}$$

This expression is nothing but (1.37):

$$H[\mathbf{\Omega}(\tau_j)] = \left\langle \mathbf{\Omega}(\tau_j)\right| H \left|\mathbf{\Omega}(\tau_j)\right\rangle = \frac{J}{2} s^2 \sum_{\langle ik\rangle} \mathbf{\Omega}_i(\tau_j)\cdot\mathbf{\Omega}_k(\tau_j). \tag{1.46}$$

Putting all together we find:

$$\left\langle \mathbf{\Omega}(\tau_{j+1})\right| e^{-\epsilon H} \left|\mathbf{\Omega}(\tau_j)\right\rangle = \exp\left\{ -\epsilon \left(-is \sum_i \dot{\phi}_i \cos[\theta_i(\tau_j)] + \frac{J}{2} s^2 \sum_{\langle ik\rangle} \mathbf{\Omega}_i(\tau_j)\cdot\mathbf{\Omega}_k(\tau_j) \right) \right\}. \tag{1.47}$$

The limit $N_\epsilon \to \infty$ and $\epsilon \to 0$ will give us a path integral, where the integration measure is defined as:

$$\mathcal{D}\mathbf{\Omega}(\tau) = \lim_{N_\epsilon \to +\infty} \prod_{j=1}^{N_\epsilon} d\mathbf{\Omega}(\tau_j). \tag{1.48}$$

Finally:

$$\begin{aligned} Z &= \oint \mathcal{D}\mathbf{\Omega}(\tau) e^{-S_E[\mathbf{\Omega}]} \\ S_E &= -is \sum_i \omega[\Omega_i] + \frac{J}{2} s^2 \sum_{\langle ij\rangle} \int_0^\beta d\tau \mathbf{\Omega}_i(\tau)\cdot\mathbf{\Omega}_j(\tau) \end{aligned} \tag{1.49}$$

where

$$s\omega[\mathbf{\Omega}_i] = s\int_0^\beta d\tau \dot{\phi}_i(\tau)\cos[\theta_i(\tau)] \tag{1.50}$$

is known as the *Berry phase* [10]. The nature of this phase is purely geometric since it depends only on the trajectory of the unit vector $\mathbf{\Omega}_i(\tau)$ on the sphere and not on its time dependence. Indeed on every lattice site i is defined an unit vector $\mathbf{\Omega}_i(\tau)$ that evolves and eventually comes back to its original

value in an imaginary time β since $\mathbf{\Omega}_i(0) = \mathbf{\Omega}_i(\beta)$. The evolution of this vector traces out a closed orbit on the unit sphere whose enclosed area is exactly equal to $\omega[\mathbf{\Omega}]$. We notice that this phase arises as a result of the non-orthogonal nature of the spin coherent states. We can express the Berry phase in a gauge invariant form introducing a vector potential $A(\mathbf{\Omega})$:

$$\omega[\mathbf{\Omega}] = \int_0^\beta d\tau \boldsymbol{A}\left(\mathbf{\Omega}\right) \cdot \dot{\mathbf{\Omega}} \tag{1.51}$$

which satisfies:

$$\nabla \times \boldsymbol{A} \cdot \mathbf{\Omega} = \epsilon^{\alpha\beta\gamma} \frac{\partial A^\beta}{\partial \Omega^\alpha} \Omega^\gamma = 1 \tag{1.52}$$

by the Stokes theorem.

1.4 Haldane's mapping

In § 1.3 we stressed that quantum fluctuations in one dimension are strong enough to completely destroy the Néel order no matter how large s is. As a result we will not expect that the dominant configurations of our path integral in the semiclassical limit will spontaneously break any symmetry, but instead we can expect that they will have at least short-range Néel order and deviate from it at longer scales.
For this reason it is useful to separate short and long length scale fluctuations and express $\mathbf{\Omega}$ in terms of two new vector fields, $\mathbf{n}$ and $\mathbf{L}$ as follows [6]:

$$\mathbf{\Omega}_i = \eta_i \mathbf{n}(x_i, \tau) \sqrt{1 - \left| \frac{\mathbf{L}(x_i, \tau)}{s} \right|^2} + \frac{\mathbf{L}(x_i, \tau)}{s} \tag{1.53}$$

where $\eta_i = (-1)^i$, $\mathbf{n}$ is the *Néel field* and it is unimodular, $\mathbf{L}$ is the *canting field* and it is orthogonal to $\mathbf{n}$:

$$|\mathbf{n}| = 1; \qquad \mathbf{L} \cdot \mathbf{n} = 0. \tag{1.54}$$

The Néel field $\mathbf{n}$ has to be slowly varying and the canting field has to be small $\left|\frac{\mathbf{L}}{s}\right| \ll 1$ if our assumption of short-length scale order and long-length scale disorder has to be satisfied. Moreover we will be interested in the continuum limit where the lattice constant becomes really small $a_0 \ll 1$ and the fields can be treated as functions of a continuous space variable $\mathbf{x}$.
If we consider the canting field small then (1.4) can be approximated as follows:

$$\mathbf{\Omega}_i \approx \eta_i \mathbf{n}(x_i, \tau) \left(1 - \frac{1}{2} \frac{\mathbf{L}^2(x_i, \tau)}{s^2}\right) + \frac{\mathbf{L}(x_i, \tau)}{s}. \tag{1.55}$$

Our goal is now to find an effective action in the continuum limit for the quantum antiferromagnet in one dimension. The first step is to substitute (1.55) in the action (1.49) found previously in order to get a new approximate path integral in terms of the fields $\mathbf{n}$ and $\mathbf{L}$. Let's start with the Hamiltonian

term, where now $j = i + 1$ and $\eta_i = -\eta_j$

$$\begin{aligned}\sum_i \mathbf{\Omega}_i \cdot \mathbf{\Omega}_{i+1} = \sum_i [&-\mathbf{n}(x_i,\tau)\cdot\mathbf{n}(x_{i+1},\tau)\left(1-\frac{1}{2}\frac{\mathbf{L}^2(x_i,\tau)}{s^2}\right)\left(1-\frac{1}{2}\frac{\mathbf{L}^2(x_{i+1},\tau)}{s^2}\right)\\ &+\frac{\eta_i}{s}\left(\mathbf{n}(x_i,\tau)\cdot\mathbf{L}(x_{i+1},\tau)-\mathbf{n}(x_{i+1},\tau)\cdot\mathbf{L}(x_i,\tau)\right)\\ &+\frac{\mathbf{L}(x_i,\tau)\cdot\mathbf{L}(x_{i+1},\tau)}{s^2}]\end{aligned} \tag{1.56}$$

The second term in the sum is of higher order and can be ignored. Indeed

$$\begin{aligned}&\sum_i [\mathbf{n}(x_i,\tau)\cdot\mathbf{L}(x_{i+1},\tau)-\mathbf{n}(x_{i+1},\tau)\cdot\mathbf{L}(x_i,\tau)]\\ &=-\sum_i \mathbf{L}(x_i,\tau)\cdot(\mathbf{n}(x_{i-1},\tau)+\mathbf{n}(x_{i+1},\tau))\\ &=-\sum_i \mathbf{L}(x_i,\tau)\cdot(2\mathbf{n}(x_i,\tau)+\mathcal{O}({a_0}^2))\\ &=-\sum_i \mathcal{O}({a_0}^2)\end{aligned} \tag{1.57}$$

where we used $\mathbf{L}\cdot\mathbf{n} = 0$.
It is useful to express

$$\mathbf{n}(x_i,\tau)\cdot\mathbf{n}(x_{i+1},\tau) \tag{1.58}$$

as

$$\mathbf{n}(x_i,\tau)\cdot\mathbf{n}(x_{i+1},\tau) = -\frac{1}{2}(\mathbf{n}(x_i,\tau)-\mathbf{n}(x_{i+1},\tau))^2+1 \tag{1.59}$$

where the difference can be approximated as follows:

$$(\mathbf{n}(x_i,\tau)-\mathbf{n}(x_{i+1},\tau))^2 \approx a_0^2(\partial_x\mathbf{n}(x_i,\tau))^2. \tag{1.60}$$

After some algebra we finally get (ignoring constat terms):

$$\sum_i \mathbf{\Omega}_i\cdot\mathbf{\Omega}_{i+1} = \frac{1}{2}\sum_i\left[a_0^2(\partial_x\mathbf{n}(x_i,\tau))^2+\frac{4\mathbf{L}^2(x_i,\tau)}{s^2}\right] \tag{1.61}$$

In the continuum limit we can replace sums by integrals, so:

$$Js^2\sum_i \mathbf{\Omega}_i\cdot\mathbf{\Omega}_{i+1} \to \frac{Js^2a_0}{2}\int dx\left[(\partial_x\mathbf{n}(x,\tau))^2+\frac{4\mathbf{L}^2(x,\tau)}{a_0^2s^2}\right]. \tag{1.62}$$

We still have to evaluate the Berry phase term in the action (1.49). It can be shown [6] that this term can be express in terms of $\mathbf{n}$ and $\mathbf{L}$ as follows:

$$-is\sum_i \omega[\Omega_i] = -is\sum_i \eta_i\omega[\mathbf{n}(x_i,\tau)] - i\sum_i \frac{\delta\omega}{\delta\mathbf{n}}(x_i,\tau)\cdot\mathbf{L}(x_i,\tau). \tag{1.63}$$

Both terms can be evaluated using this expression for the variation of the Berry phase [6]:

$$\delta\omega[\mathbf{\Omega}] = \int_0^\beta d\tau\, \mathbf{\Omega}\cdot(\dot{\mathbf{\Omega}}\times\delta\mathbf{\Omega}). \tag{1.64}$$

The first term becomes:

$$\begin{aligned} -is\sum_i \eta_i\omega[\mathbf{n}(x_i,\tau)] =& -is\sum_i \omega[\mathbf{n}(x_{2i},\tau)] - \omega[\mathbf{n}(x_{2i+1},\tau)] \\ =& ia_0 s\sum_i \frac{\delta\omega}{\delta\mathbf{n}}(x_{2i})\cdot\partial_x\mathbf{n}(x_{2i},\tau) \\ \to& \frac{is}{2}\int d^2\mathbf{x}\,\mathbf{n}(\mathbf{x})\cdot(\partial_\tau\mathbf{n}(\mathbf{x})\times\partial_x\mathbf{n}(\mathbf{x})) \\ \equiv& i2\pi s\Theta[\mathbf{n}] \end{aligned} \tag{1.65}$$

This is the *topological Berry phase* and

$$\Theta[\mathbf{n}] = \frac{1}{4\pi}\int d^2\mathbf{x}\,\mathbf{n}(\mathbf{x})\cdot(\partial_\tau\mathbf{n}(\mathbf{x})\times\partial_x\mathbf{n}(\mathbf{x})) \tag{1.66}$$

is the *Pontryagin index* [27].
The second term in (1.63) is simply:

$$-i\sum_i \frac{\delta\omega}{\delta\mathbf{n}}(x_i)\cdot\mathbf{L}(x_i,\tau) \to -\frac{i}{a_0}\int d^2\mathbf{x}\,\mathbf{L}(\mathbf{x})\cdot(\mathbf{n}(\mathbf{x})\cdot\partial_\tau\mathbf{n}(\mathbf{x})). \tag{1.67}$$

Putting all together, the action has now the form:

$$S_E = \frac{1}{2}Js^2a_0\int d^2\mathbf{x}\,\left[(\partial_x\mathbf{n})^2 + 4\frac{\mathbf{L}^2}{s^2a_0^2} - i\frac{2}{Js^2a_0^2}\mathbf{L}\cdot(\mathbf{n}\times\partial_\tau\mathbf{n})\right] + i2\pi s\Theta[\mathbf{n}]. \tag{1.68}$$

By completing the square:

$$4\frac{\mathbf{L}^2}{s^2a_0^2} - i\frac{2}{Js^2a_0^2}\mathbf{L}\cdot(\mathbf{n}\times\partial_\tau\mathbf{n}) = \left(2\frac{\mathbf{L}}{sa_0} - i\,\mathbf{n}\times\partial_\tau\mathbf{n}\right)^2 + \frac{1}{(2Jsa_0)^2}(\mathbf{n}\times\partial_\tau\mathbf{n})^2 \tag{1.69}$$

we are left with a Gaussian path-integration on $\mathbf{L}$ that can be easily performed. Ignoring the overall normalization constants and noticing that:

$$|\mathbf{n}\times\partial_\tau\mathbf{n}| = |\mathbf{n}||\partial_\tau\mathbf{n}| = |\partial_\tau\mathbf{n}| \tag{1.70}$$

we can finally write the effective long-wavelength action we were eager to find [15]:

$$\tilde{S}_E = \frac{1}{2g}\int d^2\mathbf{x}\,\left[\frac{1}{v_s}(\partial_\tau\mathbf{n}(\mathbf{x}))^2 + v_s(\partial_x\mathbf{n}(\mathbf{x}))^2\right] + i2\pi s\Theta[\mathbf{n}] \tag{1.71}$$

where we defined the *coupling constant* g and the *spin-wave velocity* v_s:

$$\begin{aligned} g =& \frac{2}{s} \\ v_s =& 2a_0 J s. \end{aligned} \tag{1.72}$$

This is the action of the *Non-linear Sigma Model* in 1+1 dimensions with an additional topological Θ term. Notice that our assumption of large s causes g to be small.

1.5 The Non-linear Sigma Model (NLσM) and the topological term

In the last section the non-linear sigma model with a topological term was found to describe a one dimensional quantum antiferromagnet in the continuum limit. Let us now have a closer look to this model [27].
The standard Lagrangian density of the NLσM in real time ($x_0 = -i\tau$) with metric $g_{\mu\nu} = \text{diag}(1, -1)$ is:

$$\mathcal{L} = \frac{1}{2g}\partial_\mu \mathbf{n} \cdot \partial^\mu \mathbf{n} = \frac{1}{2g}\left[(\partial_0 \mathbf{n})^2 - (\partial_1 \mathbf{n})^2\right] \tag{1.73}$$

which differs from (1.71) just for a rescaling of the variables so as to fix $v_s = 1$. This Lagrangian, despite its appearance, does not describe a free theory because of the constraint

$$\mathbf{n}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = 1. \tag{1.74}$$

We take into account this constraint adding a Lagrange multiplier $\lambda(\mathbf{x})$ into the Lagrangian (1.73):

$$\mathcal{L} = \frac{1}{2g}\left[\partial_\mu \mathbf{n} \cdot \partial^\mu \mathbf{n} + \lambda(\mathbf{n} \cdot \mathbf{n} - 1)\right]. \tag{1.75}$$

The field equations are then:

$$(\partial_\mu \partial^\mu + \lambda)\mathbf{n} = 0. \tag{1.76}$$

Using the constraint we get an expression for $\lambda(\mathbf{x})$:

$$\lambda = -\mathbf{n} \cdot \partial_\mu \partial^\mu \mathbf{n} \tag{1.77}$$

and thus the field equations become:

$$(\partial_\mu \partial^\mu - \mathbf{n} \cdot \partial_\mu \partial^\mu \mathbf{n})\mathbf{n} = 0. \tag{1.78}$$

Moreover, defining the conjugate momenta as:

$$\boldsymbol{\pi} = \frac{\partial \mathcal{L}}{\partial(\partial_0 \mathbf{n})} = \frac{1}{g}\partial_0 \mathbf{n} \tag{1.79}$$

it easy to write down the Hamiltonian density:

$$\mathcal{H} = \boldsymbol{\pi} \cdot \partial_0 \mathbf{n} - \mathcal{L} = \frac{1}{2}[g\boldsymbol{\pi}^2 + \frac{1}{g}(\partial_1 \mathbf{n})^2] \tag{1.80}$$

and the total energy:

$$E = \int dx_1\, dx_0\, \mathcal{H} = \frac{1}{2g} \int dx_1\, dx_0\, [(\partial_0 \mathbf{n})^2 + (\partial_1 \mathbf{n})^2]. \tag{1.81}$$

If the energy has to be finite then $\mathbf{n}$ has to tend to a constant value $\mathbf{n}_0$ at Euclidean space-time infinity:

$$\lim_{|\mathbf{x}| \to \infty} \mathbf{n}(\mathbf{x}) = \mathbf{n}_0 \tag{1.82}$$

where $|\mathbf{x}| = \sqrt{x_0^2 + x_1^2}$.
The two-dimensional manifold where the field $\mathbf{n}$ lives is therefore compactified to the sphere S^2 because all the points at infinity are identified and the value of the field there is defined and constant. The field is now a map from S^2, the spacetime manfidold, to S^2, the field space, and, as every map of this sort, it can be classified into homotopy sectors [27]. Two maps belonging to the same sector are homotopic, i.e. they can be continuously deformed into each other. Moreover every sector is characterized by an integer, the *winding number* or *Pontryagin index*, which is given by:

$$\Theta = \frac{1}{8\pi} \int dx_1\, dx_0\, \epsilon^{\mu\nu} \mathbf{n} \cdot (\partial_\mu \mathbf{n} \times \partial_\nu \mathbf{n}). \tag{1.83}$$

The winding number tells us the number of times a given map winds around S^2. This is nothing but the term (1.66) found in the effective action. The partition function can be then expressed as a sum of path integrals over configurations of distinct topological sectors and fixed winding number:

$$Z = \int \mathcal{D}\mathbf{n}\, e^{i\tilde{S}[\mathbf{n}]} = \sum_{\Theta} \int_{\Theta} \mathcal{D}\mathbf{n}\, e^{iS_{NL\sigma M}[\mathbf{n}]} e^{-i2\pi s\Theta[\mathbf{n}]} \tag{1.84}$$

where $S_{NL\sigma M}[\mathbf{n}]$ is the action of the non-linear sigma model and the subscript Θ in front of the integral just reminds us to consider only configurations with that winding number. Thus, given a configuration belonging to a definite homotopy sector, the topological term in (1.71) is equal to $2\pi s$ times an integer. As a result in our path integral it will cause quantum interferences between contributions coming from different homotopy sectors when s is *half-integer*, while it can be ignored when s is *integer*.
Indeed:

$$e^{-i2\pi s\Theta[\mathbf{n}]} = \begin{cases} 1 & \text{if s is integer} \\ \pm 1 & \text{if s is half-integer.} \end{cases} \tag{1.85}$$

This difference is at the heart of the Haldane's conjecture as we will see in the next sections.

1.5.1 The NLσM: The renormalization group

We are now interested in the role of quantum fluctuations about the slowly varying field configurations that we assume are dominant in our description of the low energy limit of the quantum antiferromagnet. We can treat these fluctuations as small in the weak coupling limit $g \ll 1$ and, being *local*, they do not alter the *global*, being topological, properties of any configuration, so for the moment we can ignore the topological term and remember that the following results will be valid in every topological sector separately.
Our goal is to get the effective action for the slow modes sequentially integrating out the faster modes through a *renormalization group transformation* [15]. In order to do so we separate the slow and fast degrees of freedom in the field $\mathbf{n}$ and assume that one component of field $\mathbf{n}$, say n_3, has only fast modes and is small, while the slow varying character of the remaining components will be described by the angle $\theta \in [0, 2\pi]$:

$$\mathbf{n}(n_3, \theta) = (\sqrt{1 - n_3^2}\cos\theta, \sqrt{1 - n_3^2}\sin\theta, n_3). \tag{1.86}$$

With this parametrization the constraint $|\mathbf{n}| = 1$ is still satisfied. We also rescale n_3 as:

$$n_3 = \sqrt{g}\phi. \tag{1.87}$$

Going back to imaginary time ($\tau = ix_0$) and Euclidean metric $g_{\mu\nu} = \mathrm{diag}(1, 1)$ the Lagrangian density (1.73) then reads:

$$\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)^2 + \frac{1}{2g}(1 - g\phi^2)(\partial_\mu\theta)^2 + \frac{1}{2}\left(\frac{g}{1 - g\phi^2}\right)(\phi\partial_\mu\phi)^2. \tag{1.88}$$

We can use the smallness of g to approximate the expression for $\mathcal{L}$:

$$\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)^2 + \frac{1}{2g}(\partial_\mu\theta)^2 - \frac{1}{2}\phi^2(\partial_\mu\theta)^2 + \mathcal{O}(g). \tag{1.89}$$

We remember that in the path integral

$$Z = \int_\Lambda \mathcal{D}\phi(\mathbf{p})\mathcal{D}\theta(\mathbf{p})\, e^{-\int d^2\mathbf{x}\,\mathcal{L}[\phi,\theta]} \tag{1.90}$$

we are integrating over all the Fourier components from 0 to an upper cut-off Λ of the order of the inverse of the lattice space constant $\Lambda \sim \frac{1}{a_0}$. In order to take into account only the low energy behavior we would to integrate out fluctuations corresponding to large momenta $\mathbf{p} \sim \Lambda$ and keep the slower modes. We consider then a momentum shell

$$b\Lambda < |\mathbf{p}| < \Lambda \tag{1.91}$$

where $b \to 1^-$, and we integrate out all the components within this shell. We assume also that $(\partial_\mu\theta)^2$ does not have Fourier components in (1.91) given

that θ is assumed slowly varying. Thus

$$\int_{b\Lambda<|\mathbf{p}|<\Lambda} \mathcal{D}\phi(\mathbf{p})\, e^{-\frac{1}{2}\int \frac{d^2\mathbf{p}}{(2\pi)^2}|\phi(\mathbf{p})|^2(\mathbf{p}^2-(\partial_\mu\theta)^2)} \approx \prod_{b\Lambda<|\mathbf{p}|<\Lambda} \left[\frac{2\pi}{\mathbf{p}^2-(\partial_\mu\theta)^2}\right]^{\frac{1}{2}}. \tag{1.92}$$

Exponentiating this result we get the contribution of the fast modes to the effective Lagrangian describing the slower modes:

$$\begin{aligned}\mathcal{L}^{eff} = &-\frac{1}{2}\int_{b\Lambda<|\mathbf{p}|<\Lambda}\frac{d^2\mathbf{p}}{2\pi}\ln\frac{2\pi}{\mathbf{p}^2}+\\ &+\frac{1}{2}(\partial_\mu\phi)^2+\frac{1}{2}\left(\frac{1}{g}-\int_{b\Lambda<|\mathbf{p}|<\Lambda}\frac{d^2\mathbf{p}}{2\pi}\frac{1}{\mathbf{p}^2}\right)(\partial_\mu\theta)^2-\frac{1}{2}\phi^2(\partial_\mu\theta)^2+\mathcal{O}(g).\end{aligned} \tag{1.93}$$

The effective Lagrangian density differs from the original (1.89) for a shift in the energy given by the first term in (1.93), a rescale of the momentum cut-off $\Lambda' = b\Lambda$ and a renormalization of the coupling constant g:

$$\begin{aligned}\frac{1}{g'} &= \frac{1}{g}-\int_{b\Lambda<|\mathbf{p}|<\Lambda}\frac{d^2\mathbf{p}}{2\pi}\frac{1}{\mathbf{p}^2}\\ \Rightarrow g' &= \frac{g}{1+\frac{g}{2\pi}\ln b}.\end{aligned} \tag{1.94}$$

From (1.94) we can get the corresponding *beta function*:

$$\beta(g) = \frac{dg}{d\ln(b)} = -\frac{g^2}{2\pi} \tag{1.95}$$

which is always negative. This means that as we average out the faster modes, the effective value of the coupling constant g for the slower modes increases or equivalently the *effective s* of the corresponding spin system decreases.

1.5.2 The NLσM: the correlation length

Under renormalization the NLσM in the weak coupling regime flows then to strong coupling. Both this regimes correspond to a particular limit of another spin system: the classical Heisenberg Model [6]:

$$\frac{J}{2}\sum_{\langle ij\rangle}\mathbf{\Omega_i}\cdot\mathbf{\Omega_j}. \tag{1.96}$$

More precisely the NLσM in d-dimensions in weak coupling coincides with the low temperature limit of the classical Heisenberg model in d-dimensions while its strong coupling regime coincides with the high temperature phase of the same model. We know that this system is disordered for all T in 2 dimensions and has an unique ground state [6]. This means that the NLσM has

exponentially decaying correlations and is massive for all g.
The correlation length ξ is what characterize this exponential decay and we can estimate its dependence on the bare, i.e. not renormalized, coupling constant $g_0 = \frac{2}{s}$ using the result of the last section. This length depends on the coupling constant g and on the momentum cut-off Λ, but it makes no difference if we evaluate it using the renormalized model or not. In other words ξ is a renormalization group invariant and should not depend on the parameter b we introduced in (1.91):

$$\xi = \xi(\Lambda(b), g(b)) = \xi(\Lambda_0, g_0) \tag{1.97}$$

Therefore the following equation should be satisfied:

$$\begin{aligned} \frac{d\xi}{d\ln b} &= \frac{\partial\xi}{\partial\Lambda}\frac{d\Lambda}{d\ln b} + \frac{\partial\xi}{\partial g}\frac{dg}{d\ln b} \\ &= \frac{\partial\xi}{\partial\Lambda}\frac{d\Lambda}{d\ln b} + \frac{\partial\xi}{\partial g}\beta = 0. \end{aligned} \tag{1.98}$$

Now ξ is dimensionally a length so it can be expressed as:

$$\xi = \frac{1}{\Lambda} f(g) \tag{1.99}$$

where f is some adimensional function of g. Taking into account that $\Lambda = b\Lambda_0$, we find then:

$$\xi = -\frac{\partial\xi}{\partial g}\beta. \tag{1.100}$$

The solution to this equation is easily found to be:

$$\xi(g) = \xi(g') \exp\left\{2\pi\left(\frac{1}{g} - \frac{1}{g'}\right)\right\}. \tag{1.101}$$

Here $\xi(g)$ and $\xi(g')$ are the correlation length of the model corresponding to two different value of the coupling constant. If we consider the strong coupling limit where $g' \gg 1$, then the correlation length for our original model defined at $g = g_0 = \frac{2}{s}$ is:

$$\xi(g_0) = \xi(g') e^{\pi s}. \tag{1.102}$$

The value of $\xi(g')$ depends on whether or not we have to take into account the topological term.

1.6 The Haldane conjecture

In these previous sections we have seen how a quantum antiferromagnetic spin chain in the limit of large s can be mapped onto a non-linear sigma model in weak coupling with an additional topological term. We know that the NLσM is always disordered and massive, i.e. has a gap in its spectrum.

How things change when we take into account the topological term?
We already know the answer for *integer* spin chains. Indeed in this case the topological term can be ingnored and all the results we found for the NLσM apply for integer spin systems. Thus there is no long-range order and the correlation length can be estimated from (1.102):

$$\xi(g_0) \approx a_0 e^{\pi s} \tag{1.103}$$

where $\xi(g') = \mathcal{O}(a_0)$ in the strong coupling limit $g' \to \infty$ we have considered. Moreover the gap Δ is [6, 15]:

$$\Delta = \frac{v_s}{\xi} = \frac{v_s}{a_0} e^{-\pi s}. \tag{1.104}$$

What really happens in the *half-integer* spin case is harder to understand because of the significant presence of the topological term which leads to interferences between different homotopy sectors in the path integral.
In this case the Lieb-Schultz-Mattis theorem can shed some light on the problem [2] . According to the theorem, quantum antiferromagnetic half-integer spin chains have a unique ground state and a gap that is $\mathcal{O}(L^{-1})$, where L is the finite length of the chain. When we consider the thermodynamic limit $L \to \infty$ either the ground state becomes degenerate or the gap vanishes. What we know for sure is that the quantum antiferromagnetic chain of spin $1/2$ is gapless and critical, as can be shown by exact Bethe-Ansatz techniques [6]. Moreover in § 1.5.1 the effective spin s was found to be decreasing as we integrated out the faster and more energetic modes. Therefore the behavior of half-integral spin chains is comparable to the lowest half-integral spin chain, for which the correlation length is infinite $\xi(g') = \infty$ being critical. Thus the same should be true for all half-integral spins:

$$\xi(g_0) = \xi(g') e^{\pi s} = \infty. \tag{1.105}$$

Therefore we expect all half-integer spin chains to be critical and gapless. This fundamental difference between integral and half-integral antiferromagnetic spin chains is what we call the Haldane conjecture.

1.7 Extension to Spin Ladders

We have seen how integral and half-integral spin chains behave quite differently. If we were trying to extend our findings to higher dimensional spin systems we would fail. It has indeed been shown that a topological term is absent in any spatial dimension greater than one [17]. Nevertheless there are some systems between 1D and 2D which behave interestingly and for which a good amount of our previous results are still valid and easy to be generalized. These systems are called *spin ladders* and are obtained by arranging a finite number of parallel spin chains and by antiferromagnetically coupling spins both along and across the chains. The striking feature of these systems, besides the differences predicted due to the different values of the spin as in

the one dimensional case, is that the number of the legs, i.e. the number of coupled parallel chains, is relevant in determining its qualitative behavior. Let's consider a general Hamiltonian for a ladder system with n_l legs of length N and with arbitrary values of the interchain J_a and intrachain $J_{a,a+1}$ coupling constants [14]:

$$H_{ladder} = \sum_{a=1}^{n_l} \sum_{i=1}^{N} \left[J_a \, \mathbf{S}_a(i) \cdot \mathbf{S}_a(i+1) + J'_{a,a+1} \, \mathbf{S}_a(i) \cdot \mathbf{S}_{a+1}(i) \right] \tag{1.106}$$

where J_a and $J'_{a,a+1}$ are assumed to be positive. The partition function for this system can be represented as a path-integral using the derivation in § 1.3.2:

$$\begin{aligned} Z(\beta) &= \int \mathcal{D}\mathbf{\Omega} \exp\{-S_E\} \\ S_E &= -is \sum_{i,a} \omega[\mathbf{\Omega}_a(i,\tau)] + s^2 \sum_{i,a} \int_0^\beta d\tau [J_a \mathbf{\Omega}_a(i,\tau) \cdot \mathbf{\Omega}_a(i+1,\tau) \\ &\quad + J'_{a,a+1} \mathbf{\Omega}_a(i,\tau) \cdot \mathbf{\Omega}_{a+1}(i,\tau)]. \end{aligned} \tag{1.107}$$

As in § 1.4 we will assume that the dominant configurations in (1.107) have short-range order but are disordered at longer wavelengths:

$$\mathbf{\Omega}_a(i,\tau) = (-1)^{a+i} \mathbf{n}(i,\tau) \sqrt{1 - \frac{|\mathbf{L}_a(i,\tau)|^2}{s^2}} + \frac{\mathbf{L}_a(i,\tau)}{s}. \tag{1.108}$$

Here the fields $\mathbf{n}$ and $\mathbf{L}$ have the same proprieties seen previously, but we have to assume further that the correlation length ξ is much bigger than the width of the ladder $\xi \gg n_l a_0$ so $\mathbf{n}$ does not depend on the index a. In order to get the effective action for this system we can follow most of the calculations of § 1.4. Indeed the interchain term in the action is:

$$s^2 \sum_{i,a} J_a \mathbf{\Omega}_a(i,\tau) \cdot \mathbf{\Omega}_a(i+1,\tau) \approx \frac{a_0 s^2}{2} \int dx \left[(\sum_a J_a)(\partial_x \mathbf{n}(x,\tau))^2 + 4 \sum_a J_a \frac{\mathbf{L}_a^2(x,\tau)}{a_0^2 s^2} \right], \tag{1.109}$$

while the intrachain term is:

$$\begin{aligned} s^2 \sum_{i,a} J'_{a,a+1} \mathbf{\Omega}_a(i,\tau) \cdot \mathbf{\Omega}_{a+1}(i,\tau) \approx \frac{a_0 s^2}{2} \sum_a \int dx \, J'_{a,a+1} \Big[& \frac{\mathbf{L}_a^2(x,\tau)}{a_0^2 s^2} + \frac{\mathbf{L}_{a+1}^2(x,\tau)}{a_0^2 s^2} \\ & + 2 \frac{\mathbf{L}_a(x,\tau) \cdot \mathbf{L}_{a+1}(x,\tau)}{a_0^2 s^2} \Big]. \end{aligned} \tag{1.110}$$

The Hamiltonian then reads:

$$H_{ladder}(\tau) = \frac{a_0}{2} \int dx \left[\left(s^2 \sum_a J_a \right) (\partial_x \mathbf{n}(x,\tau))^2 + \sum_{a,b} \mathbf{L}_a(x,\tau) \mathcal{J}_{ab} \mathbf{L}_b(x,\tau) \right] \tag{1.111}$$

where

$$\mathcal{J}_{ab} = \begin{cases} a_0^{-2}(4J_a + J'_{a,a+1} + J'_{a,a-1}) & \text{if} \quad a = b \\ a_0^{-2} J'_{a,b} & \text{if} \quad |a-b| = 1. \end{cases} \tag{1.112}$$

The Berry phase is evaluated as before:

$$-is\sum_{i,a}\omega[\mathbf{\Omega}(i,\tau)] \approx -is\sum_{i,a}(-1)^{a+i}\omega[\mathbf{n}(i,\tau)] - i\sum_{i,a}\int_0^\beta d\tau\,[\mathbf{n}(i,\tau)\times\partial_\tau\mathbf{n}(i,\tau)]\cdot\mathbf{L}_a(i,\tau). \tag{1.113}$$

We now integrate out the field $\mathbf{L}$ to get the kinetic term of the NLσM:

$$\begin{aligned} &\int \mathcal{D}\mathbf{L}\exp\Big\{\int_0^\beta d\tau\int dx\Big[-\frac{a_0}{2}\sum_{a,b}\mathbf{L}_a(x,\tau)\mathcal{J}_{ab}\mathbf{L}_b(x,\tau) \\ &+\frac{i}{a_0}\sum_a[\mathbf{n}(x,\tau)\times\partial_\tau\mathbf{n}(x,\tau)]\cdot\mathbf{L}_a(x,\tau)\Big]\Big\} \\ &\propto \exp\Big\{-\frac{1}{2}\int_0^\beta d\tau\int dx\sum_{a,b}\frac{\mathcal{J}^{-1}_{ab}}{a_0^3}(\partial_\tau\mathbf{n})^2\Big\}. \end{aligned} \tag{1.114}$$

We still need to evaluate the first term in the right hand side of (1.113). We notice that this term simply cancels out when n_l is *even* but it gives the same topological term $\Theta[\mathbf{n}]$ of the one dimensional chain when n_l is *odd*:

$$-is\sum_a(-1)^a\sum_i(-1)^i\omega[\mathbf{n}(i,\tau)] = \begin{cases} 0 & n_l \text{ even} \\ i2\pi s\Theta[\mathbf{n}] & n_l \text{ odd}. \end{cases} \tag{1.115}$$

The complete effective action can be now expressed as:

$$\tilde{S}_E = \begin{cases} \frac{1}{2g}\int d^2\mathbf{x}\left(\frac{1}{v_s}(\partial_\tau\mathbf{n}(\mathbf{x}))^2 + v_s(\partial_x\mathbf{n}(\mathbf{x}))^2\right) & n_l \text{ even} \\ \frac{1}{2g}\int d^2\mathbf{x}\left(\frac{1}{v_s}(\partial_\tau\mathbf{n}(\mathbf{x}))^2 + v_s(\partial_x\mathbf{n}(\mathbf{x}))^2\right) + i2\pi s\Theta[\mathbf{n}] & n_l \text{ odd} \end{cases} \tag{1.116}$$

where the coupling constant g and the spin-wave velocity v_s are defined as:

$$\begin{aligned} g &= \frac{a_0}{s}\frac{1}{\sqrt{\sum_{abc}J_a\mathcal{J}^{-1}_{bc}}} \\ v_s &= a_0^2 s\sqrt{\frac{\sum_a J_a}{\sum_{a,b}\mathcal{J}^{-1}_{ab}}}. \end{aligned} \tag{1.117}$$

If we fix $n_l = 1$ and $J_a = J$, $J'_{a,a+1} = 0$ we get exactly (1.72).

Therefore the continuum limit of spin ladder systems is effectively described by a NLσM if the spin is integer *or* the ladder has an even number of legs. As a result it will be gapped and the correlation functions will decay exponentially. On the other hand, the system will be gapless and critical if there is an odd number of legs *and* the spin is half-integer.

We expect that the difference between even and odd leg ladders disappears as we take into account more and more chains, because we know that in two dimensions the topological term must vanish. Indeed if we consider the case when $J_a = J$, $J'_{a,a+1} = J'$ and $J' \ll J$ then the coupling constant $g \approx \frac{2}{sn_l}$ is small when the number of legs is large and the NLσM is in weak coupling regime. Thus we can estimate the gap Δ for the even leg ladder as in (1.104):

$$\Delta = \frac{v_s}{a_0} e^{-\frac{2\pi}{g}} \approx \frac{v_s}{a_0} e^{-\pi s n_l} \tag{1.118}$$

So in the limit $n_l \to \infty$ the gap disappears and the behavior of even and odd leg ladders coincides.

Chapter 2

Spin-1 models

In the last chapter we have considered the Heisenberg Hamiltonian (1.1) as a model for quantum spin systems in one or higher dimensions. We focused our attention mainly on the corresponding antiferromagnetic chain for which Haldane predicted unexpected results for integer and half-interger spin. In the latter case these results found rigorous proof in the Lieb-Schultz-Mattis theorem [26], extended by Affleck and Lieb [2], which assure us that half-integral spin chains are gapless or have a degenerate ground state in the infinite volume limit. Given that all one-dimensional Heisenberg antiferromagnets have a unique ground state in this limit [6], Haldane's predictions for half-integer spins are confirmed. Such rigorous proofs are not available for integer spin chains, but nonetheless a lot of numerical calculations support Haldane's conclusions for $s = 1$ [25, 37, 43].
From now on we will be interested in the particular $s = 1$ case and a more general one-dimensional spin Hamiltonian which includes (1.1) as a special case, the so-called *bilinear-biquadratic* hamiltonian, will be considered:

$$H = J \sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right] \tag{2.1}$$

where β is a real parameter and J is the coupling constant.
It is worth to cite another important class of spin-1 models which includes the Heisenberg model as a special case, the class of $\lambda - D$ models:

$$H_{\lambda - D} = J \sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (\lambda - 1) S_i^z S_{i+1}^z + D (S_i^z)^2 \right] \tag{2.2}$$

but it will not be further discussed here.

2.1 The bilinear-biquadratic spin-1 model and its phases

The reason why the Hamiltonian (2.1) is of interest is in its rich phase diagram which can be probed varying the value of β and the sign of J[1]. Furthermore this is the most general SU(2)-invariant isotropic spin-1 Hamiltonian

[1] Obviuosly varying the value of $|J|$ just sets the energy scale

with nearest-neighbor interactions. Indeed a Hamiltonian with the properties above should be expressed as a sum of powers of exchange terms:

$$H = \sum_m J_m \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^m. \tag{2.3}$$

which in turn can be expressed as follows [6] :

$$(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^m = \sum_{j=0}^{2s} \left[\frac{1}{2} j(j+1) - s(s+1) \right]^m \mathcal{P}_j(i, i+1) \tag{2.4}$$

where $j(j+1)$ are the eigenvalues of the square of the total spin operator of the two neighboring sites $\mathbf{J}_i^2 = (\mathbf{S}_i + \mathbf{S}_{i+1})^2$ and $\mathcal{P}_j(i,,i+1)$ is the projector operator onto the subspace of total spin j. These relations can be inverted to give the projection operators as polynomials of $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$.
For $s = 1$ and for $m = 0, 1, 2$ we get:

$$\mathcal{P}_0(i, i+1) = -\frac{1}{3} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \tag{2.5}$$

$$\mathcal{P}_1(i, i+1) = 1 - \frac{1}{2} \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right] \tag{2.6}$$

$$\mathcal{P}_2(i, i+1) = \frac{1}{3} + \frac{1}{2} \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right] \tag{2.7}$$

Given that every other power $m > 2$ of the exchange term is still a linear combination of (2.5),(2.6) and (2.7), the highest power in (2.3) must be at most 2, therefore from trivial manipulations we can get back (2.1). It can be shown in the same fashion that the Heisenberg Hamiltonian is the most general one for spin $s = 1/2$.
We are giving now a quick overview of the different phases of the model. The coupling constant J is assumed positive if not otherwise specified. Besides the Heisenberg point $\beta = 0$ which gives us back (1.1), there is another point intimately related to the former as they share the same physics, but this time we can extract some rigorous results from the model and the consequences of the Haldane conjecture can be directly verified. It is the *AKLT point* which is given by $\beta = -1/3$ [4]:

$$H_{AKLT} = J \sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right]. \tag{2.8}$$

This is one of the several *projection points* of the phase diagram, for which a number of exact properties can be calculated with various techniques. In a projection point the Hamiltonian (2.1) can be expressed as a sum over the projection operators $\mathcal{P}_j(i, i+1)$ acting on every pair of interacting spins for a given value of $j = 0, 1, 2$. From (2.7) it is clear that the Hamiltonian (2.8) can be written as:

$$H_{AKLT} = -\frac{2}{3} NJ + 2J \sum_i \mathcal{P}_2(i, i+1). \tag{2.9}$$

Both the Heisenberg and the AKLT points belong to a wider region of the phase diagram defined by:

$$-1 < \beta < 1 \quad and \quad J > 0 \tag{2.10}$$

called the *Haldane phase* which shows an antiferromagnetic behavior with exponentially decaying correlation functions and a unique massive ground state.
The points at $\beta = 1$ and $\beta = -1$ are critical and correspond to the so-called *Takhtajan-Babujian model* [7, 44] and the *Sutherland model* [42] respectively. For both these models the ground state has been exactly calculated and it is unique and without a gap between it and the first excited state. It appears then that these models behave quite differently from the Heisenberg antiferromagnet. The point $\beta = -1$ is also a projection point, as can be seen from (2.6):

$$H_S = 2NJ - 2J \sum_i \mathcal{P}_1(i, i+1). \tag{2.11}$$

This model has also a larger SU(3) symmetry since it can be mapped explicitly into the antiferromagnetic SU(3) Heisenberg model [38].
Another SU(3)-invariant model can be realized when $\beta = \infty$, where the bilinear-biquadratic model becomes purely biquadratic:

$$H_{bq} = \lim_{\beta \to \infty} \frac{H}{\beta} = -J \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2. \tag{2.12}$$

and can still be expressed in terms of projectors:

$$H_{bq} = -NJ - 3J \sum_i \mathcal{P}_0(i, i+1). \tag{2.13}$$

Furthermore we can map this model into the antiferromagnetic SU(3) Heisenberg model with alternating fundamental and anti-fundamental representations (see appendix C). When $\beta = \infty$ and $J > 0$ the model have a two-fold degenerate ground state and a small excitation gap [8, 24] and belongs to an antiferromagnetic dimer phase region defined by:

$$\begin{array}{ll} \beta > 1 & J > 0 \\ \beta < -1 & J < 0. \end{array} \tag{2.14}$$

The two-fold degeneracy of the ground state is caused by the broken translational symmetry which is typical of a dimer phase where the system tends to split its spins in valence-bounded pairs (see § 2.2). Since there are two ways to form such pairs in a chain, then the corresponding states will both have the lowest energy and be related by a translation of one site.
There is one last antiferromagnetic region in the phase diagram for:

$$\beta < -1 \quad and \quad J > 0 \tag{2.15}$$

which is a gapless *trimerized* phase.
For every remaining combination of values of β and J:

$$\beta > -1 \quad and \quad J < 0 \tag{2.16}$$

we have a ferromagnetic gapless phase, which contains also the Heisenberg ferromagnet for $\beta = 0$. The ground state of every model in this region is the fully aligned state:

$$|\Psi_0\rangle = |+ + + + + \ldots\rangle \tag{2.17}$$

with energy $E^{(0)}$:

$$E^{(0)} = JN(1-\beta). \tag{2.18}$$

As we already know such a ground state breaks the continuous rotational symmetry of (2.1) and as a result we expect arbitrary small spin wave excitations which make the spectrum gapless. Indeed the energy of a generic spin wave excitation with momentum $k \neq 0$ and total spin $s = N - 1$ is [5]:

$$E^{(1)} = E^{(0)} + 2J(\cos(k) - 1). \tag{2.19}$$

The ferromagnetic and antiferromagnetic phases are separated by two projection points. Indeed at $\beta = \infty$ and $J < 0$ the Hamiltonian becomes purely biquadratic as in (2.12). The ground state is still the fully aligned state (2.17) with energy $E^{(0)}_{bq}$:

$$E^{(0)}_{bq} = \lim_{\beta\to\infty} \frac{E^{(0)}}{\beta} = \lim_{\beta\to\infty} \frac{JN(1-\beta)}{\beta} = -NJ. \tag{2.20}$$

From the ferromagnetic region, as we move towards this point, the energy (2.19) of the spin wave excitations gets more and more close to $\beta E^{(0)}_{bq}$, and eventually they become equal in the limit $\beta \to \infty$:

$$\frac{E^{(1)}}{\beta} \xrightarrow[\beta\to\infty]{} E^{(0)}_{bq} \tag{2.21}$$

meaning that every such excitation becomes degenerate with the ground state in this limit, but the energy of excitations of momentum k and total spin $s = N - 2$ is [5]:

$$E^{(2)} = E^{(0)} - \beta J[3 + 2\cos(k)] \tag{2.22}$$

Again in the limit $\beta \to \infty$ the energy of these excitations becomes:

$$E^{(2)}_{bq} = \lim_{\beta\to\infty} \frac{E^{(2)}}{\beta} = E^{(0)}_{bq} - J[3 + 2\cos(k)] \tag{2.23}$$

showing a gapped dispersion relation.
The second projection point between the two phases is at $\beta = -1$ and $J < 0$.

This model is SU(3)-invariant [5] and has ferromagnetic and antiferromagnetic degenerate ground states, of total spin $s = N$ and $s = 0$ respectively, with energy given by (2.18):

$$E^{(0)} = 2JN. \tag{2.24}$$

Moreover there are other ground states with arbitrary even spin between 0 and N. For each ground state we can find a corresponding excitation with momentum k and energy [5]:

$$E^{(1)} = E^{(0)} + 2J(\cos(k) - 1), \tag{2.25}$$

giving a gapless spectrum. Another exact result that can be evaluated in this case is the correlation function:

$${}_s\langle\Psi_0|\,\mathbf{S}_i \cdot \mathbf{S}_j\,|\Psi_0\rangle_s = \frac{s(s+1) - 2N}{N(N-1)}. \tag{2.26}$$

We see that for a given ground state $|\Psi_0\rangle_s$ of total spin s, it does not depend on the distance between spins.
In order to visualize better the phase diagram of this class of bilinear-biquadratic models we can express the corresponding Hamiltonian in a more convenient form. As said before, what really matters in defining the various phases of the diagram is not the absolute value of the coupling constant J but rather the value of β and the sign of J, where β is nothing more than the ratio of the biquadratic and bilinear coupling terms. Thus the Hamiltonian can be also expressed as:

$$H = J' \sum_i \left[\cos(\theta)\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \sin(\theta)\,(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2\right] \tag{2.27}$$

where now $J = J'\cos(\theta)$ and $\beta = \tan(\theta)$. The corresponding phase diagram can be drawn fixing the sign of the coupling constant J' and let the other angular parameter θ vary in the interval $[0, 2\pi]$ (see Fig.2.1).

2.2 The Valence Bonds

It is definitively worth introducing the *valence bond states* as they give us an intuitive picture of different antiferromagnetic ground states and can be used as a calculation tool to get some exact and approximate results for various models.
Let us consider two spin-1/2 variables. A suitable basis for this two-spins system is given by:

$$\begin{array}{ccc} & \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) & \\ |\uparrow\uparrow\rangle & \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) & |\downarrow\downarrow\rangle \end{array} \tag{2.28}$$

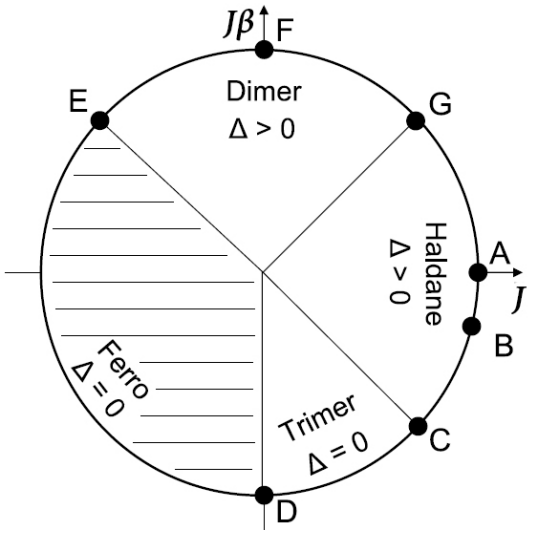


FIGURE 2.1: The phase diagram of the bilinear-biquadratic model. Varying the parameter θ on the circle we can find all the phases discussed before: in **A** we have the AF Heisenberg Model, in **B** the AKLT point, in **F** and **D** the AF and FM biquadratic models respectively, in **G** the Takhtajan-Babujian model, in **C** the Sutherland model end finally in **E** the SU(3) transition point from the antiferromagnetic dimer phase to the ferromagnetic phase [5].

FIGURE 2.2: A schematic representation of valence bonds in a dimer state on a chain of spin-$1/2$'s. Each point is a spin variable and a valence bond is depicted as a straight line connecting two spins.

so to have a singlet of total spin $s = 0$ and a triplet of total spin $s = 1$.
Now consider a spin-$1/2$ system on a lattice. A *valence-bond basis* for the spin-singlet states of the system consists of all the possible configurations in which pairs of spins are contracted to form a singlet $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ called a valence bond. Playing with valence bonds between spins we can easily construct ground states for some suitable models.
As an example let us consider a periodic spin-$1/2$ chain and the two states where only nearest-neighbor pairs of spins form valence bonds (see Fig. 2.2) [6]:

$$|d\rangle_{\pm}^{s=1/2} = \bigotimes_{i=1}^{N/2} \frac{1}{\sqrt{2}}(|\uparrow_{2i}\rangle \otimes |\downarrow_{2i\pm1}\rangle - |\downarrow_{2i}\rangle \otimes |\uparrow_{2i\pm1}\rangle). \tag{2.29}$$

In both the above states each group of three consecutive spins cannot have a total spin higher than $1/2$ since in order to have a total spin of $3/2$ at least one pair of spins should be combined to form a triplet. We can express this

property in mathematical form using a projection operator onto the subspace of total spin $s = 3/2$:

$$\mathcal{P}_{3/2}(i, i+1, i+2) \left|d\right\rangle_{\pm} = 0 \qquad \forall i \tag{2.30}$$

where

$$\begin{aligned} \mathcal{P}_{3/2}(i, i+1, i+2) =& \frac{1}{3}\left[(\mathbf{S}_i + \mathbf{S}_{i+1} + \mathbf{S}_{i+2})^2 - \frac{3}{4}\right] \\ =& \frac{1}{2} + \frac{2}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \mathbf{S}_i \cdot \mathbf{S}_{i+2} + \mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2}). \end{aligned} \tag{2.31}$$

Now we can construct a Hamiltonian ad hoc for which the states (2.29) are ground states:

$$\begin{aligned} H_{MG} =& |J| \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{2}\mathbf{S}_i \cdot \mathbf{S}_{i+2}\right) \\ =& -\frac{3}{8}N|J| + \frac{3}{4}|J| \sum_i \mathcal{P}_{3/2}(i, i+1, i+2). \end{aligned} \tag{2.32}$$

This Hamiltonian is made up of two antiferromagnetic interaction terms, where the first is between nearest-neighbor spins and the second, being between next-nearest-neighbors, partially frustrates the Heisenberg-like corresponding model. It is called the *Majumdar-Ghosh* Hamiltonian. The states (2.29) are an example of dimer states breaking the translational symmetry of the system.
As we are more interested in spin-1 models, a generalization of valence bonds for higher spin is needed. A natural way to introduce valence bonds in spin-s systems is to treat every single spin-s variable as a symmetrization of $2s$ spin-$1/2$'s [3]. Valence bonds then can be formed between these spin-$1/2$ variables on different sites as before. There will be $2s$ bonds emanating from each site and if all of them terminate on the same nearest-neighbor site we get a dimer state as in the $s = 1/2$ case, but this time the corresponding Hamiltonian is constructed as a sum with positive coefficients of projection operators acting on every group of three neighboring spins onto the subspace of each possible total spin but s.

2.2.1 The AKLT Model and the VBS ground state

If the coordination number of the lattice equals $2s$ there is another interesting way to arrange valence bonds to form a ground state, that is linking every site with all the corresponding nearest-neighbors. This ground state is called a *valence bond solid* or *VBS* as the bonds mimic the geometry of the lattice. For a given system of spin s on a given lattice there is a unique (in the infinite volume limit) VBS ground state and, unlike the dimer state, it does not break the transational symmetry. So far we have given the ground state but not the corresponding Hamiltonian so we now focus on the special case $s = 1$. In

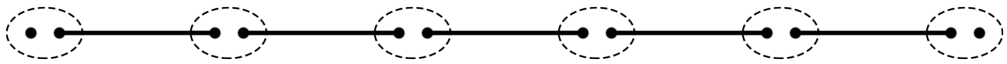


FIGURE 2.3: The spin-1 VBS state. Here each point still represents a spin-1/2 variable, but the dotted circle corresponds to the symmetrization of the two spins inside to give a spin-1. Notice the free spins at the boundaries which do not participate in any bond.

this case the lattice has to be one-dimensional, so to have the condition on the coordination number satisfied. In this chain there is always a valence bond between two neighboring spins so that each pair will never be in a quintet state, which would need all four spin-1/2 to form a triplet and never a singlet. In other words:

$$\mathcal{P}_2(i,i+1)\,|VBS\rangle = 0 \qquad \forall i, \tag{2.33}$$

where $\mathcal{P}_2(i,i+1)$ is given by (2.7). It is now clear that the Hamiltonian we are looking for is nothing but the AKLT Hamiltonian (2.8).
Since our system can be thought as made up of spin-1/2 variables, we will use for the corresponding state space the common basis $\{\psi_1 = |\uparrow\rangle, \psi_2 = |\downarrow\rangle\}$ of eigenstates of S^z, in terms of which we can construct an orthogonal basis for the $s = 1$ state space [4]. Indeed taking the symmetrized tensor products of ψ_1 and ψ_2 we get:

$$\psi_{\alpha\beta} = \frac{1}{\sqrt{2}}(\psi_\alpha \otimes \psi_\beta + \psi_\beta \otimes \psi_\alpha). \tag{2.34}$$

Notice that $\psi_{12} = \psi_{21} = |0\rangle$, $\psi_{11} = \sqrt{2}\,|+\rangle$ and $\psi_{22} = \sqrt{2}\,|-\rangle$ where $\{|0\rangle, |+\rangle, |-\rangle\}$ is the standard orthonormal basis for the spin-1 space state. In order to contract a pair of spin-1/2's to form a singlet, that is a valence bond, we have to take an antisymmetrized tensor product between the two, which we express using a ϵ tensor: $\epsilon^{\alpha\beta}\psi_\alpha \otimes \psi_\beta$. So a (un-normalized) state $\Omega_{\alpha\beta}$ with a valence bond between two spin-1/2's can be written as (see Fig. 2.3):

$$\Omega_{\alpha\beta} = \epsilon^{\gamma\delta}\psi_{\alpha\gamma} \otimes \psi_{\delta\beta}. \tag{2.35}$$

This can be thought as the ground state for the AKLT Hamiltonian on a chain of only two sites, where the subscripts α and β account for the freedom that, in an open chain, the "outer" spin-1/2's have to be in a state $|\uparrow\rangle$ or $|\downarrow\rangle$, giving a total of four different and degenerate possibilities, i.e. one singlet state and three triplet states. If we impose periodic boundary conditions there is only one ground state:

$$\Omega = \epsilon^{\alpha\beta}\epsilon^{\gamma\delta}\psi_{\alpha\gamma} \otimes \psi_{\delta\beta}. \tag{2.36}$$

It is now easy to generalize the construction of the VBS ground state for a chain of length N:

$$\begin{aligned}&\Omega_{\alpha\beta} = \epsilon^{\beta_1\alpha_2}\epsilon^{\beta_2\alpha_3}\dots\epsilon^{\beta_{N-1}\alpha_N}\psi_{\alpha\beta_1}\otimes\psi_{\alpha_2\beta_2}\otimes\dots\otimes\psi_{\alpha_N\beta} \quad ;\\ &\Omega = \epsilon^{\alpha\beta}\Omega_{\alpha\beta} = \epsilon^{\alpha\beta}\epsilon^{\beta_1\alpha_2}\epsilon^{\beta_2\alpha_3}\dots\epsilon^{\beta_{N-1}\alpha_N}\psi_{\alpha\beta_1}\otimes\psi_{\alpha_2\beta_2}\otimes\dots\otimes\psi_{\alpha_N\beta}.\end{aligned} \tag{2.37}$$

We still have four degenerate ground states for the open chain and just one ground state for the closed chain, but all of them yield the same unique ground state when considering the infinite volume limit $N \to \infty$ [4]. This means that if we are interested in evaluating an expectation value in this limit we can do the calculations on the finite closed chain and then take the limit $N \to \infty$. We can, for instance, exactly evaluate the expectation value of $S_0^a S_r^b$, i.e. the two point correlation function using the VBS state Ω [4]:

$$\lim_{N\to\infty}\langle\Omega|\, S_0^a S_r^b\,|\Omega\rangle = \delta^{ab}(-1)^r\frac{4}{3}3^{-r} \tag{2.38}$$

showing, as anticipated, an exponentially decaying correlation function with correlation length $\xi = \ln(3)^{-1}$. Also the presence of a finite gap in the spectrum of this model, i.e. the Haldane gap, can be rigorously proven[4].

2.2.2 The dimer state

The VBS ground state is the exact ground state for the AKLT model, but it can represent a good approximation for other systems in the same phase, i.e. the Haldane phase, especially for the Heisenberg model ($\beta = 0$) which is close to the AKLT point ($\beta = -1/3$). The same can be said about the dimer states constructed as specified in § 2.2:

$$\begin{aligned}|d\rangle_{\pm}^{s=1} &= \frac{1}{\mathcal{C}}\bigotimes_{i=1}^{N/2}\psi_{\alpha_{2i}\beta_{2i}}\otimes\psi_{\alpha_{2i\pm1}\beta_{2i\pm1}}\epsilon^{\alpha_{2i}\alpha_{2i\pm1}}\epsilon^{\beta_{2i}\beta_{2i\pm1}}\\ &= \bigotimes_{i=1}^{N/2}\frac{1}{\sqrt{3}}(|+\rangle_{2i}\otimes|-\rangle_{2i\pm1} + |-\rangle_{2i}\otimes|+\rangle_{2i\pm1} - |0\rangle_{2i}\otimes|0\rangle_{2i\pm1})\end{aligned} \tag{2.39}$$

where $\mathcal{C}$ is a normalization constant. Here in the first line we have explicated how the virtual spin-1/2's have to be contracted to give the dimer state: each valence bond (there are two of them) emanating from the site $2i$ has to terminate on the neighboring site $2i \pm 1$ (see Fig. 2.4). There is no value of β in

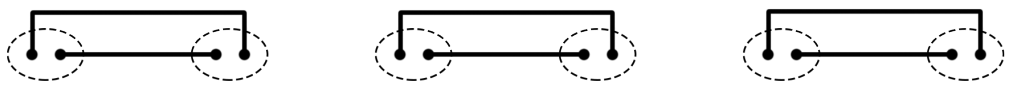


FIGURE 2.4: The spin-1 dimer state. Here the valence bonds form singlet pairs of neighboring spin-1's.

(2.1) giving a model for which (2.39) is the exact ground state. Indeed, as we know from § 2.2, the correct Hamiltonian should be expressed as a sum of projection operators onto $s = 0, 2$ and 3 for each group of three neighboring spins. Nevertheless this ground state may approximate the ground state for the dimer phase defined in (2.14). Indeed let us now consider the following Hamiltonian:

$$\mathcal{H}_\delta = \sum_i J_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right]. \tag{2.40}$$

where $J_i = J$ on *odd* sites and $J_i = J\delta \leq J$ on *even* sites. Clearly for $\delta = 1$ we get back (2.1) but varying continuously this parameter from 1 to another value $\delta' < 1$ we may still face no phase transitions. Indeed this is what happens for those values of β in which (2.1) is in the dimer phase, i.e. varying δ from 1 to 0 causes no phase transitions (see Fig.2.5) [21]. It is easy to show that $|d\rangle_-^{s=1}$ in (2.39) is the ground state of (2.40) if $\delta = 0$ and $\beta > -\frac{1}{3}$.

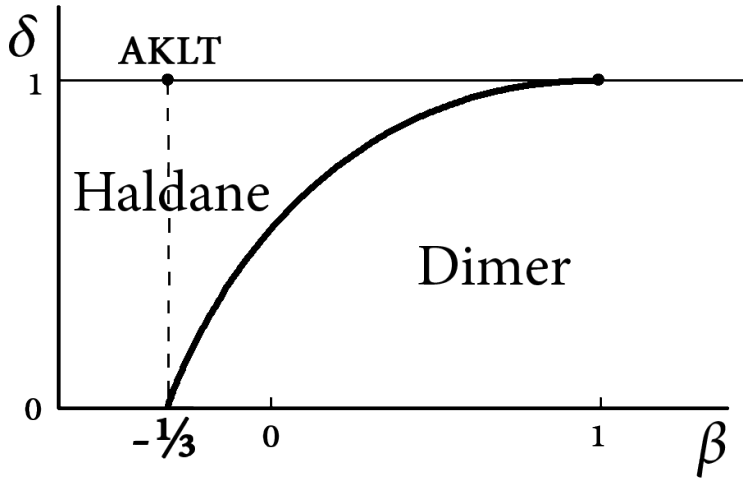


FIGURE 2.5: A qualitative phase diagram of the Hamiltonian H_δ. We can see that if $\beta > 1$ the new parameter δ can be continuously varied from 1 to 0 without incurring a phase transition [21].

2.3 The $Z_2 \times Z_2$ symmetry and the string order parameter

Both the Haldane and the dimer phases are antiferromagnetic gapped phases separated by a continuous transition at $\beta = 1$. What characterize the former from the latter is a hidden symmetry breaking, related to the $Z_2 \times Z_2$ symmetry. In the previous section we have seen that the AKLT model has exponentially decaying correlations and this applies to the whole Haldane phase. Therefore we may conclude that there is no order in this antiferromagnetic phase but, as we will see, a different kind of *hidden* order is actually there. We are going to show this on the VBS state. First of all we re-express the VBS state $\Omega_{\alpha\beta}$ in terms of the standard basis of eigenstates of S_i^z in the spin-1

representation in each site:

$$\Omega_{\alpha\beta} = \sum_{\sigma} \Omega_{\alpha\beta}(\sigma)\Phi_{\sigma}. \tag{2.41}$$

Here σ is a string of $+$'s, $-$'s and 0's and defines the corresponding state Φ_σ which can be expressed as a tensor product of single site states $|+\rangle, |-\rangle$ and $|0\rangle$. $\Omega_{\alpha\beta}(\sigma)$ is the coefficient relative to the state Φ_σ, and it is different from zero just for few σ's, the form of which depends on α and β. For instance, if $\alpha = 1$ and $\beta = 2$ it means that the first spin-1/2 of the chain is in the $|\uparrow\rangle$ state, and thus there cannot be a $|-\rangle$ state in the first site, which must be a $|+\rangle$ or a $|0\rangle$. In the latter case we still must have the first non-zero character to be a $+$ in σ in order to satisfy the construction of the VBS state (2.37). It can be verified that there has to be the same number of $+$'s and $-$'s alternating all along the σ string, with no further restrictions on the number of 0's between them. If $\alpha = \beta = 1$ the form of σ is still the same, i.e. with alternating $+$'s and $-$'s but this time the numer of 0's must accommodate for one more $+$ than $-$. When α and β are reversed then $+$'s and $-$'s are too. So a typical permitted state Φ_σ for, let's say, $\alpha = 1$ and $\beta = 2$ could look like this:

$$\Phi_\sigma = |000+-0+-+0-+0-+-0\rangle\,. \tag{2.42}$$

It can be shown that the VBS state can be written as follows [3]:

$$\Omega_{\alpha\beta} = \sum_{\sigma} (-1)^{z(\sigma)} 2^{n(\sigma)/2} \Phi_\sigma \tag{2.43}$$

where $z(\sigma)$ is the number of 0 characters in odd sites and $n(\sigma)$ is the number of non-zero characters in σ. If we take a look at (2.42) it is apparent that there is a sort of Néel order if we ignore the 0's. Still we cannot predict what the spins will be in two distant sites as we have no control on the number of the 0's. Indeed there is no *local* order parameter that can be found to be non-zero in the Haldane phase and that can be used to distinguish this phase from the others. As it turned out, there actually is a *non-local* order parameter, the *string order parameter*, that reveals the hidden order of the Haldane phase. It is defined as follows [22, 28][2]:

$$\mathcal{O}^{\alpha}_{S}(H) = \lim_{|j-k|\to\infty} \left\langle S^{\alpha}_{j} \exp\left(i\pi \sum_{l=j+1}^{k-1} S^{\alpha}_{l} \right) S^{\alpha}_{k} \right\rangle_{H} \tag{2.44}$$

where $\alpha = x, y$ or z and $< \cdots >_H$ is the expectation value in the infinite volume ground state of H, that we know has to be unique in the Haldane phase even though the VBS state in a finite chain is four-fold degenerate due to the effective spin-1/2's at the boundaries. For a generic model in the Haldane phase the ground state is not four-fold degenerate, but it shows a *nearly* degeneracy, i.e. the lowest four eigenvalues are very close, and they all converge to the same value as we take the infinite volume limit. Both the hidden

[2] We are discarding a minus sign from the original definition.

order and the near or exact degeneracy of the ground state in the Haldane phase are consequences of the hidden $Z_2 \times Z_2$ symmetry breaking [22]. In order to make manifest this symmetry breaking we have to introduce a non-local unitary transformation $\mathcal{U}$:

$$\mathcal{U} = \prod_{j<k} \exp\left(i\pi S_j^z S_k^x\right) \tag{2.45}$$

such that:

$$\mathcal{U}\Phi_\sigma = (-1)^{z(\sigma)}\Phi_{\bar{\sigma}}. \tag{2.46}$$

Here the configuration $\bar{\sigma}$ is defined as follow:

- if $\sigma_i = +(-)$ and the number of non-zero charachters to the left of the site i is odd then $\bar{\sigma}_i = -(+)$
- $\bar{\sigma}_i = \sigma_i$ otherwise

where σ_i is the i-th character of the string. We give an example of the action of $\mathcal{U}$ on a random state:

$$|0+-+++0+-+0++0\rangle \to -\,|0+++-+0---0+-0\rangle\,. \tag{2.47}$$

Notice that if applied on a state with alternating $+$'s and $-$'s as in a permitted state in (2.43), this unitary transformation aligns all the non-zero spins, i.e. if the first non zero character is $+(-)$ all the other non zero characters become $+(-)$. It is also evident that $\mathcal{U}^{-1} = \mathcal{U}$.
Let us show now how the spin operators transform under the action of $\mathcal{U}$ [22]:

$$\begin{aligned}
\mathcal{U}S_j^x\mathcal{U}^{-1} &= S_j^x \exp\left(i\pi \sum_{l>j} S_l^x\right) \\
\mathcal{U}S_j^y\mathcal{U}^{-1} &= \exp\left(i\pi \sum_{l<j} S_l^z\right) S_j^y \exp\left(i\pi \sum_{l>j} S_l^x\right) \\
\mathcal{U}S_j^z\mathcal{U}^{-1} &= \exp\left(i\pi \sum_{l<j} S_l^z\right) S_j^z.
\end{aligned} \tag{2.48}$$

Notice that *local* operators have been mapped onto *non-local* operators as they contain a sum of spin operators acting on different sites. This is not surprising given that $\mathcal{U}$ itself is a non-local unitary transformation. For the same reason we should expect that, in general, also the transformed Hamiltonian $\tilde{H} = \mathcal{U}H\mathcal{U}^{-1}$ will be non-local and thus have long-range interactions but, using the transformed spin operators (2.48), it actually turns out to be a local operator:

$$\tilde{H} = J\sum_j [h_j - \beta(h_j)^2] \tag{2.49}$$

where

$$h_j = -S_j^x S_{j+1}^x + S_j^y \exp\left(i\pi(S_j^z + S_{j+1}^x)\right) S_{j+1}^y - S_j^z S_{j+1}^z. \tag{2.50}$$

The transformed Hamiltonian $\tilde{H}$ still has the same symmetries of the original Hamiltonian H, but they may not be local symmetries anymore. Actually the only local symmetry $\tilde{H}$ has is related to its invariance under rotations of π about each coordinate axis. This symmetry group is equivalent to $Z_2 \times Z_2$. Indeed the product of two π-rotations about two different axes produce a π-rotation about the third axis, so we can take as generators of this symmetry $\prod_j \exp\left(i\pi S_j^z\right)$ and $\prod_j \exp\left(i\pi S_j^x\right)$.

2.3.1 The symmetry breaking

Now we want to show how this symmetry is spontaneously broken in the transformed AKLT model. The key feature of this model is the presence of effective spin-1/2 degrees of freedom at the boundaries, which is reflected in the four-fold degeneracy of its ground state. For instance we can fix the z component of both these free spins giving in this way the four different states (2.37):

$$\Omega_{11} \qquad \Omega_{22} \qquad \Omega_{12} \qquad \Omega_{21}, \tag{2.51}$$

or equivalently we can ask the ground states to be in a singlet or in triplet state:

$$\underbrace{(\Omega_{12} - \Omega_{21})}_{singlet} \qquad \underbrace{\Omega_{11} \qquad \Omega_{22} \qquad (\Omega_{12} + \Omega_{21})}_{triplet}, \tag{2.52}$$

but the four ground states of H_{AKLT} that will transform under $\mathcal{U}$ into the four symmetry-breaking ground states of $\tilde{H}_{AKLT}$ are defined fixing the z component and the x component of the spin-1/2's at the left and right end of the chain respectively [33]:

$$\begin{array}{ll} |\uparrow\rightarrow\rangle = (\Omega_{11} + \Omega_{12}) & |\uparrow\leftarrow\rangle = (\Omega_{11} - \Omega_{12}) \\ |\downarrow\rightarrow\rangle = (\Omega_{22} + \Omega_{21}) & |\downarrow\leftarrow\rangle = (\Omega_{21} - \Omega_{21}) \end{array} . \tag{2.53}$$

Let us consider for instance a VBS state where the free spin-1/2 at the left is fixed at $|\uparrow\rangle$. In this case, as discussed before, the first spin-1 not in a $|0\rangle$ state must be in a $|+\rangle$ state, the second in a $|-\rangle$ state and so on. When $\mathcal{U}$ is applied to such a state, every second non-zero spin is flipped, so every site is in a $|+\rangle$ or $|0\rangle$ state. If we now fix the free spin-1/2 at the right to be in a $|\rightarrow\rangle$ state, using a basis in which S_i^x, instead of S_i^z, is diagonal, we can likewise expect that the transformed state must be in a $|+\rangle_x$ or $|0\rangle_x$ state, where obviously:

$$S^x |+\rangle_x = |+\rangle_x \qquad S^x |0\rangle_x = \mathbf{0} \qquad S^x |-\rangle_x = -|-\rangle_x . \tag{2.54}$$

Thus in each site there cannot be $|-\rangle$ or $|-\rangle_x$ states, and this condition determine uniquely the exact state in every site:

$$|\phi\rangle_1 = \sqrt{\frac{2}{3}} |+\rangle + \frac{1}{\sqrt{3}} |0\rangle = \sqrt{\frac{2}{3}} |+\rangle_x + \frac{1}{\sqrt{3}} |0\rangle_x . \tag{2.55}$$

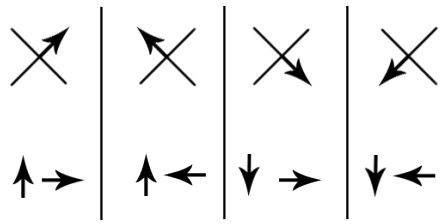


FIGURE 2.6: The direction of the bulk magnetization in the four symmetry broken states (upper panel) and the corresponding ground states of the original Hamiltonian with the different polarization of the spins at the boundaries (lower panel) [33].

Following the same principle we can write the state in each site for the remaining ways to arrange the spin-1/2's at the boundaries:

$$\begin{aligned} |\uparrow\leftarrow\rangle \rightarrow |\phi\rangle_2 &= \sqrt{\frac{2}{3}}\,|+\rangle - \frac{1}{\sqrt{3}}\,|0\rangle \\ |\downarrow\rightarrow\rangle \rightarrow |\phi\rangle_3 &= \sqrt{\frac{2}{3}}\,|-\rangle + \frac{1}{\sqrt{3}}\,|0\rangle \\ |\downarrow\leftarrow\rangle \rightarrow |\phi\rangle_4 &= \sqrt{\frac{2}{3}}\,|-\rangle - \frac{1}{\sqrt{3}}\,|0\rangle\,. \end{aligned} \tag{2.56}$$

The complete ground state for $\tilde{H}_{AKLT}$ is simply obtained tensoring together as many copies of $|\phi\rangle_\nu$ as required by the length of the chain, with $\nu = 1,2,3,4$. Let us recall that the four degenerate ground states of H_{AKLT} will converge to a single infinite volume ground state as required by the Lieb-Schultz-Mattis theorem and as proven in [4] but the same is not true for the ground states of $\tilde{H}_{AKLT}$, as they will converge to four distinct infinite volume states, even though the two Hamiltonians are related by a unitary transformation. Indeed it is the non-locality of the transformation that does not guarantee us a one-to-one correspondence between the ground states. It is apparent now that each of these ground states break the $Z_2 \times Z_2$ symmetry, and show a ferromagnetic order in the z and x directions as revealed by the corresponding non-vanishing order parameters:

$$\mathcal{O}^\alpha_{ferro}(\tilde{H}_{AKLT}) = \lim_{|j-k|\rightarrow\infty} \left\langle S^\alpha_j S^\alpha_k \right\rangle_{\tilde{H}_{AKLT}} = \frac{4}{9} \qquad \alpha = x,z \tag{2.57}$$

Notice that the ground states of the transformed Hamiltonian have a non-vanishing bulk magnetization along diagonal directions given by the original polarizations of the free spin-1/2's at the edges (see Fig. 2.6).

Finally we can understand the role of the string order parameter (2.44). Indeed if we apply the unitary transformation $\mathcal{U}$ on the string operator we get:

$$\mathcal{U}\left(S^\alpha_j \exp\left(i\pi \sum_{l=j+1}^{k-1} S^\alpha_l\right) S^\alpha_k\right)\mathcal{U}^{-1} = -S^\alpha_j S^\alpha_k \qquad \alpha = x,z \tag{2.58}$$

providing us an important identity between the order parameters:

$$\mathcal{O}^{\alpha}_{ferro}(\tilde{H}_{AKLT}) = -\mathcal{O}^{\alpha}_{S}(H_{AKLT}) \qquad \alpha = x, z. \tag{2.59}$$

This means that the presence of ferromagnetic order in the transformed Hamiltonian $\tilde{H}_{AKLT}$ corresponds to a non-vanishing value for the string order parameter $O^{\alpha}_{S}(H_{AKLT})$ which can be then used to reveal the breaking of the hidden symmetry in the original system. Such a symmetry breaking is not peculiar to the AKLT model, but to the whole Haldane phase it belongs to. Indeed, for instance, in the dimer phase the symmetry is completely unbroken and the string order parameter will vanish for every α. On the other hand we can define a different non-local order parameter called *parity* [9]:

$$\mathcal{O}^{\alpha}_{P} = \lim_{|j-k|\to\infty} \left\langle \exp\left(i\pi \sum_{l=j+1}^{k-1} S^{\alpha}_{l} \right) \right\rangle \qquad \alpha = x, y, z \tag{2.60}$$

which is non zero in the dimer phase, while it vanishes in the Haldane phase or in any other non trivial topological phase for every α. We will come back to this in chapter 3.

Chapter 3

Classification and Detection of SPT Phases

3.1 Beyond Landau's theory of symmetry breaking

In the last decades with the discovery of new phases sharing the same symmetries it has been made clear that Landau's theory could not describe all different phases in materials. Indeed the only mechanism in Landau's theory that characterize the various phases is the symmetry breaking. We now know that the phase diagram of many materials is far richer than expected, as a new kind of *topological* order is to be considered.

3.1.1 Quantum phases and quantum phase transitions

In order to give a rigorous definition of quantum phases we consider a class of Hamiltonians $\mathcal{H}(\mathbf{g})$ which have a smooth dependence on a parameter $\mathbf{g}$. We say that the corresponding quantum system described by $\mathcal{H}(\mathbf{g})$ has a phase transition in $\mathbf{g} = \mathbf{g}_c$ if the ground state expectation value $\langle O(\mathbf{g}_c)\rangle$ of a local operator O has a singularity in the thermodynamic limit. Thus the Hamiltonians $\mathcal{H}(\mathbf{g}_0)$ and $\mathcal{H}(\mathbf{g}_1)$ belong to the same quantum phase if we can find a smooth path $\mathcal{H}(\mathbf{g}_t)$, $0 \leq t \leq 1$ connecting $\mathcal{H}(\mathbf{g}_0)$ and $\mathcal{H}(\mathbf{g}_1)$ without facing a phase transition. The existence of such a path connecting two Hamiltonians defines an equivalence relation. A quantum phase is thus an equivalence class of Hamiltonians.
If we are interested in gapped systems then the closure of the gap is a sign of phase transition and two Hamiltonians belong to the same gapped phase if we can find a smooth path of gapped Hamiltonians connecting the two [13].
All the above definitions can be restated in terms of ground states. We say that two gapped ground states $|\psi_0\rangle$ and $|\psi_1\rangle$ are in the same phase, and thus in the same equivalence class, if and only if they are related by a *local unitary evolution*:

$$|\psi_0\rangle \sim |\psi_1\rangle \quad \textit{iff} \quad |\psi_1\rangle = \mathcal{T}\left[e^{-i\int_0^1 dt\tilde{H}(t)}\right]|\psi_0\rangle \tag{3.1}$$

where $\mathcal{T}$ denotes a time-ordered integral and $\tilde{H}(t)$ is a local Hamiltonian, i.e. a sum of local Hermitian operators $\sum_i h_i(t)$.

3.1.2 Topological order

With the given definition of quantum phases it is clear that there is no need to have a symmetry breaking in order to have different phases. Indeed we have not introduce any kind of symmetry so far: the Landau theory of symmetry breaking is not enough to describe all possible orders. Thus, even in absence of any symmetry constraint, we can still have different quantum phases corresponding to different *topological* orders. Two gapped ground states have then the same topological order if they are related by a local unitary evolution (3.1). This order is said to be *trivial* if any state in that phase is equivalent to a *direct-product state*, a state which has no entanglement. States with this kind of order are said to have only *short-range entanglement*. On the other hand, states with non-trivial topological order have *long-range entaglement*.

3.1.3 Symmetry Protected Topological Order

So far we have not introduced any kind of symmetry constraint, meaning that two Hamiltonians with different symmetries could belong to the same phase. If such constraints are taken into account then we have to slightly modify our previous definition of quantum phase, more precisely we will say that the ground states of two Hamiltonians with the same symmetries are in the same phase if and only if they are related by a *symmetric* local unitary evolution (3.1) where now $\tilde{H}(t)$ have the same symmetries of the Hamiltonians. The resulting phase diagram will be inevitably richer as, in the presence of symmetries, states with short-range entanglement are not necessarily in the same phase[1]. Indeed the ground states may partly break the symmetry and different symmetry breaking give rise to different quantum phases which are well described by Landau's theory. According to the latter, states with the same symmetries are always in the same phase so it fails to detect the existence of distinct phases with the same symmetries of the Hamiltonians, i.e. without symmetry breaking involved. Correspondingly we have a new kind of order, also known as *symmetry protected topological* (SPT) order.
Notice that according to the previous section this type of order is topologically trivial as it possesses only short-range entanglement but in our current context, that is when long-range entanglement is not involved, we treat as trivial a symmetric phase in which every state is equivalent to a direct-product state according to the new definition of equivalence given here. Indeed it can be shown that one dimensional gapped spin systems do not have long-range entanglement [12, 11].

3.2 Classification of SPT phases

Now we want to give a classification of these SPT phases when the symmetry involved could be an on-site symmetry described by a group G, parity symmetry or time reversal symmetry. Translational invariance will be always

[1] States with long-range entanglement in the same topological phase may also belong to different phases in presence of symmetries, but we will not be interested in them here.

assumed instead. In order to get this classification we need to exploit a particular representation of quantum states, the MPS representation, which we introduce in § 3.2.1. Another key concept is the projective representation of a symmetry group which is presented in § 3.2.2.

3.2.1 Matrix Product States

Let us consider spin-s variables localized on the sites of a chain of length L. On each site the local state space $|i_k\rangle$ is $d = 2s+1$ dimensional, so $i_k = 1 \dots d$ and $k = 1 \dots L$. A generic quantum state on this chain reads:

$$|\psi\rangle = \sum_{i_1 \dots i_L} c_{i_1 \dots i_L} |i_1 \dots i_L\rangle \tag{3.2}$$

where $c_{i_1 \dots i_L}$ is a tensor with d^L components. Using repeatedly the singular value decomposition (see appendix B) this tensor can be expressed as [39]:

$$c_{i_1 \dots i_L} = \begin{cases} A^{[1]}_{i_1} \dots A^{[k]}_{i_k} \dots A^{[L]}_{i_L} & \textit{with Open Boundary Conditions (OBC)} \\ \mathrm{Tr}\left[A^{[1]}_{i_1} \dots A^{[k]}_{i_k} \dots A^{[L]}_{i_L} \right] & \textit{with Periodic Boundary Conditions (PBC)} \end{cases} \tag{3.3}$$

where, for a fixed i_k, $A^{[k]}_{i_k}$ is a $\chi_k \times \chi_{k+1}$ matrix. Then in each site are defined d matrices of this type. In case of OBC the first $A^{[1]}_{i_1}$ and last matrix $A^{[L]}_{i_L}$ are respectively $1 \times \chi_2$ and $\chi_L \times 1$ matrices, i.e. a row and a column vector. Thus the corresponding representation of the quantum state (3.2) in terms of these matrices is called *Matrix Product State* (MPS) and reads(see Fig.3.1):

$$\begin{aligned} |\psi\rangle &= \sum_{i_1 \dots i_L} A^{[1]}_{i_1} \dots A^{[L]}_{i_L} |i_1 \dots i_L\rangle \qquad \textit{OBC} \\ |\psi\rangle &= \sum_{i_1 \dots i_L} \mathrm{Tr}\left[A^{[1]}_{i_1} \dots A^{[L]}_{i_L} \right] |i_1 \dots i_L\rangle \qquad \textit{PBC} \end{aligned} \tag{3.4}$$

Moreover we say that $\chi = \max_k \chi_k \leq d^{\frac{L}{2}}$ is the *bond dimension* of the MPS and if we express explicitly each tensor $A^{[k]}_{i_k}$ with all his indexes

$$\left(A^{[k]}_{i_k} \right)^{\alpha_k \alpha_{k+1}} \tag{3.5}$$

then we say that $i_k = 1 \dots d$ is the *physical* index while $\alpha_k = 1 \dots \chi_k$ and $\alpha_{k+1} = 1 \dots \chi_{k+1}$ are the *bond* indexes.
The MPS representation of a given state $|\psi\rangle$ is not unique. Indeed it is clear that if we redefine each $A^{[k]}_{i_k}$ as:

$$A^{[k]}_{i_k} \to X_k^{-1} A^{[k]}_{i_k} X_{k+1} \tag{3.6}$$

where X_k is a $\chi_k \times \chi_k$ invertible matrix, then (3.4) does not change. Using this properties the MPS can be put in *canonical form*, i.e. the matrices can be

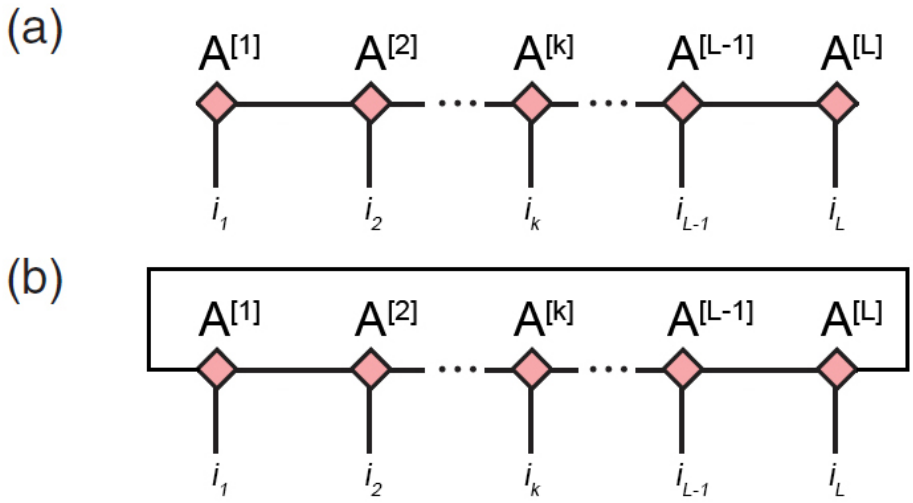


FIGURE 3.1: Diagrammatic representation of the MPS with (a) open boundary conditions and (b) periodic boundary conditions in terms of the matrices $A_i^{[k]}$. Every line corresponds to an index: the vertical open line selects one of the d matrices on each site, while the horizontal lines represent the other indexes $1 \dots \chi_k$. The contraction of indexes is represented by linked lines.

chosen such that $\forall k$ [29] (see Fig.3.2):

$$\begin{aligned} \sum_i A_i^{[k]} A_i^{[k]\dagger} &= \mathbb{I}_{\chi_k} \\ \sum_i A_i^{[k]\dagger} (\Lambda^{[k-1]})^2 A_i^{[k]} &= (\Lambda^{[k]})^2 \end{aligned} \tag{3.7}$$

where $\Lambda^{[k]}$ is a $\chi_{k+1} \times \chi_{k+1}$ positive diagonal matrix with $\mathrm{Tr}\left[(\Lambda^{[k]})^2\right] = 1$.

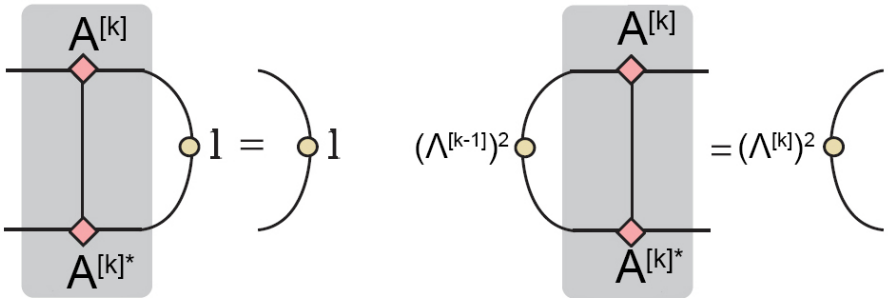


FIGURE 3.2: The conditions satisfied by the MPS matrices in canonical form.

Actually the entries of $(\Lambda^{[k]})^2$ are the non-zero eigenvalues of the reduced density matrix $\rho = \mathrm{Tr}_A |\psi\rangle \langle\psi| = \mathrm{Tr}_B |\psi\rangle \langle\psi|$ related to a bipartion of the system in two halves [29][2]. Notice that $\Lambda^{[0]} = \Lambda^{[L]} = 1$.

[2]In reference [29] the matrix $\Lambda^{[k]}$ is equal to $(\Lambda^{[k]})^2$ in our notation.

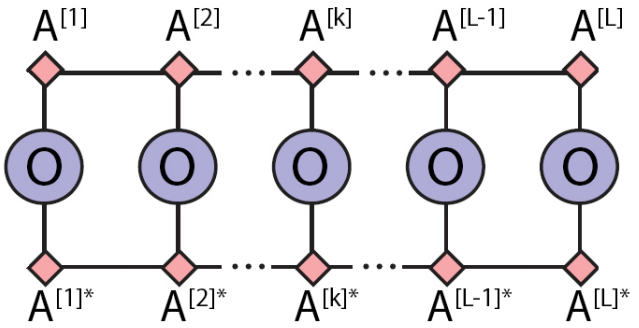


FIGURE 3.3: The expectation value of $\prod_k O(k)$ with OBC.

If we define the linear maps $\mathcal{E}^{[k]}$, also called *transfer matrices*, as follow (see Fig.3.4):

$$\mathcal{E}^{[k]}(X) = \sum_i A_i^{[k]} X A_i^{[k]\dagger} \tag{3.8}$$

where X is a $\chi_{k+1} \times \chi_{k+1}$ matrix, then (3.7) can be restated as:

$$\begin{aligned} &\mathcal{E}^{[k]}(\mathbb{I}_{\chi_{k+1}}) = \mathbb{I}_{\chi_k} \\ &\mathcal{E}^{*[k]}((\Lambda^{[k-1]})^2) = (\Lambda^{[k]})^2 \end{aligned} \tag{3.9}$$

where in $\mathcal{E}^{*[k]}$ $A_i^{[k]}$ and $A_i^{[k]\dagger}$ are interchanged.
Matrix product states can be easily manipulated in order to give expectation values of product of local operators $O(k)$ (see Fig.3.3):

$$\begin{aligned} \langle\psi| \prod_{k=1}^{L} O(k) |\psi\rangle &= \prod_{k=1}^{L} \mathcal{E}_O^{[k]} \qquad OBC \\ \langle\psi| \prod_{k=1}^{L} O(k) |\psi\rangle &= \mathrm{Tr}\left[\prod_{k=1}^{L} \mathcal{E}_O^{[k]}\right] \qquad PBC \end{aligned} \tag{3.10}$$

where (see Fig.3.4):

$$\mathcal{E}_O^{[k]}(X) = \sum_{ij} \langle i| O(k) |j\rangle A_j^{[k]} X A_i^{[k]\dagger}. \tag{3.11}$$

Notice that with OBC $\mathcal{E}_O^{[1]}$ and $\mathcal{E}_O^{[L]}$ can be treated respectively as row and column vectors of dimension $(\chi_2)^2$ and $(\chi_{L-1})^2$. When $O(k) = \mathbb{I}_k$ the canonical form conditions (3.9) guarantee us that the norm of $|\psi\rangle$ with OBC is already normalized.
Let us now focus on MPS's where the matrices $A_i^{[k]} = A_i$ are site-independent, or can be blocked together to give a new site-independent matrix, so to drop the index k. When we have translational invariance this is certainly the case. With OBC we have site-independent matrices in the bulk but still have to take into account the two vectors at the edges.

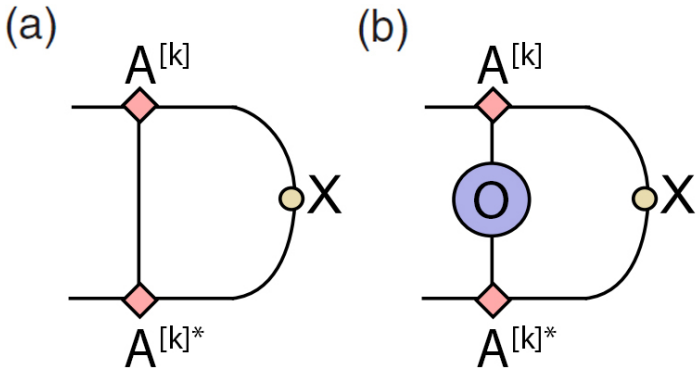


FIGURE 3.4: The linear maps (a) $\mathcal{E}^{[k]}(X)$ and (b) $\mathcal{E}_O^{[k]}(X)$.

These $\chi \times \chi$ matrices in canonical form now satisfy:

$$\begin{aligned} \sum_i A_i A_i^\dagger &= \mathbb{I} \\ \sum_i A_i^\dagger (\Lambda)^2 A_i &= (\Lambda)^2 \end{aligned} \tag{3.12}$$

so the transfer matrix $\mathcal{E}(\mathcal{E}^*)$ have $\mathbb{I}((\Lambda)^2)$ as eigenvector corresponding to the eigenvalue 1. Since from now on we will be interested in the ground states of gapped Hamiltonians, which have a finite correlation length ξ, we can assume that $\mathcal{E}$ has a non-degenerate largest eigenvalue of modulus one $\epsilon_1 = 1$, while the second largest eingenvalue ϵ_2 gives us the correlation length [39]:

$$\xi = -\frac{1}{\ln|\epsilon_2|}. \tag{3.13}$$

Furthermore the ground states of gapped Hamiltonians can be approximated to a given accuracy with an MPS of bond dimension χ which is always finite even in the thermodynamic limit $L \to \infty$ [45].
If $\mathcal{A}$ is a linear map with the largest non-degenerate eigenvalue $\epsilon_1 = 1$ then

$$\mathcal{A}^L = |\epsilon_1\rangle\langle\epsilon_1| + \sum_{k=2}^{n} \epsilon_k^L |\epsilon_k\rangle\langle\epsilon_k| \xrightarrow{L\to\infty} |\epsilon_1\rangle\langle\epsilon_1|, \tag{3.14}$$

thus it is now easy to check that the norm of a gapped ground state with PBC is normalized to one in the thermodynamic limit $L \to \infty$:

$$\langle\psi|\psi\rangle = \mathrm{Tr}\left[\mathcal{E}^L\right] \xrightarrow{L\to\infty} 1. \tag{3.15}$$

3.2.2 Projective Representations

Let G be a group. We say that the operator $R(g)$ form a *projective representation* of G if $\forall g, h \in G$:

$$R(g) \cdot R(h) = \omega(g,h) R(g \cdot h) \tag{3.16}$$

where $\omega(g,h) \in \mathbb{C}$, $|\omega(g,h)| = 1$ is called the *factor system* and distinguishes different projective representations. Furthermore it satisfies:

$$\omega(h,t)\omega(g,h\cdot t) = \omega(g,h)\omega(g\cdot h,t) \qquad \forall g,h,t \in G. \tag{3.17}$$

The common representation of a group is then a trivial projective, also said linear, representation with $\omega(g,h) = 1$ in (3.16).
If we redefine the phase of the operators in the representation $R'(g) = \beta(g)R(g)$ then the corresponding factor system $\omega'(g,h)$ becomes:

$$\omega'(g,h) = \frac{\beta(gh)}{\beta(g)\beta(h)}\omega(g,h). \tag{3.18}$$

We consider as equivalent projective representations which differ for a redefinition of the phase of its operators and the corresponding factor systems $\omega(g,h)$, $\omega'(g,h)$ as belonging to the same equivalence class ω [11].
Given two projective representations $R_1(g)$ and $R_2(g)$ we can form a new projective representation $\tilde{R}(g) = R_1(g) \otimes R_2(g)$ of G satisfying:

$$\tilde{R}(g)\cdot\tilde{R}(h) = \omega_1(g,h)\omega_2(g,h)\tilde{R}(g\cdot h) \tag{3.19}$$

so the corresponding factor system is $\tilde{\omega}(g,h) = \omega_1(g,h)\omega_2(g,h)$. The set of equivalence classes of factor systems together with this operation forms an abelian group called the *second cohomology group* of G and is denoted as $H^2(G,\mathbb{C})$.

3.2.3 On-site symmetry transformation of the MPS

The ground state of a gapped Hamiltonian admits an MPS representation of bond dimension χ of the form:

$$|\psi\rangle = \sum_{i_1\dots i_L} \mathrm{Tr}\left[A_{i_1}\dots A_{i_L}\right]|i_1\dots i_L\rangle \tag{3.20}$$

where translational invariance and PBC are considered for convenience.[3] Let us assume that the ground state is symmetric under a group G of on-site unitary transformations, that is:

$$\bigotimes_{k=1}^{L}\Sigma^{[k]}(g)\,|\psi\rangle = e^{iL\theta_\Sigma(g)}\,|\psi\rangle \qquad \forall g \in G \tag{3.21}$$

where $\Sigma^{[k]}(g)$ is a d-dimensional unitary representation of G[4] acting on the k-th site while $e^{iL\theta_\Sigma(g)}$ is a phase.

[3] The results that follow in this section are valid also if translational invariance is not required and if we consider OBC.

[4] This representation has to be linear. If we consider also projective representations of G acting on the physical sites then it becomes determinant asking non-translational invariance for what follows. See [11] for further details.

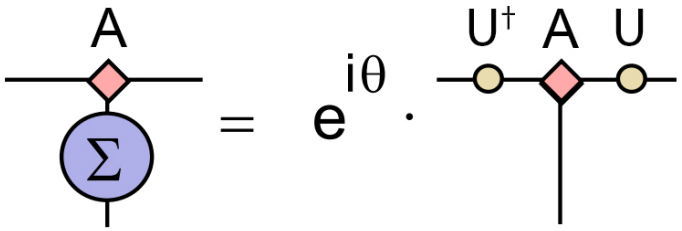


FIGURE 3.5: Symmetry transformation of the matrix A_i.

How do the matrices A_i of the MPS transform under $\Sigma(g)$? It can be shown that in order to satisfy (3.21) A_i must transform like (see Fig.3.5) [11, 12, 31]:

$$\sum_j \Sigma_{ij}(g) A_j = e^{i\theta_\Sigma(g)} U_\Sigma^\dagger(g) A_i U_\Sigma(g) \tag{3.22}$$

where now $U_\Sigma(g)$ is a χ-dimensional unitary *projective* representation of G of a certain class $\omega \in H^2(G, \mathbb{C})$, and $e^{i\theta_\Sigma(g)}$ is a one dimensional representation of G.
The key point for the classification of the various SPT phases for a given symmetry G is that two ground states belong to the same phase if the corresponding projective representations belong to the same class ω. Indeed as shown in [11, 12] it is possible to construct explicitly a local unitary transformation (3.1) that connects the two ground states without breaking the symmetry or facing a phase transition when the corresponding MPS are related to equivalent projective representations, while it is not possible when they are inequivalent. When translational invariance is assumed then also $\theta_\Sigma(g)$ has to be considered for the classification of the possible SPT phases, indeed it cannot be changed without breaking translational symmetry.
Thus the SPT phases of spin systems with only translational and on-site unitary symmetry G are labeled by $\{\omega, \theta_\Sigma(g)\}$ where $\omega \in H^2(G, \mathbb{C})$ and $e^{i\theta_\Sigma(g)}$ is a one dimensional representation of G.

3.2.4 Parity and Time-Reversal Symmetry

Consider now a system which possesses only parity and translational symmetry [5]. The parity transformation on the quantum state (3.20) reads [11, 12]:

$$\left(\bigotimes_{k=1}^{L} \Sigma_P^{[k]} \right) \mathcal{P} \left| \psi \right\rangle = \pm \left| \psi \right\rangle \tag{3.23}$$

where Σ_P is an on-site unitary operation satisfying $(\Sigma_P)^2 = 1$ and $\mathcal{P}$ exchange the sites of the chain. This operations transform the matrices of the

[5] Translational symmetry is inevitable for a system invariant under parity transformations.

MPS in a way similar to that seen previously in (3.22):

$$\sum_j (\Sigma_P)_{ij} A_j^T = e^{i\theta_P} U_P^\dagger A_i U_P \tag{3.24}$$

where the only difference is in the left side of the equation where we used A_i^T in order to take into account the reflection of the chain under parity. If we transpose the equation (3.24) and then apply again $(\Sigma_P)_{li}$ we get:

$$A_l = e^{2i\theta} U_P^T U_P^\dagger A_l U_P U_P^* \tag{3.25}$$

then from (3.12):

$$\mathbb{I} = \sum_l A_l A_l^\dagger = e^{2i\theta} U_P^T U_P^\dagger A_l U_P U_P^* A_l^\dagger \tag{3.26}$$

or equivalently:

$$\mathcal{E}(U_P U_P^*) = e^{-2i\theta_P} U_P U_P^*. \tag{3.27}$$

This last equation tells us that $U_P U_P^*$ is a eigenvector of $\mathcal{E}$ with eigenvalue $e^{-2i\theta_P}$, but we know that the only unimodular eigenvalue of $\mathcal{E}$ is 1, then:

$$e^{-2i\theta_P} = 1 \quad \Rightarrow \quad e^{i\theta_P} = \pm 1 \qquad (\theta_P = 0, \pi). \tag{3.28}$$

On the other hand $U_P U_P^* = e^{i\phi_P}\mathbb{I}$ then:

$$\begin{aligned} U_P &= e^{i\phi_P} U_P^T = e^{i\phi_P}(e^{i\phi_P} U_P) = e^{2i\phi_P} U_P \\ &\Rightarrow \quad e^{i\phi_P} = \pm 1 \qquad (\phi_P = 0, \pi). \end{aligned} \tag{3.29}$$

Thus the matrix U_P of the projective representation of the parity transformation can be either symmetric ($\phi_P = 0$) or antisymmetric ($\phi_P = \pi$).
Thus the SPT phases of systems with only parity symmetry are labeled by $\{\theta_P, \phi_P\}$.
If we consider only time-reversal symmetry instead, the corresponding symmetry transformation on $|\psi\rangle$ is represented by the antiunitary operator [12, 11]:

$$\left(\bigotimes_{k=1}^{L} \Sigma_T^{[k]} \right) \mathcal{T} |\psi\rangle = e^{iL\theta_T} |\psi\rangle \tag{3.30}$$

where Σ_T is an on-site unitary operator satisfying $\Sigma_T^* \Sigma_T = \mathbb{I}$ and $\mathcal{T}$ is the complex conjugate operator. Correspondingly the matrices of the MPS transform as [12, 32]:

$$\sum_j (\Sigma_T)_{ij} A_j^* = e^{i\theta_T} U_T^\dagger A_i U_T. \tag{3.31}$$

Taking the complex conjugate of the previous expression and applying again $(\Sigma_T)_{li}$ we get:

$$A_l = U_T^T U_T^\dagger A_l U_T U_T^*. \tag{3.32}$$

In analogy with the previous case we find:

$$e^{i\phi_T} = \pm 1 \qquad (\phi_T = 0, \pi) \tag{3.33}$$

while we do not obtain any condition on θ_T which is arbitrary and then can be fixed to 1. Thus there are two SPT phases with only time-reversal symmetry, and they are labeled by $\{\phi_T\}$.

3.3 Detection of SPT phases

So far we have shown what are the possible SPT phases in one dimension in presence of various symmetries, and how to classify them looking at the matrices U_Σ of the projective representation of the symmetry involved. How can we find the matrices U_Σ? If we have access to the MPS representation of a quantum ground state, that is if we know the matrices A_i, we can obtain the matrix U_Σ representing projectively the symmetry transformation Σ. Before showing how it is done, let us introduce an alternative form of the matrices in the MPS, a form that will be convenient in the next sections. Indeed we can factorize the matrix $\Lambda^{[k]}$ from $A_i^{[k]}$ and write [46]:

$$A_i^{[k]} = \Gamma_i^{[k]} \Lambda^{[k]} \tag{3.34}$$

and drop the index k as we are considering translation invariant MPS's. The state $|\psi\rangle$ in (3.20) is then represented as:

$$|\psi\rangle = \sum_{i_1 \dots i_L} \mathrm{Tr}\left[\Gamma_{i_1} \Lambda \dots \Gamma_{i_L} \Lambda\right] |i_1 \dots i_L\rangle \tag{3.35}$$

and the canonical form conditions (3.12) can be restated as:

$$\sum_i \Gamma_i \Lambda^2 \Gamma_i^\dagger = \sum_i \Gamma_i^\dagger \Lambda^2 \Gamma_i = \mathbb{I}. \tag{3.36}$$

We now go back to determine U_Σ. First of all if Σ is a symmetry then $|\langle\psi|\tilde{\psi}\rangle| = 1$ where $|\tilde{\psi}\rangle$ is the transformed state. But this norm can be evaluated in analogy with (3.15) (see Fig. 3.6):

$$|\langle\psi|\tilde{\psi}\rangle| = \left|\mathrm{Tr}\left[\mathcal{E}_\Sigma^L\right]\right| \xrightarrow{L\to\infty} 1. \tag{3.37}$$

Thus also $\mathcal{E}_\Sigma$ have a unimodular non-degenerate dominant eigenvalue. It is

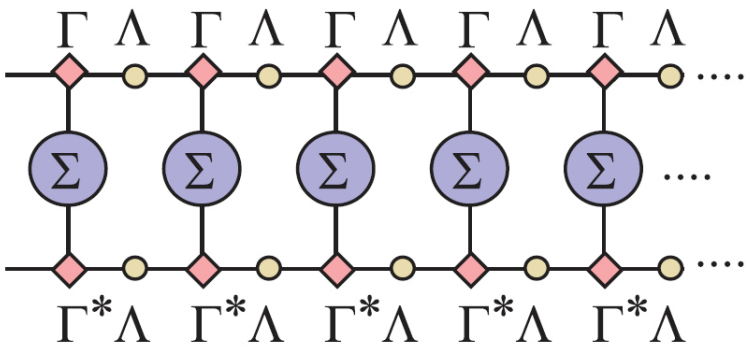


FIGURE 3.6: The norm of the overlap between $|\psi\rangle$ and the corresponding transformed state $|\tilde{\psi}\rangle$ [31].

now easy to show that the corresponding eigenvector is $U_\Sigma^\dagger$:

$$\begin{aligned}\mathcal{E}_\Sigma(U_\Sigma^\dagger) =& \sum_{ij}\Sigma_{ji}\Gamma_i\Lambda U_\Sigma^\dagger\Lambda\Gamma_j^\dagger \\ =& \sum_j\left(\sum_i\Sigma_{ji}\Gamma_i\right)\Lambda U_\Sigma^\dagger\Lambda\Gamma_j^\dagger \\ =& e^{i\theta_\Sigma}\sum_j U_\Sigma^\dagger\Gamma_j U_\Sigma\Lambda U_\Sigma^\dagger\Lambda\Gamma_j^\dagger \\ =& e^{i\theta_\Sigma}\sum_j U_\Sigma^\dagger\Gamma_j\Lambda^2\Gamma_j^\dagger \\ =& e^{i\theta_\Sigma}U_\Sigma^\dagger.\end{aligned} \tag{3.38}$$

where we have used (3.22) and a general property of the Λ's matrices, that is $[\Lambda, U_\Sigma] = 0$ [46]. Notice that if parity or time-reversal symmetries are involved, then the definition of $\mathcal{E}_\Sigma$ has to be slightly changed, according to (3.24) and (3.31):

$$\begin{aligned}\mathcal{E}_P(X) &= \sum_i(\Sigma_P)_{ij}\Gamma_i^T\Lambda X\Lambda\Gamma_j^\dagger \\ \mathcal{E}_T(X) &= \sum_i(\Sigma_T)_{ij}\Gamma_i^*\Lambda X\Lambda\Gamma_j^\dagger.\end{aligned} \tag{3.39}$$

Knowing the U_Σ matrices for each symmetry operation, we can easily read off the factor system ω and thus determine the corresponding phase.

3.3.1 The Generalized Non-Local Order Parameters

In chapter 2 we have introduced two non-local order parameters:

$$\begin{aligned}\mathcal{O}_S^\alpha &= \lim_{|j-k|\to\infty}\left\langle S_j^\alpha\exp\left(i\pi\sum_{l=j+1}^{k-1}S_l^\alpha\right)S_k^\alpha\right\rangle \\ \mathcal{O}_P^\alpha &= \lim_{|j-k|\to\infty}\left\langle\exp\left(i\pi\sum_{l=j+1}^{k-1}S_l^\alpha\right)\right\rangle\end{aligned} \tag{3.40}$$

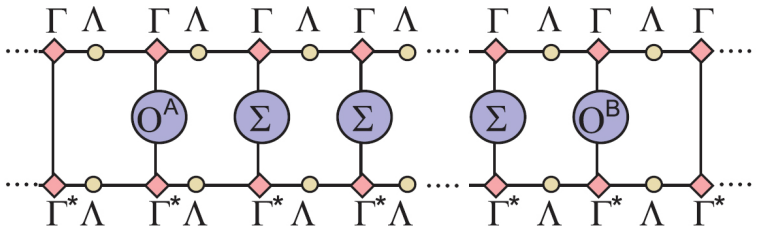


FIGURE 3.7: The generalized non-local order parameter $\mathcal{O}_\Sigma(O^A, O^B)$ [31].

asserting that they are non-zero in the (non-trivial) Haldane phase and in the (trivial) dimerized phase respectively, while they vanish elsewhere. Thus they can be useful to distinguish these two phases, both symmetric under SU(2) symmetry transformations. We can generalize these non-local order parameters for systems with other symmetries. Indeed if Σ is a symmetry transformation then [31](see Fig. 3.7):

$$\mathcal{O}_\Sigma(O^A, O^B) = \lim_{n\to\infty} \langle\psi| O^A(1) \left(\prod_{k=2}^{n-1} \Sigma(k)\right) O^B(n) |\psi\rangle \tag{3.41}$$

where O^A and O^B are two local operators. This expression for generic O^A,O^B is non-vanishing if Σ is a symmetry operation [30], so in general it cannot distinguish among different topological phases with the same symmetry. Nevertheless if those local operators are suitably chosen the non-local order parameter just defined can distinguish some topological states. We now show how to choose appropriately O^A and O^B. To begin with it is easy to check that (3.41) can be expressed as (see Fig. 3.8):

$$\begin{aligned}\mathcal{O}_\Sigma(O^A, O^B) &= \lim_{n\to\infty} \mathrm{Tr}\left[\Lambda^2 \mathcal{E}_{O^A} \mathcal{E}_\Sigma^n \mathcal{E}_{O^B}(\mathbb{I})\right] \\ &= \mathrm{Tr}\left[\Lambda^2 \mathcal{E}_{O^A}(U_\Sigma^\dagger)\right] \cdot \mathrm{Tr}[\Lambda U_\Sigma \Lambda \mathcal{E}_{O^B}(\mathbb{I})] \\ &= \mathrm{Tr}\left[\Lambda^2 U_\Sigma^\dagger \bar{O}^A\right] \cdot \mathrm{Tr}\left[\Lambda^2 U_\Sigma \bar{O}^B\right]\end{aligned} \tag{3.42}$$

where:

$$\begin{aligned}\bar{O}^A &= \sum_{ij} O^A_{ij} \Gamma_i^\dagger \Lambda^2 \Gamma_j; \\ \bar{O}^B &= \sum_{ij} O^B_{ij} \Gamma_j \Lambda^2 \Gamma_i^\dagger.\end{aligned} \tag{3.43}$$

Thus in order to let $\mathcal{O}_\Sigma$ vanish in some phase we need to find in which conditions $\mathrm{Tr}\left[\Lambda^2 U_\Sigma^\dagger \bar{O}^A\right]$ or $\mathrm{Tr}\left[\Lambda^2 U_\Sigma \bar{O}^B\right]$ gives zero. Then suppose we have an additional symmetry Σ' that commutes with the previous one $[\Sigma', \Sigma] = 0$, but when represented projectively by $U_{\Sigma'}$ may give a non-trivial commutation relation with U_Σ :

$$U_{\Sigma'} U_\Sigma = e^{i\phi} U_\Sigma U_{\Sigma'}. \tag{3.44}$$

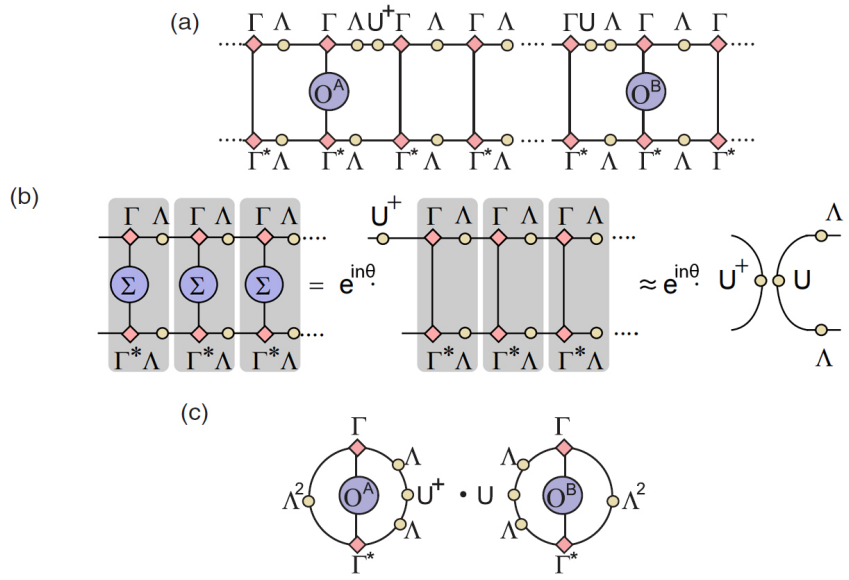


FIGURE 3.8: Evaluation of the string order paramter $\mathcal{O}_\Sigma(O^A, O^B)$. (a) The matrices U_Σ and $U_\Sigma^\dagger$ involved in the transformation of the Γ's all vanish except the ones at the edges. (b,c) If the segment in between the two local operators O^A and O^B is large then $\mathcal{E}_\Sigma^n(X)$ can be approximated by $e^{in\theta_\Sigma} U_\Sigma^\dagger \operatorname{Tr}\left[\Lambda^2 U_\Sigma X\right]$. We are ignoring the overall phase $e^{in\theta_\Sigma}$ [31].

Now we can choose a local operator, say O^A, such that it has a particular quantum number under the new symmetry Σ':

$$\Sigma' O^A \Sigma'^\dagger = e^{i\sigma} O^A. \tag{3.45}$$

It is not difficult to show that $\bar{O}^A$ transforms in the same fashion:

$$U_{\Sigma'} \bar{O}^A U_{\Sigma'}^\dagger = e^{i\sigma} \bar{O}^A. \tag{3.46}$$

Then it follows that:

$$\operatorname{Tr}\left[\Lambda^2 U_\Sigma^\dagger \bar{O}^A\right] = e^{i\sigma} \operatorname{Tr}\left[\Lambda^2 U_\Sigma^\dagger U_{\Sigma'}^\dagger \bar{O}^A U_{\Sigma'}\right] = e^{i(\sigma-\phi)} \operatorname{Tr}\left[\Lambda^2 U_\Sigma^\dagger \bar{O}^A\right]. \tag{3.47}$$

Now if $\sigma \neq \phi$ this equality tells us that the non-local order parameter must vanish. If $\sigma = \phi$ then it will generally be non-zero, but it could still accidentally vanish.

Chapter 4

Analytical evaluation of the non local order parameters

We are ready now to use the methods described in the last chapter to get new non-local order parameters which are able to detect the massive phases of the bilinear-biquadratic class of Hamiltonians (2.1), and evaluate them analytically. We have shown how to evaluate this non local order parameters using the MPS representation of the ground state. Clearly, without numerical methods, it is a difficult task to find the exact ground state of a given Hamiltonian and even more to find its corresponding MPS representation. For these reasons we will consider only two special points as representatives of the Haldane and dimer phase. Indeed we will show in the next sections how to find the exact MPS representation of the AKLT state and of the dimer state. As discussed in § 2.2.2, the latter is not the ground state of any of the Hamiltonians (2.1) but since it belongs anyway to the dimer phase then any non-local order parameter we may find to be non-vanishing when evaluated on the dimer state works well also in detecting that massive phase of the bilinear-biquadratic model.

4.1 Exact MPS representations

4.1.1 MPS representation of the AKLT state

In § 2.2.1 the AKLT state was thought as a symmetrical combination of two spin-1/2's in the same sites and as an antisymmetrical combination of two spin-1/2's on nearest neighbors sites. Here we show how a MPS representation of this state can be found following the same thinking [39].
A generic quantum state on a chain of length L made of $2L$ spin-1/2's can be expressed as:

$$|\psi\rangle = \sum_{\substack{a_1 \dots a_L \\ b_1 \dots b_L}} \psi_{a_1 \dots a_L b_1 \dots b_L} |a_1 \dots a_L\rangle |b_1 \dots b_L\rangle \tag{4.1}$$

where $|a_k\rangle, |b_k\rangle = |\uparrow\rangle, |\downarrow\rangle$ form a pair of spins on the k-th site. In the AKLT state we need to create singlet bonds between spins b_k and a_{k+1} so we apply

a matrix of the form:

$$\Sigma^{b_k a_{k+1}} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \tag{4.2}$$

which antisymmetrize these two spins. The state (4.1) with singlet bonds between each site now reads:

$$\begin{aligned} |\psi\rangle &= \sum_{\substack{a_1 \dots a_L \\ b_1 \dots b_L}} \Sigma^{b_1 a_2} \dots \Sigma^{b_L a_1} |a_1 \dots a_L\rangle |b_1 \dots b_L\rangle \qquad \text{PBC} \\ |\psi\rangle &= \sum_{\substack{a_2 \dots a_L \\ b_1 \dots b_{L-1}}} \Sigma^{b_1 a_2} \dots \Sigma^{b_{L-1} a_L} |a_1 \dots a_L\rangle |b_1 \dots b_L\rangle \qquad \text{OBC} \end{aligned} \tag{4.3}$$

where the four degenerate ground states with open boundary conditions are retrieved fixing a_1 and b_L. We now require that each pair of spins on the same site k represents a spin-1 variable, thus we have to introduce a set of three matrices $M_{i_k}^{a_k b_k}$ which encode the correct symmetrization:

$$M_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad M_0 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \qquad M_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{4.4}$$

and such that $M_{i_k}^{a_k b_k} |i_k\rangle \langle a_k b_k|$ project the local state $|a_k b_k\rangle$ onto $|i_k\rangle = |+\rangle, |0\rangle, |-\rangle$. After such a projection the AKLT state can be finally expressed as:

$$\begin{aligned} |\psi\rangle_{AKLT} &= \sum_{\substack{a_1 \dots a_L \\ b_1 \dots b_L}} \sum_{i_1 \dots i_L} M_{i_1}^{a_1 b_1} \Sigma^{b_1 a_2} \dots M_{i_L}^{a_L b_L} \Sigma^{b_L a_1} |i_1 \dots i_L\rangle \qquad \text{PBC} \\ |\psi\rangle_{AKLT} &= \sum_{\substack{a_2 \dots a_L \\ b_1 \dots b_{L-1}}} \sum_{i_1 \dots i_L} M_{i_1}^{a_1 b_1} \Sigma^{b_1 a_2} \dots \Sigma^{b_{L-1} a_L} M_{i_L}^{a_L b_L} |i_1 \dots i_L\rangle \qquad \text{OBC} \end{aligned} \tag{4.5}$$

or equivalently:

$$\begin{aligned} |\psi\rangle_{AKLT} &= \sum_{i_1 \dots i_L} \mathrm{Tr}\left[M_{i_1} \Sigma \dots M_{i_L} \Sigma\right] |i_1 \dots i_L\rangle \qquad \text{PBC} \\ |\psi\rangle_{AKLT} &= \sum_{i_1 \dots i_L} M_{i_1}^{a_1} \Sigma \dots M_{i_{L-1}} \Sigma M_{i_L}^{b_L} |i_1 \dots i_L\rangle \qquad \text{OBC.} \end{aligned} \tag{4.6}$$

Now the MPS matrices of the corresponding representation are easily found to be given by $A_{i_k} = M_{i_k} \Sigma$:

$$A_+ = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix} \qquad A_0 = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \qquad A_- = \begin{pmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}. \tag{4.7}$$

With open boundary conditions the row index a_1 and the column index b_L are fixed, so the first and the last matrices are respectively row and column vectors. We now want our MPS representation to satisfy the canonical form

(3.12). Since:

$$\sum_i A_i A_i^\dagger = \frac{3}{4}\mathbb{I} \tag{4.8}$$

we are led to re-scale the A_i matrices by a factor of $\frac{2}{\sqrt{3}}$:

$$A_+ = \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{pmatrix} \qquad A_0 = \begin{pmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \qquad A_- = \begin{pmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0. \end{pmatrix} \tag{4.9}$$

Furthermore (3.36) is satisfied defining the Λ matrix as:

$$\Lambda = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}\mathbb{I} \tag{4.10}$$

thus the corresponding Γ_i matrices in (3.34) are:

$$\Gamma_+ = \begin{pmatrix} 0 & \frac{2}{\sqrt{3}} \\ 0 & 0 \end{pmatrix} \qquad \Gamma_0 = \begin{pmatrix} -\sqrt{\frac{2}{3}} & 0 \\ 0 & \sqrt{\frac{2}{3}} \end{pmatrix} \qquad \Gamma_- = \begin{pmatrix} 0 & 0 \\ -\frac{2}{\sqrt{3}} & 0 \end{pmatrix} \tag{4.11}$$

In the next sections we will use a different basis for the local Hilbert space on each site, that is a basis whose elements are:

$$|x\rangle = -\frac{1}{\sqrt{2}}(|+\rangle - |-\rangle) \qquad |y\rangle = \frac{i}{\sqrt{2}}(|+\rangle + |-\rangle) \qquad |z\rangle = |0\rangle\,. \tag{4.12}$$

In this basis the spin matrices become:

$$S^x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad S^y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \qquad S^z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4.13}$$

and correspondingly the Γ_i matrices are:

$$\Gamma_x = -\sqrt{\frac{2}{3}}\sigma_x \qquad \Gamma_y = -\sqrt{\frac{2}{3}}\sigma_y \qquad \Gamma_z = -\sqrt{\frac{2}{3}}\sigma_z. \tag{4.14}$$

4.1.2 MPS representation of the dimer state

In the basis just introduced the dimer state (2.39) can be expressed as:

$$|d\rangle_- = \bigotimes_i \frac{1}{\sqrt{3}}\left(|x\rangle_{2i-1} \otimes |x\rangle_{2i} + |y\rangle_{2i-1} \otimes |y\rangle_{2i} + |z\rangle_{2i-1} \otimes |z\rangle_{2i}\right) \tag{4.15}$$

Clearly this state is no longer invariant under translations of one site and correspondingly we do not expect to find a site-independent MPS representation. On the other hand it is still invariant under translations of *two* sites and thus we should find two sets of matrices A_i, $\tilde{A}_i$ defined in odd and even

sites respectively. Given that the dimer state is the product state of singlets (dimers), and that the MPS representation of a product state is made up of 1×1 matrices, i.e. scalars, we expect the matrices A_i, $\tilde{A}_i$ to actually be χ-dimensional row and column vectors, so to give a scalar upon contraction. It can be easily verified that a possible choice is:

$$A_x = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \qquad A_y = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \qquad A_z = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \tag{4.16}$$

$$\tilde{A}_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \tilde{A}_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \tilde{A}_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{4.17}$$

We can find a 3×3 matrix Λ and a 1×1 matrix $\tilde{\Lambda}$:

$$\Lambda = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \tilde{\Lambda} = 1. \tag{4.18}$$

such that the conditions (3.36) are satisfied. The Γ_i, $\tilde{\Gamma}_i$ matrices are then:

$$\Gamma_x = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \qquad \Gamma_y = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \qquad \Gamma_z = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \tag{4.19}$$

$$\tilde{\Gamma}_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \tilde{\Gamma}_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \tilde{\Gamma}_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{4.20}$$

4.2 Characterization of the phases

The two massive phases of the bilinear-biquadratic model are symmetry protected topological phases, indeed as it turns out [33] the Haldane phase is protected by either $Z_2 \times Z_2$ symmetry, parity symmetry or time reversal symmetry meaning that we can add small symmetry breaking terms in the Hamiltonian without causing phase transitions, provided that at least one of the mentioned protecting symmetries is preserved. For instance we expect that a small parity-breaking parameter as δ in (2.40) does not wipe out the Haldane phase as it is indeed shown in Fig.2.5.
On the other hand, in the dimer phase the parity symmetry is spontaneously broken but as just explained this is not at the root of the phase transition. Moreover it is a topological trivial phase given that the dimer state is a product state. Therefore we expect these phases to be characterized by non-equivalent projective representations of the symmetries. With the exact MPS representations of the AKLT and dimer states in our hands it is easy to find the various matrices that represent projectively the symmetries and thus their classes of equivalence.
To begin with let us consider the AKLT state and the symmetry operation

given by a π-rotation about the α-axis ($\alpha = x, y, z$). In order to find the corresponding projective representation we have to find the eigenvector of (3.11) relative to the unimodular eigenvalue, and it easy to verify that the matrix we are looking for is σ_α. Indeed fixing for instance $\alpha = z$:

$$\begin{aligned}\mathcal{E}_z(\sigma_z) &= \sum_{ij} \left(e^{i\pi S^z}\right)_{ji} \Gamma_i \Lambda \sigma_z \Lambda \Gamma_j^\dagger \\ &= \frac{1}{2}\left(-\Gamma_x \sigma_z \Gamma_x^\dagger - \Gamma_y \sigma_z \Gamma_y^\dagger + \Gamma_z \sigma_z \Gamma_z^\dagger\right) \\ &= \frac{1}{3}\left(-\sigma_x \sigma_z \sigma_x - \sigma_y \sigma_z \sigma_y + \sigma_z \sigma_z \sigma_z\right) \\ &= \frac{1}{3}\left(\sigma_z + \sigma_z + \sigma_z\right) \\ &= \sigma_z\end{aligned} \tag{4.21}$$

where we can also read off the phase $e^{i\theta} = 1$ which together with the system factor ω labels the different SPT phases. It is clear that this is a non-trivial projective representation of the commutative $Z_2 \times Z_2$ group given that the σ matrices anti-commute:

$$\sigma_\alpha \sigma_\beta = 2\delta_{\alpha\beta} - \sigma_\beta \sigma_\alpha. \tag{4.22}$$

If we define $e^{i\phi}$ as in (3.44) where $\Sigma = \sigma_\alpha$, $\Sigma' = \sigma_\beta$ ($\alpha \neq \beta$) then the AKLT state is characterized by $\theta = 0$ and $\phi = \pi$, and as they cannot change without facing a phase transition, they characterize also the whole Haldane phase.
In order to find the projective representations of the same symmetry group acting on the dimer state we have to take into account that we do not have a site-independent MPS and thus we will find two different, but equivalent, representations acting on the left and on the right bond indexes of the MPS matrices:

$$\begin{aligned}\sum_j \Sigma_{ij} \Gamma_j &= e^{i\theta_\Sigma} \tilde{R}_\Sigma^\dagger \Gamma_i R_\Sigma \\ \sum_j \Sigma_{ij} \tilde{\Gamma}_j &= e^{i\theta_\Sigma} R_\Sigma^\dagger \tilde{\Gamma}_i \tilde{R}_\Sigma\end{aligned} \tag{4.23}$$

where now R_Σ is a 3×3 matrix and $\tilde{R}_\Sigma$ is a 1×1 matrix. Again we can easily verify that each element of $Z_2 \times Z_2$ possesses the following matrices as projective representations:

$$\begin{aligned} R_x &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \tilde{R}_x = 1 \\ R_y &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \tilde{R}_y = 1 \\ R_z &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \tilde{R}_z = 1. \end{aligned} \tag{4.24}$$

Notice that $R_\alpha = e^{i\pi S^\alpha}$, thus this is a trivial projective representation with $\theta = 0, \phi = 0$ which characterize the dimer state and the whole dimer phase. From the comparison of θ and ϕ we can conclude that the Haldane and dimer phases are indeed distinct massive phases.
Another symmetry we can consider is the time reversal Σ_T which transforms the components of the spin as:

$$S^\alpha \to -S^\alpha \qquad\qquad \alpha = x, y, z \tag{4.25}$$

and thus acts on the physical index of the MPS through $\Sigma_T = e^{i\pi S^y}$:

$$\Gamma_i \to \left(e^{i\pi S^y}\right)_{ij} \Gamma_j. \tag{4.26}$$

We already know that this transformation corresponds to a non-trivial projective representation when acting on the AKLT state, while it is trivially represented in the dimer state, thus also ϕ_T introduced in (3.33) can correctly used to distinguish the non-trivial Haldane phase ($\phi_T = \pi$) from the trivial dimer phase ($\phi_T = 0$).

4.3 Definition and evaluation of new non-local order parameters

In section § 3.3.1 we illustrated how to find generalized non-local order parameters which can detect different symmetric phases. Following those guidelines we want now to define and analytically evaluate new non-local order parameters in both the massive phases of the bilinear-biquadratic model, clearly using the exact MPS representations of the AKLT state and of the dimer state just found.
As previously shown, a generic non-local order parameter should have the form:

$$\mathcal{O}_\Sigma(O^A, O^B) = \lim_{n\to\infty} \langle\psi| O^A(1) \left(\prod_{k=2}^{n-1} \Sigma(k)\right) O^B(n) |\psi\rangle \tag{4.27}$$

where Σ is a symmetry transformation and O^A, O^B are local operators. We also recall that in order to predict in which phase this order parameter should vanish we need another[1] symmetry Σ' which commutes with Σ. Then for our purposes we can use the symmetry transformations of the abelian $Z_2 \times Z_2$ group, fixing from now on $\Sigma = e^{i\pi S^z}$ and $\Sigma' = e^{i\pi S^\alpha}$, with $\alpha = x, y$. The local operators O^A and O^B are 3×3 matrices, thus we choose the following basis for this 9-dimensional vector space:

$$\begin{array}{lll} S^x & S^y & S^z \\ S^y S^z & S^x S^z & S^x S^y \\ (S^x)^2 & (S^y)^2 & (S^z)^2 \end{array} \tag{4.28}$$

[1] different from the identity $\mathbb{I}$.

such that any other local operator we may choose in (4.27) can be expressed as linear combination of the previous. Each of these operators transform under a π-rotation about the x-axis as follows:

$$\begin{array}{lll} S^x \to S^x & S^y \to -S^y & S^z \to -S^z \\ S^y S^z \to S^y S^z & S^x S^z \to -S^x S^z & S^x S^y \to -S^x S^y \\ (S^x)^2 \to (S^x)^2 & (S^y)^2 \to (S^y)^2 & (S^z)^2 \to (S^z)^2 \end{array} \tag{4.29}$$

and under the same rotation about the y-axis as follows:

$$\begin{array}{lll} S^x \to -S^x & S^y \to S^y & S^z \to -S^z \\ S^y S^z \to -S^y S^z & S^x S^z \to S^x S^z & S^x S^y \to -S^x S^y \\ (S^x)^2 \to (S^x)^2 & (S^y)^2 \to (S^y)^2 & (S^z)^2 \to (S^z)^2. \end{array} \tag{4.30}$$

We see that we can separate those nine operators into three classes:

1. Operators which are odd under Σ' for both $\alpha = x, y$, like S^z and $S^x S^y$;
2. Operators which are even under Σ' for both $\alpha = x, y$, like $(S^x)^2$, $(S^y)^2$ and $(S^z)^2$;
3. Operators which may be even or odd under Σ', depending on the axis of rotation chosen, like the $S^y S^z$, $S^x S^z$, S^x and S^y.

According to (3.45) the first two classes correspond to $\sigma = \pi$ and $\sigma = 0$ respectively, thus we expect to be able to define new non-local order parameters certainly vanishing in:

- the Haldane phase ($\phi = \pi$) if O^A or O^B are chosen within the second class ($\sigma = 0$);
- the dimer phase ($\phi = 0$) if O^A or O^B are chosen within the first class ($\sigma = \pi$);
- both Haldane phase and dimer phase if O^A or O^B are chosen within the third class.

Obviously a non-local order parameter which is zero everywhere would not be of much use, thus we have to explicitly verify that if they are vanishing in a phase they do not vanish in the other as well. Indeed as we pointed out in 3.3.1, they may still be vanishing even if $\phi = \sigma$.
In the following we will always assume that $O^A = O^B$ for convenience, but the case $O^A \neq O^B$ will be easily deducible from our calculations, as (3.42) can be seen to factorize into two terms, each depending only on O^A or O^B.
In Fig.4.1 it is shown the numerical evaluation of some of these non-local order parameters as we vary the angle θ in the bilinear-biquadratic Hamiltonian. For the calculations we have used the DMRG code (see appendix E for a review of the DMRG algorithm) of the C++ library ITensor [19] on a chain of 64 sites, fixing the higher bond dimension of the MPS to $\chi = 500$. As it can be seen, the two massive phases of the model are clearly visible, but the precision of the simulation decreases really rapidly as we get closer to the critical point at $\theta = \frac{\pi}{4}$, thus it is hard to locate precisely the transition.

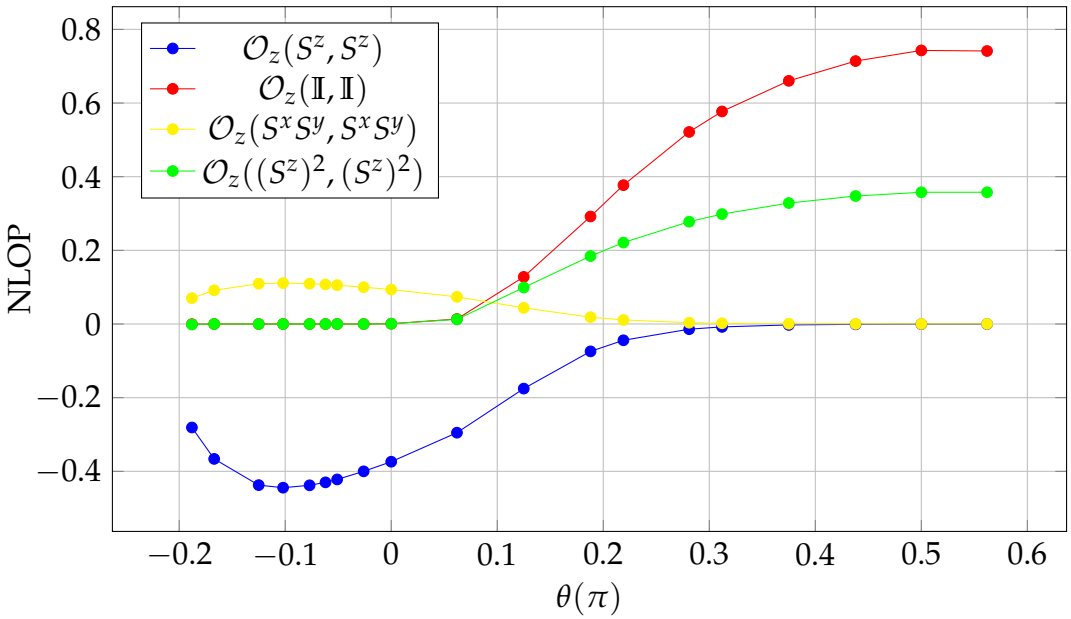


FIGURE 4.1: Numerical evaluation of the non-local order parameters defined in this chapter. It is clear that they can indeed detect the two massive phases of the bilinear-biquadratic model. The transition point is hard to locate as the precision of the simulation is quite low near critical points.

4.3.1 Evaluation in the AKLT point

In (3.3.1) we have shown that the evaluation of the non-local order parameters can be reduced to the evaluation of the following traces:

$$\mathcal{O}_\Sigma(O^A, O^B) = \mathrm{Tr}\left[\Lambda^2 U_\Sigma^\dagger \bar{O}^A\right] \cdot \mathrm{Tr}\left[\Lambda^2 U_\Sigma \bar{O}^B\right]. \tag{4.31}$$

where

$$\begin{aligned} \bar{O}^A &= \sum_{ij} O^A_{ij} \Gamma_i^\dagger \Lambda^2 \Gamma_j; \\ \bar{O}^B &= \sum_{ij} O^B_{ij} \Gamma_j \Lambda^2 \Gamma_i^\dagger. \end{aligned} \tag{4.32}$$

We recall that for the AKLT point we use:

$$\begin{aligned} &\Sigma = e^{i\pi S^z} && U_\Sigma = U_z = \sigma_z && \Lambda = \frac{1}{\sqrt{2}}\mathbb{I} \\ &\Gamma_x = -\sqrt{\frac{2}{3}}\sigma_x && \Gamma_y = -\sqrt{\frac{2}{3}}\sigma_y && \Gamma_z = -\sqrt{\frac{2}{3}}\sigma_z \end{aligned} \tag{4.33}$$

We first verify that choosing O^A and O^B within the second class ($\sigma = 0$) we indeed get vanishing non-local order parameters. So let for instance $O^A = O^B = (S^z)^2$:

$$\mathcal{O}_z((S^z)^2, (S^z)^2) = \mathrm{Tr}\left[\Lambda^2 U_z^\dagger (S^{\bar{z}})^2{}_A\right] \cdot \mathrm{Tr}\left[\Lambda^2 U_z (S^{\bar{z}})^2{}_B\right] \tag{4.34}$$

where

$$\begin{aligned}(\bar{S^z})^2{}_A &= \sum_{ij}((S^z)^2)_{ij}\Gamma_i^\dagger\Lambda^2\Gamma_j \\ &= \frac{1}{2}\left(\Gamma_x^\dagger\Gamma_x + \Gamma_y^\dagger\Gamma_y\right) \\ &= \frac{1}{3}\left(\sigma_x\sigma_x + \sigma_y\sigma_y\right) \\ &= \frac{2}{3}\mathbb{I}\end{aligned} \tag{4.35}$$

$$\begin{aligned}(\bar{S^z})^2{}_B &= \sum_{ij}((S^z)^2)_{ij}\Gamma_j\Lambda^2\Gamma_i^\dagger \\ &= \frac{1}{2}\left(\Gamma_x\Gamma_x^\dagger + \Gamma_y\Gamma_y^\dagger\right) \\ &= \frac{1}{3}\left(\sigma_x\sigma_x + \sigma_y\sigma_y\right) \\ &= \frac{2}{3}\mathbb{I}\end{aligned} \tag{4.36}$$

thus we find:

$$\mathcal{O}_z((S^z)^2,(S^z)^2) = \frac{1}{2}\,\mathrm{Tr}\left[\sigma_z\left(\frac{2}{3}\mathbb{I}\right)\right]\frac{1}{2}\,\mathrm{Tr}\left[\sigma_z\left(\frac{2}{3}\mathbb{I}\right)\right] = 0 \tag{4.37}$$

as expected. In the same fashion we can show that choosing $(S^x)^2$ or $(S^y)^2$ gives the same vanishing result.
Equivalently if O^A or O^B are taken within the third class we expect to get a vanishing non-local order parameter. Indeed if $O^A = O^B = S^x$, then:

$$\mathcal{O}_z(S^x,S^x) = \mathrm{Tr}\left[\Lambda^2 U_z^\dagger \bar{S}_A^x\right]\cdot\mathrm{Tr}\left[\Lambda^2 U_z \bar{S}_B^x\right] \tag{4.38}$$

where

$$\begin{aligned}\bar{S}_A^x &= \sum_{ij}(S^x)_{ij}\Gamma_i^\dagger\Lambda^2\Gamma_j \\ &= \frac{1}{2}\left(-i\Gamma_y^\dagger\Gamma_z + i\Gamma_z^\dagger\Gamma_y\right) \\ &= \frac{1}{3}\left(-i\sigma_y\sigma_z + i\sigma_z\sigma_y\right) \\ &= \frac{2}{3}\sigma_x\end{aligned} \tag{4.39}$$

$$\begin{aligned}\bar{S}_B^x &= \sum_{ij}(S^x)_{ij}\Gamma_j\Lambda^2\Gamma_i^\dagger \\ &= \frac{1}{2}\left(-i\Gamma_z\Gamma_y^\dagger + i\Gamma_y\Gamma_z^\dagger\right) \\ &= \frac{1}{3}\left(-i\sigma_z\sigma_y + i\sigma_y\sigma_z\right) \\ &= -\frac{2}{3}\sigma_x\end{aligned} \tag{4.40}$$

thus we get:

$$\mathcal{O}_z(S^x, S^x) = \frac{1}{2}\,\mathrm{Tr}\left[\sigma_z\left(\frac{2}{3}\sigma_x\right)\right]\cdot\frac{1}{2}\,\mathrm{Tr}\left[\sigma_z\left(-\frac{2}{3}\sigma_x\right)\right] = 0. \tag{4.41}$$

Choosing $O^A = O^B = S^y$ would similarly give a term proportional to $\mathrm{Tr}\left[\sigma_z\sigma_y\right]$ which is still zero. On the other hand if we use $O^A = O^B = S^yS^z$ we get:

$$\mathcal{O}_z(S^yS^z, S^yS^z) = \mathrm{Tr}\left[\Lambda^2 U_z^\dagger \overline{S^yS^z}_A\right]\cdot\mathrm{Tr}\left[\Lambda^2 U_z \overline{S^yS^z}_B\right] \tag{4.42}$$

where

$$\begin{aligned}\overline{S^yS^z}_A &= \sum_{ij}(S^yS^z)_{ij}\Gamma_i^\dagger\Lambda^2\Gamma_j\\ &= -\frac{1}{2}\left(\Gamma_z^\dagger\Gamma_y\right)\\ &= -\frac{1}{3}\left(\sigma_z\sigma_y\right)\\ &= \frac{i}{3}\sigma_x\end{aligned} \tag{4.43}$$

$$\begin{aligned}\overline{S^yS^z}_B &= \sum_{ij}(S^yS^z)_{ij}\Gamma_j\Lambda^2\Gamma_i^\dagger\\ &= -\frac{1}{2}\left(\Gamma_y\Gamma_z^\dagger\right)\\ &= -\frac{1}{3}\left(\sigma_y\sigma_z\right)\\ &= -\frac{i}{3}\sigma_x\end{aligned} \tag{4.44}$$

thus we find:

$$\mathcal{O}_z(S^yS^z, S^yS^z) = \frac{1}{2}\,\mathrm{Tr}\left[\sigma_z\left(\frac{i}{3}\sigma_x\right)\right]\cdot\frac{1}{2}\,\mathrm{Tr}\left[\sigma_z\left(-\frac{i}{3}\sigma_x\right)\right] = 0. \tag{4.45}$$

Again if $O^A = O^B = S^xS^z$ we still get zero from a term proportional to $\mathrm{Tr}\left[\sigma_z\sigma_y\right]$.

Let us now verify that there are non-vanishing non-local order parameters in the Haldane phase constructed from operators within the first class. Notice that if we use $O^A = O^B = S^z$ we get back the string order parameter (2.44), which was found to be equal to $-\frac{4}{9}$. We can here double check this result exploiting our MPS representation of the AKLT state:

$$\mathcal{O}_z(S^z, S^z) = \mathrm{Tr}\left[\Lambda^2 U_z^\dagger \bar{S}_A^z\right]\cdot\mathrm{Tr}\left[\Lambda^2 U_z \bar{S}_B^z\right] \tag{4.46}$$

where

$$\begin{aligned}\bar{S}^z_A &= \sum_{ij} (S^z)_{ij} \Gamma_i^\dagger \Lambda^2 \Gamma_j \\ &= \frac{1}{2}\left(-i\Gamma_x^\dagger \Gamma_y + i\Gamma_y^\dagger \Gamma_x\right) \\ &= \frac{1}{3}\left(-i\sigma_x\sigma_y + i\sigma_y\sigma_x\right) \\ &= \frac{2}{3}\sigma_z\end{aligned} \tag{4.47}$$

$$\begin{aligned}\bar{S}^z_B &= \sum_{ij} (S^z)_{ij} \Gamma_j \Lambda^2 \Gamma_i^\dagger \\ &= \frac{1}{2}\left(-i\Gamma_y \Gamma_x^\dagger + i\Gamma_x \Gamma_x^\dagger\right) \\ &= \frac{1}{3}\left(-i\sigma_y\sigma_x + i\sigma_x\sigma_y\right) \\ &= -\frac{2}{3}\sigma_z\end{aligned} \tag{4.48}$$

thus we get:

$$\mathcal{O}_z(S^z, S^z) = \frac{1}{2}\operatorname{Tr}\left[\sigma_z\left(\frac{2}{3}\sigma_z\right)\right] \cdot \frac{1}{2}\operatorname{Tr}\left[\sigma_z\left(-\frac{2}{3}\sigma_z\right)\right] = -\frac{4}{9}. \tag{4.49}$$

A new non-local order parameter can be defined using instead $O^A = O^B = S^x S^y$:

$$\mathcal{O}_z(S^x S^y, S^x S^y) = \operatorname{Tr}\left[\Lambda^2 U_z^\dagger \overline{S^x S^y}_A\right] \cdot \operatorname{Tr}\left[\Lambda^2 U_z \overline{S^x S^y}_B\right] \tag{4.50}$$

where

$$\begin{aligned}\overline{S^x S^y}_A &= \sum_{ij} (S^x S^y)_{ij} \Gamma_i^\dagger \Lambda^2 \Gamma_j \\ &= -\frac{1}{2}\left(\Gamma_y^\dagger \Gamma_x\right) \\ &= -\frac{1}{3}\left(\sigma_y\sigma_x\right) \\ &= \frac{i}{3}\sigma_z\end{aligned} \tag{4.51}$$

$$\begin{aligned}\overline{S^x S^y}_B &= \sum_{ij} (S^x S^y)_{ij} \Gamma_j \Lambda^2 \Gamma_i^\dagger \\ &= -\frac{1}{2}\left(\Gamma_x \Gamma_y^\dagger\right) \\ &= -\frac{1}{3}\left(\sigma_x\sigma_y\right) \\ &= -\frac{i}{3}\sigma_z\end{aligned} \tag{4.52}$$

and eventually we get:

$$\mathcal{O}_z(S^x S^y, S^x S^y) = \frac{1}{2}\operatorname{Tr}\left[\sigma_z\left(\frac{i}{3}\sigma_z\right)\right] \cdot \frac{1}{2}\operatorname{Tr}\left[\sigma_z\left(-\frac{i}{3}\sigma_z\right)\right] = \frac{1}{9}. \tag{4.53}$$

This non-vanishing order parameter can therefore be used to distinguish the Haldane phase from the trivial phase where it vanishes instead, as we will verify in the next section.
As mentioned before we can construct other local operators starting from the basis (4.28), and define other non-local order parameters correspondingly. For instance we can express $S^y S^x$ as $S^y S^x = [S^y, S^x] - S^x S^y = -iS^z - S^x S^y$ and find:

$$\begin{aligned}\mathcal{O}_z(S^y S^x, S^y S^x) = &-\mathcal{O}_z(S^z, S^z) + \mathcal{O}_z(S^x S^y, S^x S^y) \\ &-i\mathcal{O}_z(S^z, S^x S^y) - i\mathcal{O}_z(S^x S^y, S^z) \\ = &\frac{1}{9}\end{aligned} \tag{4.54}$$

where each term in the right hand side of the last equation is known from previous calculations. Similarly we could use $\{S^x, S^y\} = S^x S^y + S^y S^x$, but it turns out to be zero even though it belongs to the first class of operators, as it is clearly odd under π-rotation about both x and y axes.

4.3.2 Evaluation in the dimer state

We are now taking into account the dimer state, and an important observation is in order. Contrary to the AKLT state, the dimer state is not translational invariant and has not a site independent MPS representation as showed before. Thus in evaluating the different non-local order parameters we have to specify *where* we place the local operators O^A and O^B. More precisely we have four possibilities:

1. O^A on an even site and O^B on an odd site;
2. O^A on an odd site and O^B on an even site;
3. O^A and O^B on even sites;
4. O^A and O^B on odd sites.

Consequently we have four different expressions for the non-local order parameters:

1. EVEN-ODD

$$\mathcal{O}_\Sigma(O^A, O^B) = \mathrm{Tr}\left[\tilde{\Lambda}^2 \tilde{R}_\Sigma^\dagger \bar{O}^A\right] \mathrm{Tr}\left[\tilde{\Lambda}^2 \tilde{R}_\Sigma \bar{O}^B\right] \tag{4.55}$$

where

$$\begin{aligned}\bar{O}^A &= \sum_{ij} (O^A)_{ij} \tilde{\Gamma}_i^\dagger \Lambda^2 \tilde{\Gamma}_j \\ \bar{O}^B &= \sum_{ij} (O^B)_{ij} \Gamma_j \Lambda^2 \Gamma_i^\dagger.\end{aligned} \tag{4.56}$$

2. ODD-EVEN

$$\mathcal{O}_\Sigma(O^A, O^B) = \mathrm{Tr}\left[\Lambda^2 R_\Sigma^\dagger \bar{O}^A\right] \mathrm{Tr}\left[\Lambda^2 R_\Sigma \bar{O}^B\right] \tag{4.57}$$

where

$$\begin{aligned}\bar{O}^A &= \sum_{ij} (O^A)_{ij} \Gamma_i^\dagger \tilde{\Lambda}^2 \Gamma_j \\ \bar{O}^B &= \sum_{ij} (O^B)_{ij} \tilde{\Gamma}_j \tilde{\Lambda}^2 \tilde{\Gamma}_i^\dagger .\end{aligned} \tag{4.58}$$

3. EVEN-EVEN

$$\mathcal{O}_\Sigma(O^A, O^B) = \mathrm{Tr}\left[\tilde{\Lambda}^2 \tilde{R}_\Sigma^\dagger \bar{O}^A\right] \mathrm{Tr}\left[\Lambda^2 R_\Sigma \bar{O}^B\right] \tag{4.59}$$

where

$$\begin{aligned}\bar{O}^A &= \sum_{ij} (O^A)_{ij} \tilde{\Gamma}_i^\dagger \Lambda^2 \tilde{\Gamma}_j \\ \bar{O}^B &= \sum_{ij} (O^B)_{ij} \tilde{\Gamma}_j \tilde{\Lambda}^2 \tilde{\Gamma}_i^\dagger .\end{aligned} \tag{4.60}$$

4. ODD-ODD

$$\mathcal{O}_\Sigma(O^A, O^B) = \mathrm{Tr}\left[\Lambda^2 R_\Sigma^\dagger \bar{O}^A\right] \mathrm{Tr}\left[\tilde{\Lambda}^2 \tilde{R}_\Sigma \bar{O}^B\right] \tag{4.61}$$

where

$$\begin{aligned}\bar{O}^A &= \sum_{ij} (O^A)_{ij} \Gamma_i^\dagger \tilde{\Lambda}^2 \Gamma_j \\ \bar{O}^B &= \sum_{ij} (O^B)_{ij} \Gamma_j \Lambda^2 \Gamma_i^\dagger .\end{aligned} \tag{4.62}$$

Once again, it is not necessary to evaluate each case, but it suffices to consider only the first two, given that the last two can be deduced immediately from the traces already calculated. Thus we start with the case where we place O^A and O^B, again taken equal, on an even site and on an odd site respectively. The matrices used for the dimer case are:

$$\begin{aligned}&R_\Sigma = R_z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \Lambda = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &\tilde{R}_\Sigma = \tilde{R}_z = 1 \qquad \tilde{\Lambda} = 1 \\ &\Gamma_x = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \qquad \Gamma_y = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \qquad \Gamma_z = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \\ &\tilde{\Gamma}_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \tilde{\Gamma}_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \tilde{\Gamma}_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.\end{aligned} \tag{4.63}$$

As before, we first verify that the non-local order parameters containing operators of the first class ($\sigma = \pi$) vanish in the dimer phase ($\phi = 0$). Indeed taking $O^A = O^B = S^z$ gives:

$$\mathcal{O}_z(S^z, S^z) = \mathrm{Tr}\left[\tilde{\Lambda}^2 \tilde{R}_z^\dagger \bar{S}_A^z\right] \mathrm{Tr}\left[\tilde{\Lambda}^2 \tilde{R}_z \bar{S}_B^z\right] \tag{4.64}$$

where

$$\begin{aligned}\bar{S}^z_A &= \sum_{ij} (S^z)_{ij} \tilde{\Gamma}^\dagger_i \Lambda^2 \tilde{\Gamma}_j \\ &= \frac{1}{3}\left(-i\tilde{\Gamma}^\dagger_x \tilde{\Gamma}_y + i\tilde{\Gamma}^\dagger_y \tilde{\Gamma}_x\right) \\ &= \frac{1}{3}(0+0) \\ &= 0\end{aligned} \tag{4.65}$$

$$\begin{aligned}\bar{S}^z_B =& \sum_{ij} (S^z)_{ij} \Gamma_j \Lambda^2 \Gamma^\dagger_i \\ =& \frac{1}{3}(-i\Gamma_y \Gamma^\dagger_x + i\Gamma_x \Gamma^\dagger_y) \\ =& \frac{1}{3}(0+0) \\ =& 0\end{aligned} \tag{4.66}$$

thus we find:

$$\mathcal{O}_z(S^z, S^z) = \mathrm{Tr}[1 \cdot 0]\,\mathrm{Tr}[1 \cdot 0] = 0. \tag{4.67}$$

Taking $O^A = O^B = S^x S^y$ gives instead:

$$\mathcal{O}_z(S^x S^y, S^x S^y) = \mathrm{Tr}\left[\tilde{\Lambda}^2 \tilde{R}^\dagger_z \overline{S^x S^y}_A\right] \mathrm{Tr}\left[\tilde{\Lambda}^2 \tilde{R}_z \overline{S^x S^y}_B\right] \tag{4.68}$$

where

$$\begin{aligned}\overline{S^x S^y}_A &= \sum_{ij} (S^x S^y)_{ij} \tilde{\Gamma}^\dagger_i \Lambda^2 \tilde{\Gamma}_j \\ &= -\frac{1}{3}\left(\tilde{\Gamma}^\dagger_x \tilde{\Gamma}_y\right) \\ &= -\frac{1}{3}(0) \\ &= 0\end{aligned} \tag{4.69}$$

$$\begin{aligned}\overline{S^x S^y}_B &= \sum_{ij} (S^x S^y)_{ij} \Gamma_j \Lambda^2 \Gamma^\dagger_i \\ &= -\frac{1}{3}(\Gamma_x \Gamma^\dagger_y) \\ &= -\frac{1}{3}(0) \\ &= 0\end{aligned} \tag{4.70}$$

thus we get:

$$\mathcal{O}_z(S^x S^y, S^x S^y) = \mathrm{Tr}[1 \cdot 0]\,\mathrm{Tr}[1 \cdot 0] = 0. \tag{4.71}$$

It is clear from these two examples that every operator which is not diagonal in our base, like any operator of the first and third class, would give a vanishing non-local order parameter.
The operators in the second class ($\sigma = 0$) are diagonal instead, thus they may

give a non-zero value in the dimer phase. Indeed for $O^A = O^B = (S^z)^2$:

$$\mathcal{O}_z((S^z)^2,(S^z)^2) = \mathrm{Tr}\Big[\tilde{\Lambda}^2\tilde{R}_z^\dagger\overline{(S^z)^2}_A\Big]\,\mathrm{Tr}\Big[\tilde{\Lambda}^2\tilde{R}_z\overline{(S^z)^2}_B\Big] \tag{4.72}$$

where

$$\begin{aligned}\overline{(S^z)^2}_A &= \sum_{ij}((S^z)^2)_{ij}\tilde{\Gamma}_i^\dagger\Lambda^2\tilde{\Gamma}_j\\ &= \frac{1}{3}\left(\tilde{\Gamma}_x^\dagger\tilde{\Gamma}_x+\tilde{\Gamma}_y^\dagger\tilde{\Gamma}_y\right)\\ &= \frac{1}{3}(1+1)\\ &= \frac{2}{3}\end{aligned} \tag{4.73}$$

$$\begin{aligned}\overline{(S^z)^2}_B =& \sum_{ij}((S^z)^2)_{ij}\Gamma_j\Lambda^2\Gamma_i^\dagger\\ =&\frac{1}{3}(\Gamma_x\Gamma_x^\dagger+\Gamma_y\Gamma_y^\dagger)\\ =&\frac{1}{3}(1+1)\\ =&\frac{2}{3}\end{aligned} \tag{4.74}$$

thus we find:

$$\mathcal{O}_z((S^z)^2,(S^z)^2) = \mathrm{Tr}\left[1\cdot\frac{2}{3}\right]\mathrm{Tr}\left[1\cdot\frac{2}{3}\right] = \frac{4}{9}. \tag{4.75}$$

It is easy to see that the other operators, $(S^x)^2$ and $(S^y)^2$, give exactly the same value. From this results we can evaluate the parity order parameter (2.60), given that $\mathbb{I} = \frac{1}{2}\left((S^x)^2+(S^y)^2+(S^z)^2\right)$:

$$\mathcal{O}_z(\mathbb{I},\mathbb{I}) = \frac{1}{4}\sum_{\alpha\beta}\mathcal{O}_z((S^\alpha)^2),(S^\beta)^2) = \frac{1}{4}\left(9\cdot\frac{4}{9}\right) = 1 \tag{4.76}$$

which as expected does not vanish in a trivial phase.
In conclusion we can try to place all the above operators in odd-even sites and see how the values of the corresponding non-local order parameters change. In order to avoid tedious calculations we will not here explicitly check that we have vanishing values when we already expect so, thus we will focus only on $(S^x)^2$, $(S^y)^2$ and $(S^z)^2$. Then if $O^A = O^B = (S^z)^2$, we have:

$$\mathcal{O}_z((S^z)^2,(S^z)^2) = \mathrm{Tr}\Big[\Lambda^2R_z^\dagger(S^{\bar{z}})^2{}_A\Big]\,\mathrm{Tr}\Big[\Lambda^2R_z(S^{\bar{z}})^2{}_B\Big] \tag{4.77}$$

where

$$
\begin{aligned}
(S^{\bar{z}})^2{}_A &= \sum_{ij}((S^z)^2)_{ij}\Gamma_i^\dagger\tilde{\Lambda}^2\Gamma_j \\
&= \left(\Gamma_x^\dagger\Gamma_x + \Gamma_y^\dagger\Gamma_y\right) \\
&= \left[\begin{pmatrix}1\\0\\0\end{pmatrix}\otimes\begin{pmatrix}1&0&0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\otimes\begin{pmatrix}0&1&0\end{pmatrix}\right] \\
&= \left[\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix} + \begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix}\right] \\
&= \begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix} = (S^z)^2
\end{aligned}
\tag{4.78}
$$

$$
\begin{aligned}
(S^{\bar{z}})^2{}_B &= \sum_{ij}((S^z)^2)_{ij}\tilde{\Gamma}_j^\dagger\tilde{\Lambda}^2\tilde{\Gamma}_i \\
&= \left(\tilde{\Gamma}_x\tilde{\Gamma}_x^\dagger + \tilde{\Gamma}_y\tilde{\Gamma}_y^\dagger\right) \\
&= \left[\begin{pmatrix}1\\0\\0\end{pmatrix}\otimes\begin{pmatrix}1&0&0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\otimes\begin{pmatrix}0&1&0\end{pmatrix}\right] \\
&= \left[\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix} + \begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix}\right] \\
&= \begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix} = (S^z)^2
\end{aligned}
\tag{4.79}
$$

thus we get:

$$
\begin{aligned}
\mathcal{O}_z((S^z)^2,(S^z)^2) &= \mathrm{Tr}\left[\Lambda^2\tilde{R}_z^{-1}(S^z)^2\right]\mathrm{Tr}\left[\Lambda^2\tilde{R}_z(S^z)^2\right] \\
&= \left\{\frac{1}{3}\,\mathrm{Tr}\left[\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix}\right]\right\}^2 \\
&= \left\{\frac{1}{3}\,\mathrm{Tr}\left[\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&0\end{pmatrix}\right]\right\}^2 = (-\frac{2}{3})(-\frac{2}{3}) = \frac{4}{9}.
\end{aligned}
\tag{4.80}
$$

	$\mathcal{O}_z((S^z)^2,(S^z)^2)$	$\mathcal{O}_z((S^x)^2,(S^x)^2)$	$\mathcal{O}_z((S^y)^2,(S^y)^2)$	$\mathcal{O}_z(\mathbb{I},\mathbb{I})$
EVEN-ODD	$4/9$	$4/9$	$4/9$	1
ODD-EVEN	$4/9$	0	0	$1/9$
EVEN-EVEN	$-4/9$	0	0	$-1/3$
ODD-ODD	$-4/9$	0	0	$-1/3$

TABLE 4.1: The values of the non-local order parameters evaluated on the dimer state for different placements of the operators.

However, if we choose $O^A = O^B = (S^x)^2$ or $O^A = O^B = (S^y)^2$ we get:

$$\begin{aligned}\mathcal{O}_z((S^x)^2,(S^x)^2) &= \mathrm{Tr}\left[\Lambda^2 R_z^\dagger (S^x)^2\right]\mathrm{Tr}\left[\Lambda^2 R_z (S^x)^2\right] \\ &= \left\{\frac{1}{3}\mathrm{Tr}\left[\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}\begin{pmatrix}0&0&0\\0&1&0\\0&0&1\end{pmatrix}\right]\right\}^2 \\ &= \frac{1}{9}\left\{\mathrm{Tr}\left[\begin{pmatrix}0&0&0\\0&-1&0\\0&0&1\end{pmatrix}\right]\right\}^2 = 0.\end{aligned} \tag{4.81}$$

$$\begin{aligned}\mathcal{O}_z((S^y)^2,(S^y)^2) &= \mathrm{Tr}\left[\Lambda^2 R_z^\dagger (S^y)^2\right]\mathrm{Tr}\left[\Lambda^2 R_z (S^y)^2\right] \\ &= \left\{\frac{1}{3}\mathrm{Tr}\left[\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}\begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}\right]\right\}^2 \\ &= \frac{1}{9}\left\{\mathrm{Tr}\left[\begin{pmatrix}-1&0&0\\0&0&0\\0&0&1\end{pmatrix}\right]\right\}^2 = 0.\end{aligned} \tag{4.82}$$

Thus only $\mathcal{O}_z((S^z)^2,(S^z)^2)$ is different from zero, and correspondingly the parity order parameter is now $\mathcal{O}_z(\mathbb{I},\mathbb{I}) = \frac{1}{9}$. In table 4.1 are summarized all the possible values of the non-local order parameters in the dimer phase for different placements of the operators within the second class.
It is obvious now that all the previous results can be straightforwardly generalized for a different choice of Σ, which may be fixed to be $e^{i\pi S^x}$ or $e^{i\pi S^y}$.

4.3.3 Analysis of the SU(2) and SU(3) Heisenberg points using non-local order parameters

In § 2.2.2 we have introduced the Hamiltonians (2.40):

$$H_\delta = \sum_i J_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2\right]. \tag{4.83}$$

with

$$J_i = \begin{cases} J & i \text{ odd} \\ J\delta & i \text{ even} \end{cases} \qquad 0 \leq \delta \leq 1. \tag{4.84}$$

If we redefine both J and δ as follows:

$$J \to J(1+\gamma) \qquad \delta \to \frac{1-\gamma}{1+\gamma} \tag{4.85}$$

where $0 \leq \gamma \leq 1$, then:

$$H_\delta \to H_\gamma = \sum_i J_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right] \tag{4.86}$$

where now:

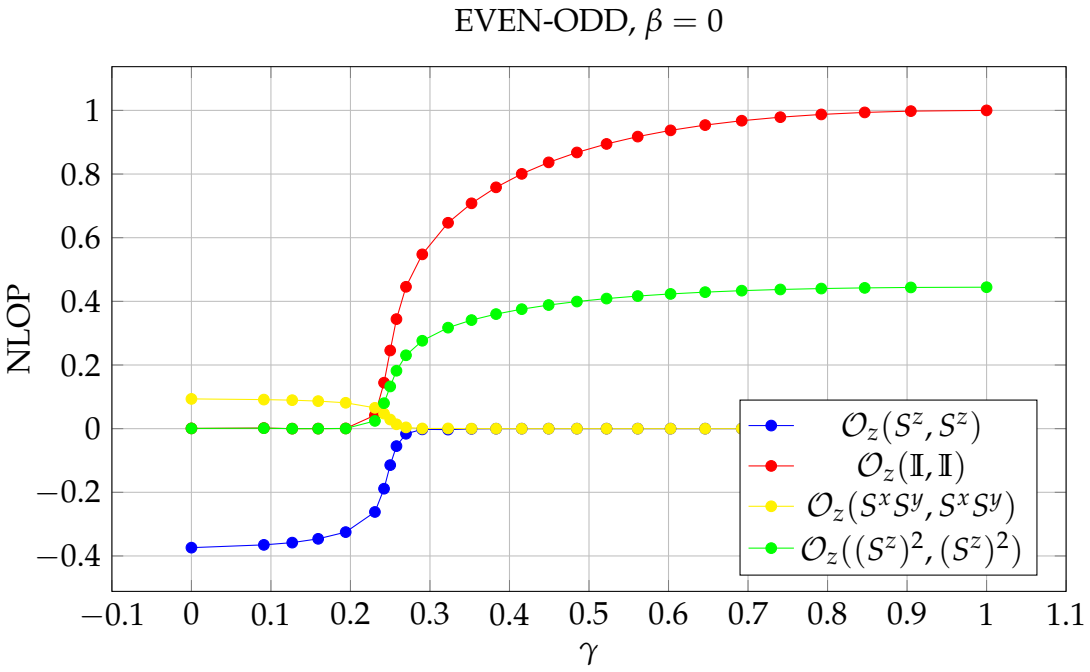
$$J_i = (1 - (-1)^i \gamma). \tag{4.87}$$

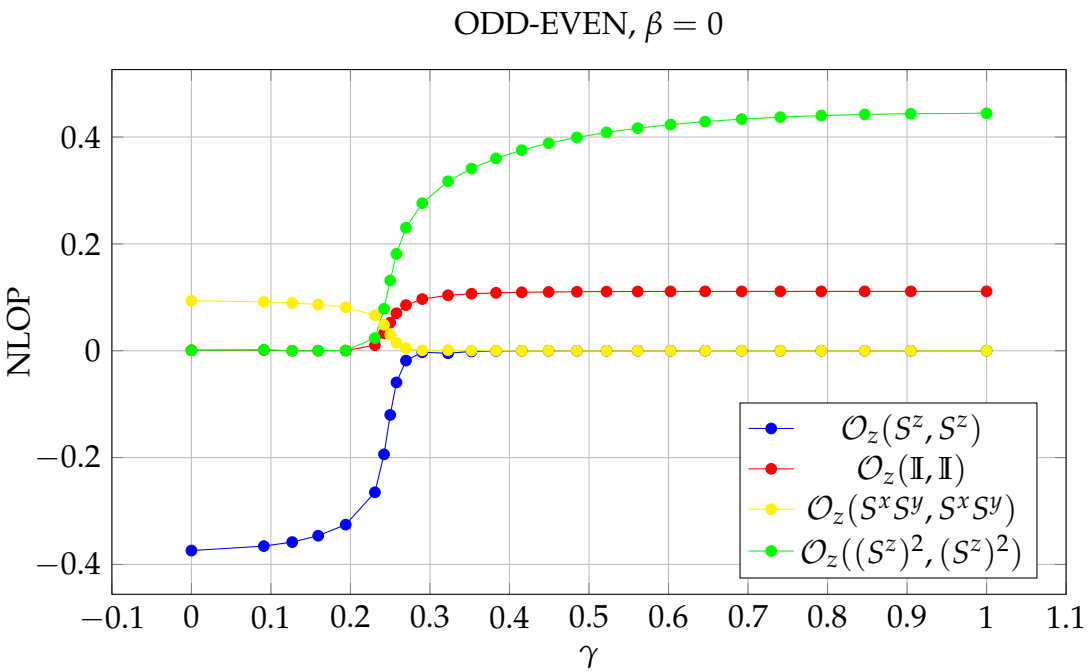
We are interested in two special points, specifically $\beta = 0$ and $\beta = \infty$, assuming always J positive, which correspond respectively to the antiferromagnetic SU(2) and SU(3) Heisenberg models with bond alternation and alternated fundamental and antifundamental representations (see appendix C):[2]

$$\begin{aligned} &\boxed{\beta = 0} \\ &\qquad H_\gamma = \sum_i J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} \\ &\boxed{\beta = \infty} \\ &\qquad \frac{2}{\beta} H_\gamma = \sum_i \left[J_{2i-1} (\boldsymbol{\lambda}_{2i-1} \cdot \bar{\boldsymbol{\lambda}}_{2i}) \right] + \sum_i \left[J_{2i} (\bar{\boldsymbol{\lambda}}_{2i} \cdot \boldsymbol{\lambda}_{2i+1}) \right]. \end{aligned} \tag{4.88}$$

They are both massive points for $\gamma = 0$, belonging to the Haldane and dimer phase respectively as we already know. Here we want to check that varying γ from 0 to 1 we get the expected behavior mentioned in § 2.2.2, i.e. we expect a phase transition when $\beta = 0$ but no phase transitions when $\beta = \infty$. We can use the non-local order parameters to detect a phase transition from the Haldane to the dimer phase, and indeed numerical simulations show a critical value of $\gamma \approx 0.25$ (Fig. 4.2). Here we have chosen a longer chain with 120 sites, keeping $\chi = 500$, in order to get a clear localization of the transition. Also we have placed the operators $O^A = O^B$ defining the corresponding non-local order parameters in sites with different "parity" (even/odd) and it can be easily seen that in the dimer state, which is the ground state of the SU(2) Heisenberg point when $\gamma = 1$, the value of the non-local order parameters are in perfect agreement with our analytical evaluation (see Table 4.1).
On the other hand when $\beta = \infty$ and γ increase from 0 to 1 the non-local order parameters do not detect any phase transition. As it can be seen from further numerical simulations in Fig. 4.3, the non-zero order parameters change just slightly their values, and once again our analytical calculation are in agreement with the numerical results.

[2] In SU(2) the fundamental and antifundamental representations are equivalent.


EVEN-ODD, $\beta = 0$
NLOP
γ
$\mathcal{O}_z(S^z, S^z)$
$\mathcal{O}_z(\mathbb{I}, \mathbb{I})$
$\mathcal{O}_z(S^xS^y, S^xS^y)$
$\mathcal{O}_z((S^z)^2, (S^z)^2)$


ODD-EVEN, $\beta = 0$
NLOP
γ
$\mathcal{O}_z(S^z, S^z)$
$\mathcal{O}_z(\mathbb{I}, \mathbb{I})$
$\mathcal{O}_z(S^xS^y, S^xS^y)$
$\mathcal{O}_z((S^z)^2, (S^z)^2)$

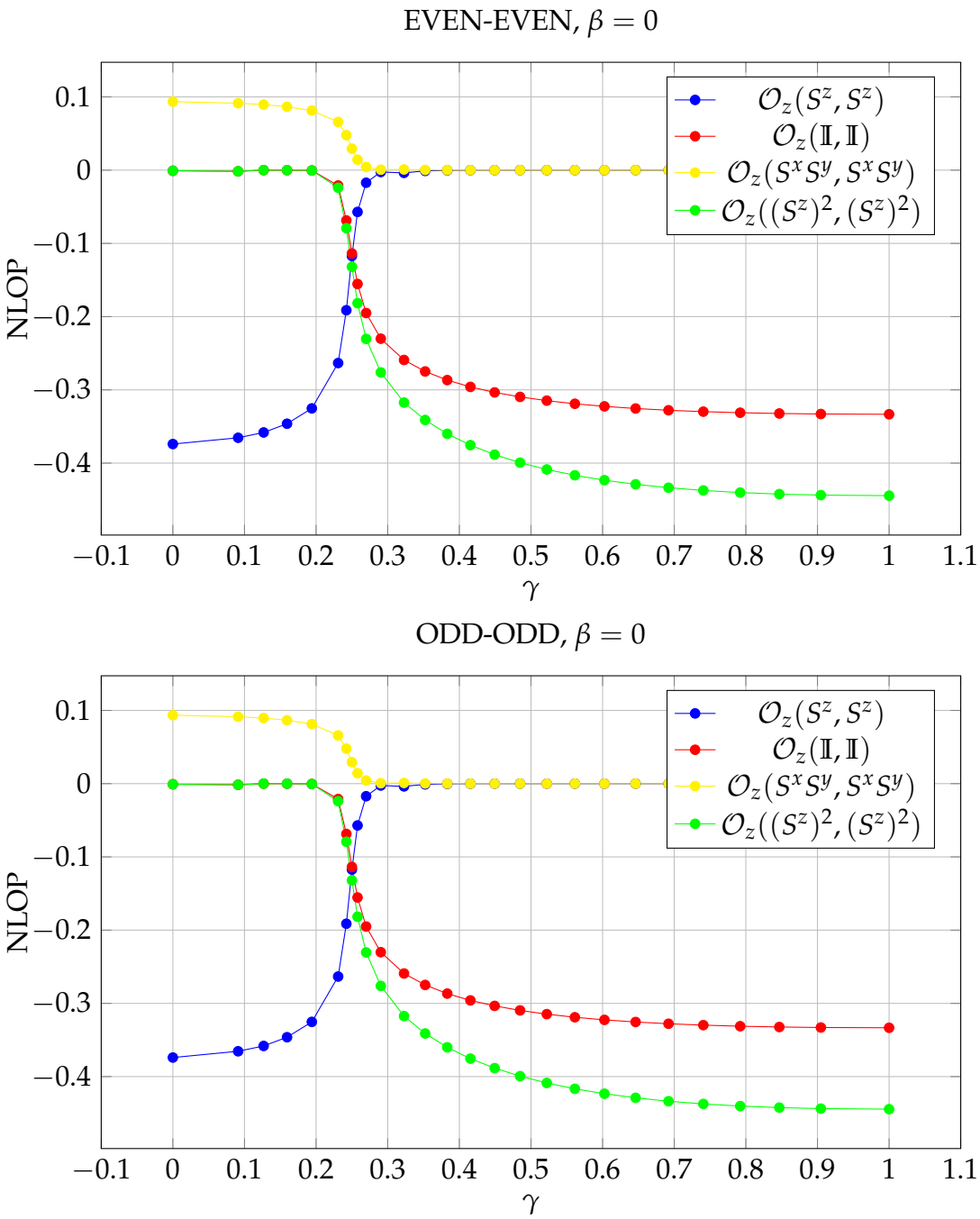
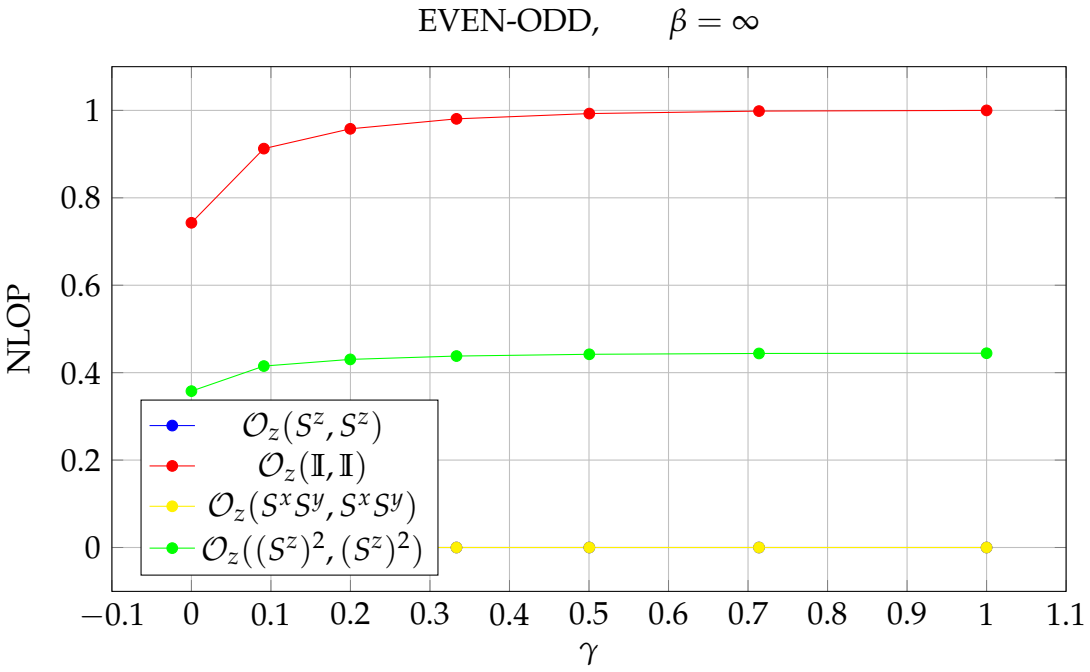
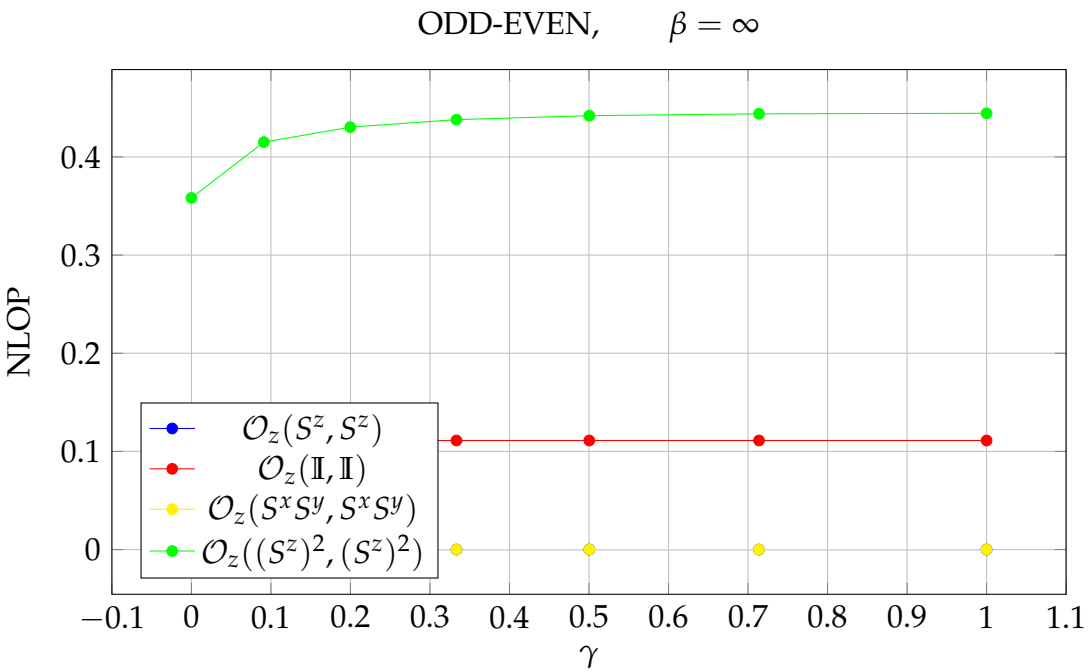


FIGURE 4.2: Numerical evaluation of the non-local order parameters in the SU(2) Heisenberg point. As we increase the value of γ from 0 to 1 we face a transition near $\gamma = 0.25$.


EVEN-ODD, $\beta = \infty$
NLOP
γ
$\mathcal{O}_z(S^z, S^z)$
$\mathcal{O}_z(\mathbb{I}, \mathbb{I})$
$\mathcal{O}_z(S^xS^y, S^xS^y)$
$\mathcal{O}_z((S^z)^2, (S^z)^2)$


ODD-EVEN, $\beta = \infty$
NLOP
γ
$\mathcal{O}_z(S^z, S^z)$
$\mathcal{O}_z(\mathbb{I}, \mathbb{I})$
$\mathcal{O}_z(S^xS^y, S^xS^y)$
$\mathcal{O}_z((S^z)^2, (S^z)^2)$

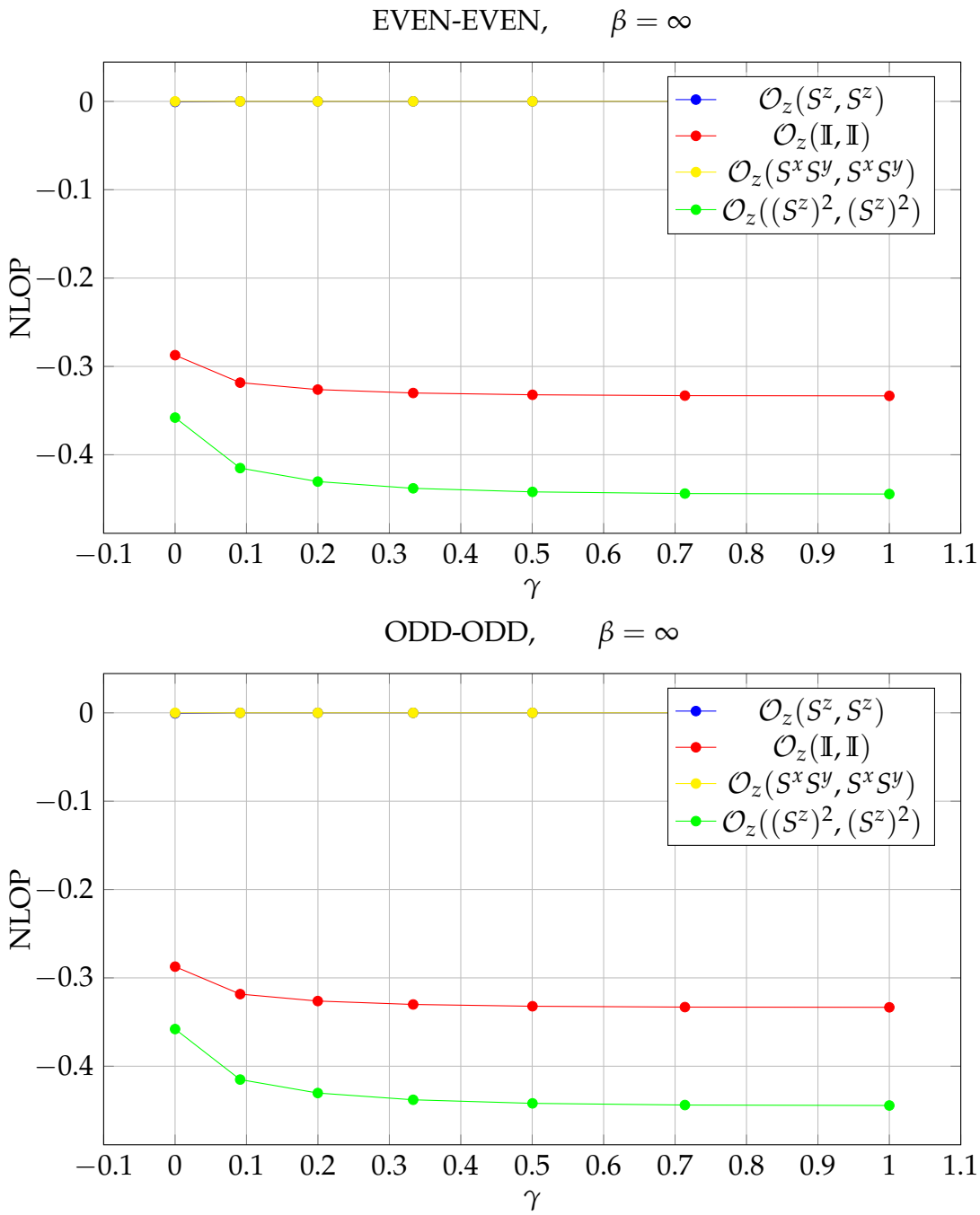


FIGURE 4.3: Numerical evaluation of the non-local order parameters in the SU(3) Heisenberg point. As we increase the value of γ from 0 to 1 we face no transitions.

4.4 Semiclassical limit of Heisenberg-like models with bond alternation

In chapter 1 we have found that the SU(2) Heisenberg model in the semiclassical limit $s \to \infty$ can be mapped onto a $O(3)$ non-linear sigma model with a topological term which is given by $2\pi s$ times an integer (see 1.71). We want now to extend this approach to the general case of a SU(N) antiferromagnetic Heisenberg models with bond alternation, i.e. with coupling constants of the form $J_i = (1 - (-1)^i\gamma)$, and with a given representation alternating with its conjugate. We will thus find the effective low-energy field theory which describes the two models in (4.88) for $N = 2, 3$, at least in their semiclassical limit. We will present a less specific approach than the one we used for the SU(2) case, which is although easier to generalize, following [35]. In any case we will reformulate the already known SU(2) case in order to make more clear the generalization for generic N.

4.4.1 SU(N) antiferromagnetic Heisenberg Hamiltonian

We start by re-expressing the SU(2) Hamiltonian (4.88) in terms of the matrix $\hat{S}$:

$$\hat{S} = \begin{pmatrix} \hat{S}_1^1 & \hat{S}_2^1 \\ \hat{S}_1^2 & \hat{S}_2^2 \end{pmatrix} = \begin{pmatrix} S^z & S^- \\ S^+ & -S^z \end{pmatrix}. \tag{4.89}$$

Indeed the exchange term $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$ can now be expressed as:

$$\frac{1}{2}\mathbf{S}_i \cdot \mathbf{S}_{i+1} = \sum_{\alpha\beta} \hat{S}_\alpha^\beta(i)\hat{S}_\beta^\alpha(i+1) = \mathrm{Tr}\left[\hat{S}_i\hat{S}_{i+1}\right] \tag{4.90}$$

thus:

$$H_\gamma = \frac{1}{2}\sum_i \sum_{\alpha\beta} J_i \hat{S}_\alpha^\beta(i)\hat{S}_\beta^\alpha(i+1) = \sum_i J_i \,\mathrm{Tr}\left[\hat{S}_i\hat{S}_{i+1}\right]. \tag{4.91}$$

We have been interested in the spin-1 representation of SU(2) so far, which is given by the symmetric product of two fundamental representations of SU(2), i.e. two spin-1/2 representations. All the other irreducible representations of spin-s can be formed taking symmetric product of $2s$ spin-1/2 fundamental representations. In order to generalize our results to higher SU(N) symmetries and to different irreducible representation of these groups, we use fermionic creation $c^\dagger_{\alpha,a}$ and annihilation $c^{\alpha,a}$ operators to define the spin operators $\hat{S}_\alpha^\beta$ in (4.89):

$$\hat{S}_\alpha^\beta = \sum_{a=1}^{2s} c^\dagger_{\alpha,a} c^{\beta,a} - \delta_\alpha^\beta s \tag{4.92}$$

where $a = 1, \ldots 2s$ is a "color" index, so that each fundamental representation needed to form the spin-s representation correspond to a color of the fermionic operators. Thus a spin-1 representation requests two colors, a spin-3/2 three colors, and so on.

On each site are imposed the following constraints:

$$\sum_{\alpha} c^{\dagger}_{\alpha,a} c^{\alpha,b} = \delta^{\beta}_{\alpha} \tag{4.93}$$

so that in total we have $2s$ fermionic operators, i.e. one for each color.
Now we can write down straightforwardly the SU(N) generalization of the SU(2) Hamiltonian (4.91):

$$\mathcal{H} = \frac{1}{N} \sum_{i} \sum_{\alpha\beta} J_i \hat{S}^{\beta}_{\alpha}(i) \hat{S}^{\alpha}_{\beta}(i+1) = \sum_{i} J_i \operatorname{Tr}\left[\hat{S}_i \hat{S}_{i+1}\right] \tag{4.94}$$

where now:

$$\hat{S}^{\beta}_{\alpha} = \sum_{a=1}^{n_c} c^{\dagger}_{\alpha,a} c^{\beta,a} - \delta^{\beta}_{\alpha} \frac{n_c}{2}. \tag{4.95}$$

The SU(N) index α can now take N different values, while the color index a runs from 1 to n_c. We now recall that we want alternated representations, and precisely we ask to have an irreducible representation on a sublattice A and the correspondent conjugate representation on sublattice B. If we choose the fundamental representation on sublattice A, then this request is equivalent to ask the antifundamental representation on sublattice B. In order to get such representations we impose suitable constraints:

$$\sum_{\alpha} c^{\dagger}_{\alpha,a} c^{\alpha,b} = \begin{cases} m\delta^{b}_{a} & \text{sublattice A} \\ (N-m)\delta^{b}_{a} & \text{sublattice B.} \end{cases} \tag{4.96}$$

where $1 \leq m \leq N-1$ tells us how many fermions of a given color we have in the chosen representation in A, while we have correspondingly $N-m$ fermions of a given color in the conjugate representation in B. Thus the two representations are given once we fix n_c and m.
In SU(2) $n_c = 2s$, while $m = 1$ always, therefore the different representations are given by n_c (or s) alone, and they are all equivalent to their conjugate. In SU(3) instead we can have $m = 1, 2$ and thus non-equivalent conjugate representations. For instance the fundamental representation corresponds to $n_c = 1$ and $m = 1$, while the antifundamental to $n_c = 1$ and $m = 2$.

4.4.2 SU(N) coherent states

Highest weight states

We can generalize the construction of a SU(N) coherent state using the fermionic operators just introduced in the last section. As before we begin with the familiar SU(2) case, comparing the present formulation with that already given in § 1.3.1.
First of all, in order to define a coherent state we need a highest weight state,

which in the SU(2) case is:

$$|s,s\rangle = c^\dagger_{1,1}c^\dagger_{1,2}\dots c^\dagger_{1,2s}|0\rangle = \frac{1}{(2s)!}\epsilon^{ab\dots}c^\dagger_{1,a}c^\dagger_{1,b}\dots|0\rangle\,. \tag{4.97}$$

This state clearly contains $2s$ fermions, one for each color, and all of them are in the 1-state.
This state is found asking that it is an eigenvector of S^z with eigenvalue s. Recalling that $S^z = \hat{S}^1_1 = -\hat{S}^2_2$, we can restate the previous request as:

$$H_\alpha|s,s\rangle = \begin{cases} s|s,s\rangle & \text{if } \alpha = 1 \\ -s|s,s\rangle & \text{if } \alpha = 2 \end{cases} \tag{4.98}$$

where $\{H_\alpha\}$ is the *Cartan subalgebra* of SU(2):

$$H_\alpha = \hat{S}^\alpha_\alpha = \sum_a c^\dagger_{\alpha,a}c^{\alpha,a} - s. \tag{4.99}$$

In § 1.3.1 we used the same highest weight state on both sublattices, here instead we choose to consider $|s,-s\rangle$ in sublattice B for convenience:

$$|s,-s\rangle = c^\dagger_{2,1}c^\dagger_{2,2}\dots c^\dagger_{2,2s}|0\rangle = \frac{1}{(2s)!}\epsilon^{ab\dots}c^\dagger_{2,a}c^\dagger_{2,b}\dots|0\rangle\,. \tag{4.100}$$

Obviously (4.98) changes accordingly. Thus, with this choice, a Néel state would be given by the product of the highest weight states on each site.
We can easily generalize this construction of a highest weight state for the SU(N) case. Thus in sublattice A we can define:

$$|\psi_0\rangle = C\underbrace{[\epsilon^{ab\dots}\underbrace{c^\dagger_{1,a}c^\dagger_{1,b}\dots}_{n_c \text{ times}}]\dots[\epsilon^{cd\dots}c^\dagger_{m,c}c^\dagger_{m,d}\dots]}_{m \text{ square brackets}}|0\rangle \tag{4.101}$$

where C is a normalization constant, and the number of colors n_c and m depend on the representation specified. For each m we have n_c fermions, one for each color, and they are all in the m-state. This state satisfy:

$$H_\alpha|\psi_0\rangle = \begin{cases} \frac{n_c}{2}|\psi_0\rangle & \text{if } \alpha \in [1,m] \\ -\frac{n_c}{2}|\psi_0\rangle & \text{if } \alpha \in [m+1,N] \end{cases} \tag{4.102}$$

where now the Cartan subalgebra of SU(N) is:

$$H_\alpha = \hat{S}^\alpha_\alpha = \sum_a c^\dagger_{\alpha,a}c^{\alpha,a} - \frac{n_c}{2}. \tag{4.103}$$

In sublattice B we define instead the following highest weight state:

$$|\psi_0\rangle = C \underbrace{[\epsilon^{ab\dots} \underbrace{c^\dagger_{m+1,a} c^\dagger_{m+1,b} \dots}_{n_c \text{ times}}] \dots [\epsilon^{cd\dots} c^\dagger_{N,c} c^\dagger_{N,d} \dots]}_{N-m \text{ square brackets}} |0\rangle \tag{4.104}$$

such that:

$$H_\alpha |\psi_0\rangle = \begin{cases} -\frac{n_c}{2} |\psi_0\rangle & \text{if } \alpha \in [1, m] \\ \frac{n_c}{2} |\psi_0\rangle & \text{if } \alpha \in [m+1, N] \, . \end{cases} \tag{4.105}$$

Coherent states

In § 1.3.1 we have defined a SU(2) coherent state $|\mathbf{\Omega}\rangle$ applying a given rotation to the highest weight state:[3]

$$|\mathbf{\Omega}\rangle = \mathcal{R}(\phi, \theta, \chi) |\psi_0\rangle \tag{4.106}$$

where ϕ, θ, χ are three Euler angles which parametrize the rotation and:

$$\mathbf{\Omega} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta). \tag{4.107}$$

As χ can be fixed to any value with no harm, we fix it to be $\chi = -\phi$. Thus we have:

$$\begin{aligned} |\mathbf{\Omega}\rangle &= e^{-i\phi S^z} e^{-i\theta S^y} e^{i\phi S^z} |\psi_0\rangle \\ &= \exp[i\theta(S^x \sin\phi - S^y \cos\phi)] |\psi_0\rangle \\ &= \exp\left[\left(-\frac{\theta}{2} e^{-i\phi}\right) S^+ - \left(-\frac{\theta}{2} e^{i\phi}\right) S^-\right] |\psi_0\rangle \\ &= \exp\left[\hat{\Omega}^1_2 \hat{S}^2_1 - (\hat{\Omega}^1_2)^* \hat{S}^1_2\right] |\psi_0\rangle \, . \end{aligned} \tag{4.108}$$

where in the last line we have defined the complex number $\hat{\Omega}^1_2 = -\frac{\theta}{2} e^{-i\phi}$ and re-expressed the spin operators in terms of the components of the matrix $\hat{S}$.
An important identity satisfied by the SU(2) coherent states is:

$$\langle \mathbf{\Omega}| \mathbf{S} |\mathbf{\Omega}\rangle = \begin{cases} & s\mathbf{\Omega} & \text{sublattice A} \\ - & s\mathbf{\Omega} & \text{sublattice B} \end{cases} \tag{4.109}$$

which in terms of $\hat{S}^\beta_\alpha$ becomes:

$$\langle \mathbf{\Omega}| \hat{S}^\beta_\alpha |\mathbf{\Omega}\rangle = \begin{cases} & s\hat{Q}^\beta_\alpha & \text{sublattice A} \\ - & s\hat{Q}^\beta_\alpha & \text{sublattice B} \end{cases} \tag{4.110}$$

[3] here $|\psi_0\rangle = |s, \pm s\rangle$, depending on the sublattice considered.

where we have introduced the $\hat{Q}$ matrix:

$$\hat{Q} = \begin{pmatrix} \hat{Q}_1^1 & \hat{Q}_2^1 \\ \hat{Q}_1^2 & \hat{Q}_1^2 \end{pmatrix} = \begin{pmatrix} \Omega^z & \Omega^- \\ \Omega^+ & -\Omega^z \end{pmatrix} = \begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix}. \tag{4.111}$$

This matrix is actually defined as follows:

$$\hat{Q} = U\Lambda U^\dagger \tag{4.112}$$

where

$$U = \exp\left[\begin{pmatrix} 0 & \hat{\Omega}_2^1 \\ -(\hat{\Omega}_2^1)^* & 0 \end{pmatrix}\right] = \begin{pmatrix} \cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2} \\ -e^{i\phi}\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \tag{4.113}$$

is the matrix which realize the rotation $\mathcal{R}(\theta,\phi)$ on the fundamental representation of SU(2), and

$$\Lambda = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.114}$$

Once again this special SU(2) case can be generalized to SU(N) with minimum effort as follows:

$$|\Omega\rangle = \mathcal{R}(\hat{\Omega}_\mu^\lambda)\,|\psi_0\rangle = \exp\left\{\hat{\Omega}_\mu^\lambda \hat{S}_\lambda^\mu - (\hat{\Omega}_\mu^\lambda)^* \hat{S}_\mu^\lambda\right\}|\psi_0\rangle \tag{4.115}$$

where now $\hat{\Omega}_\mu^\lambda$ are the entries of a $m \times (N-m)$ complex matrix $\hat{\Omega}$, with $\lambda = 1,\dots m$ and $\mu = m+1,\dots N$.
The identity (4.110) remains essentially unchanged, recalling that for SU(2) $n_c = 2s$:

$$\langle\Omega|\,\hat{S}_\alpha^\beta\,|\Omega\rangle = \begin{cases} \frac{n_c}{2}\hat{Q}_\alpha^\beta & \text{sublattice A} \\ -\frac{n_c}{2}\hat{Q}_\alpha^\beta & \text{sublattice B} \end{cases} \tag{4.116}$$

where now $\hat{Q}$ is still defined by $U\Lambda U^\dagger$ but:

$$U = \exp\left[\begin{pmatrix} 0 & \hat{\Omega} \\ -\hat{\Omega}^\dagger & 0 \end{pmatrix}\right] \tag{4.117}$$

and

$$\Lambda = \begin{pmatrix} \mathbb{I}_m & 0 \\ 0 & -\mathbb{I}_{N-m} \end{pmatrix}. \tag{4.118}$$

Notice also that $\hat{Q}^2 = \mathbb{I}_N$. Now we are ready to find the path integral formulation of these SU(N) models.

4.4.3 SU(N) path integral

Following § 1.3.2, we can express the partition function as:

$$\mathcal{Z} = \int \mathcal{D}\hat{Q}(\tau)e^{-S_E} = \int \mathcal{D}\hat{Q}(\tau)\exp\left\{\int_0^\beta d\tau\,\left[\sum_i \langle\Omega_i(\tau)|\dot{\Omega}_i(\tau)\rangle - \mathcal{H}(\hat{Q}(\tau))\right]\right\} \tag{4.119}$$

where $\hat{Q}(0) = \hat{Q}(\beta)$ and:

$$\mathcal{H}(\hat{Q}(\tau)) = -\frac{n_c^2}{4N}\sum_i\sum_{\alpha\beta} J_i \hat{Q}^{\beta}_{\alpha}(i,\tau)\hat{Q}^{\alpha}_{\beta}(i+1,\tau). \tag{4.120}$$

Exploiting the following identity satisfied by every operator O:

$$e^{-O(\tau)}\frac{d}{d\tau}e^{O(\tau)} = \int_0^1 du\, e^{-uO(\tau)}\frac{dO(\tau)}{dt}e^{uO(\tau)} \tag{4.121}$$

we can re-express the term $\langle\Omega(\tau)|\dot{\Omega}(\tau)\rangle$ as:

$$\begin{aligned}\int_0^\beta d\tau\,\langle\Omega(\tau)|\dot{\Omega}(\tau)\rangle &= \int_0^\beta d\tau\,\langle\psi_0|\,\mathcal{R}^\dagger\frac{d}{d\tau}\mathcal{R}\,|\psi_0\rangle \\ &= \int_0^\beta d\tau\int_0^1 du\;\langle\psi_0|\,\mathcal{R}_u^\dagger\left(\frac{\partial\hat{\Omega}^\lambda_\mu}{\partial\tau}\hat{S}^\mu_\lambda - \frac{\partial(\hat{\Omega}^\lambda_\mu)^*}{\partial\tau}\hat{S}^\lambda_\mu\right)\mathcal{R}_u\,|\psi_0\rangle \\ &= \eta_i\frac{n_c}{2}\int_0^\beta d\tau\int_0^1 du\;\left(\frac{\partial\hat{\Omega}^\lambda_\mu}{\partial\tau}\hat{Q}^\mu_\lambda(\tau,u) - \frac{\partial(\hat{\Omega}^\lambda_\mu)^*}{\partial\tau}\hat{Q}^\lambda_\mu(\tau,u)\right) \\ &= \eta_i i n_c\omega\end{aligned} \tag{4.122}$$

where

$$\begin{aligned}&\mathcal{R}_u = \exp\Big\{u[\hat{\Omega}^\lambda_\mu\hat{S}^\mu_\lambda - (\hat{\Omega}^\lambda_\mu)^*\hat{S}^\lambda_\mu]\Big\} \\ &\hat{Q}(\tau,u) = U(\tau,u)\Lambda U^\dagger(\tau,u) \\ &U(\tau,u) = \exp\left\{u\begin{pmatrix}0 & \hat{\Omega}(\tau)\\ -\hat{\Omega}^\dagger(\tau) & 0\end{pmatrix}\right\} \\ &\eta_i = \begin{cases}1 & \text{if i} \in \text{sublattice A}\\ -1 & \text{if i} \in \text{sublattice B}\end{cases}\end{aligned} \tag{4.123}$$

and $\hat{Q}(\tau,0) = \Lambda$, $\hat{Q}(\tau,1) = \hat{Q}(\tau)$. Integrating by parts (4.122) we get:

$$\begin{aligned}\omega &= -\frac{1}{2i}\int_0^\beta d\tau\int_0^1 du\;\mathrm{Tr}\left[\begin{pmatrix}0 & \hat{\Omega}(\tau)\\ -\hat{\Omega}^\dagger(\tau) & 0\end{pmatrix}\partial_\tau\hat{Q}(\tau,u)\right] \\ &= \frac{1}{4i}\int_0^\beta d\tau\int_0^1 du\;\mathrm{Tr}\big[\hat{Q}(\tau,u)\partial_u\hat{Q}(\tau,u)\partial_\tau\hat{Q}(\tau,u)\big]\end{aligned} \tag{4.124}$$

where we used the identity:

$$\begin{pmatrix}0 & \hat{\Omega}(\tau)\\ -\hat{\Omega}^\dagger(\tau) & 0\end{pmatrix} = -\frac{1}{2}\hat{Q}(\tau,u)\partial_u\hat{Q}(\tau,u). \tag{4.125}$$

Thus the action S in the integral becomes:

$$S_E = -in_c\sum_i\eta_i\omega_i - \frac{n_c^2}{4N}\sum_i J_i\int_0^\beta d\tau\,\mathrm{Tr}\big[\hat{Q}(i,\tau)\hat{Q}(i+1,\tau)\big]. \tag{4.126}$$

In the semiclassical limit $n_c \to \infty$ we can decompose $\hat{Q}(2i)$ e $\hat{Q}(2i+1)$ as follows:

$$\begin{aligned}\hat{Q}(2i) =& \hat{N}(x)\sqrt{1-a^2\hat{L}^2(x)} - a\hat{L}(x)\\ \hat{Q}(2i+1) =& \hat{N}(x)\sqrt{1-a^2\hat{L}^2(x)} + a\hat{L}(x)\end{aligned} \tag{4.127}$$

where $a \ll 1$ is the lattice spacing and $\hat{N}(x)$, $\hat{L}(x)$ are slowly varying functions of x. Notice that this time the variable x is defined on the link between sites i and $i+1$. Moreover it easy to check that:

$$\begin{aligned}&\hat{N}(x)^2 = \mathbb{I};\\ &\hat{N}(x)\hat{L}(x) + \hat{L}(x)\hat{N}(x) = 0\end{aligned} \tag{4.128}$$

exploiting the identity $\hat{Q}(2i)^2 = \hat{Q}(2i+1)^2 = \mathbb{I}$. Thus we find:

$$\begin{aligned}\mathrm{Tr}\big[\hat{Q}(2i)\hat{Q}(2i+1)\big] &= \mathrm{Tr}\left[\left(\hat{N}(x)\sqrt{1-a^2\hat{L}^2(x)} - a\hat{L}(x)\right)\left(\hat{N}(x)\sqrt{1-a^2\hat{L}^2(x)} + a\hat{L}(x)\right)\right]\\ &= \mathrm{Tr}\Big[\hat{N}(x)^2(1-a^2\hat{L}(x)^2) - a^2\hat{L}^2(x)\Big]\\ &= \mathrm{Tr}\Big[1 - 2a^2\hat{L}(x)^2\Big].\\ \mathrm{Tr}\big[\hat{Q}(2i)\hat{Q}(2i-1)\big] &= \mathrm{Tr}\Bigg[\left(\hat{N}(x)\sqrt{1-a^2\hat{L}^2(x)} - a\hat{L}(x)\right)\\ &\qquad\left(\hat{N}(x-2)\sqrt{1-a^2\hat{L}^2(x-2)} + a\hat{L}(x-2)\right)\Bigg]\\ &= \mathrm{Tr}\left[\hat{N}(x)\hat{N}(x-2)\sqrt{\left(1-a^2\hat{L}(x)^2\right)\left(1-a^2\hat{L}(x-2)^2\right)}\right]\\ &+ \mathrm{Tr}\left[a\hat{N}(x)\hat{L}(x-2)\sqrt{1-a^2\hat{L}(x)^2} - a\hat{L}(x)\hat{N}(x-2)\sqrt{1-a^2\hat{L}(x-2)^2}\right]\\ &- \mathrm{Tr}\Big[a^2\hat{L}(x)\hat{L}(x-2)\Big].\end{aligned} \tag{4.129}$$

Now if we consider the following approximations:

$$\begin{aligned}\hat{N}(x-2) &\approx \hat{N}(x) - 2a\partial_x\hat{N}(x)\\ \hat{L}(x-2) &\approx \hat{L}(x) - 2a\partial_x\hat{L}(x)\end{aligned} \tag{4.130}$$

we get

$$\begin{aligned}
\mathrm{Tr}\left[\hat{Q}(2i)\hat{Q}(2i-1)\right] &\approx \mathrm{Tr}\left[\left(1-\frac{1}{2}\left(\hat{N}(x)-\hat{N}(x-2)\right)^2\right)\left(1-a^2\hat{L}(x)^2\right)\right] \\
&+ \mathrm{Tr}\left[-2a^2\hat{N}(x)\partial_x\hat{L}(x)\sqrt{1-a^2\hat{L}(x)^2}+2a^2\hat{L}(x)\partial_x\hat{N}(x)\sqrt{1-a^2\hat{L}(x)^2}\right] \\
&- \mathrm{Tr}\left[a^2\hat{L}(x)^2\right] \\
&\approx \mathrm{Tr}\left[\left(1-2a^2(\partial_x\hat{N}(x))^2\right)\left(1-a^2\hat{L}(x)^2\right)\right] \\
&+ \mathrm{Tr}\left[2a^2\partial_x\hat{N}(x)\hat{L}(x)+2a^2\hat{L}(x)\partial_x\hat{N}(x)\right] \\
&- \mathrm{Tr}\left[a^2\hat{L}(x)^2\right] \\
&\approx \mathrm{Tr}\left[-2a^2\hat{L}(x)^2-2a^2(\partial_x\hat{N}(x))^2+4a^2\hat{L}(x)\partial_x\hat{N}(x)\right].
\end{aligned} \tag{4.131}$$

In the previous expressions $\hat{N}$,$\hat{L}$ and their derivatives have been treated as commuting given that they are evaluated inside a trace, which is cyclic. Exploiting this propriety and:

$$\partial_x(\hat{N}\hat{L}+\hat{L}\hat{N}) = \partial_x\hat{N}\hat{L}+\hat{N}\partial_x\hat{L}+\partial_x\hat{L}\hat{N}+\hat{L}\partial_x\hat{N} = 0 \tag{4.132}$$

we also find:

$$\hat{N}\partial_x\hat{L} = -\partial_x\hat{N}\hat{L}. \tag{4.133}$$

Now putting together the expressions above, ignoring constant terms we get:

$$\begin{aligned}
&\mathrm{Tr}\left[J_{2i}\hat{Q}(2i)\hat{Q}(2i+1)+J_{2i-1}\hat{Q}(2i)\hat{Q}(2i-1)\right] = \\
&= -\mathrm{Tr}\left[2a^2\hat{L}(x)^2(J_{2i}+J_{2i-1})-J_{2i-1}(4a^2\hat{L}(x)\partial_x\hat{N}(x)-2a^2(\partial_x\hat{N}(x))^2)\right] \\
&= -J\,\mathrm{Tr}\left[4a^2\hat{L}(x)^2+2a^2(1-\gamma)(\partial_x\hat{N}(x))^2-4a^2(1-\gamma)\hat{L}(x)\partial_x\hat{N}(x)\right] \\
&= -4a^2J\,\mathrm{Tr}\left[\hat{L}(x)^2+\frac{(1-\gamma)}{2}(\partial_x\hat{N}(x))^2-(1-\gamma)\hat{L}(x)\partial_x\hat{N}(x)\right]
\end{aligned} \tag{4.134}$$

Therefore the Hamiltonian (4.120) in the continuum limit becomes:

$$\mathcal{H} = \frac{Jn_c^2a}{2N}\int_0^\beta d\tau\int dx\,\mathrm{Tr}\left[\hat{L}(x,\tau)^2+\frac{(1-\gamma)}{2}(\partial_x\hat{N}(x,\tau))^2-(1-\gamma)\hat{L}(x,\tau)\partial_x\hat{N}(x,\tau)\right] \tag{4.135}$$

Let us evaluate now the Berry's phase (4.126):

$$\begin{aligned} in_c \sum_i \eta_i \omega(\hat{Q}(i)) &= in_c \left(\sum_i \omega(\hat{Q}(2i)) - \sum_i \omega(\hat{Q}(2i+1)) \right) \\ &= in_c \left(\sum_x \omega(\hat{N}(x) - a\hat{L}(x)) - \sum_x \omega(\hat{N}(x) + a\hat{L}(x)) \right) \\ &= -i2an_c \sum_x \frac{\delta\omega}{\delta\hat{N}}(x)\hat{L}(x) \end{aligned} \tag{4.136}$$

which in the continuum limit becomes:

$$in_c \sum_i \eta_i \omega_i \to -in_c \int dx \frac{\delta\omega}{\delta\hat{N}}(x)\hat{L}(x). \tag{4.137}$$

We use this identity:

$$\omega(\hat{Q}) = \frac{1}{2i}\int_0^\beta d\tau \int_0^1 du\, \mathrm{Tr}\left[\hat{Q}\partial_u\hat{Q}\partial_\tau\hat{Q}\right] = \frac{1}{i}\int_0^\beta d\tau \mathrm{Tr}\left[\Lambda U^\dagger \partial_\tau U\right] \tag{4.138}$$

to show that $\delta\omega$ gives:

$$\begin{aligned} \delta\omega =& \delta\left(\frac{1}{2i}\int_0^\beta d\tau \mathrm{Tr}\left\{\Lambda U^\dagger\partial_\tau U\right\}\right) \\ =& \frac{1}{2i}\int_0^\beta d\tau \mathrm{Tr}\left\{\Lambda\delta U^\dagger\partial_\tau U + \Lambda U^\dagger\partial_\tau(\delta U)\right\} \\ =& \frac{1}{2i}\int_0^\beta d\tau \mathrm{Tr}\left\{\Lambda\delta U^\dagger\partial_\tau U + \Lambda U^\dagger\partial_\tau(\delta U) + \Lambda\partial_\tau U^\dagger\delta U - \Lambda\partial_\tau U^\dagger\delta U\right\} \\ =& \frac{1}{2i}\int_0^\beta d\tau\partial_\tau \cancel{\mathrm{Tr}\left\{\Lambda U^\dagger\delta U\right\}} + \frac{1}{2i}\int_0^\beta d\tau \mathrm{Tr}\left\{\delta\hat{Q}\partial_\tau U U^\dagger\right\} \\ =& \frac{1}{4i}\int_0^\beta d\tau \mathrm{Tr}\left\{\delta\hat{Q}\left[\partial_\tau U U^\dagger - U\partial_\tau U^\dagger\right]\right\} \\ =& \frac{1}{4i}\int_0^\beta d\tau \mathrm{Tr}\left\{\delta\hat{Q}\left[\partial_\tau U\left(\Lambda U^\dagger U\Lambda\right)U^\dagger - U\left(\Lambda U^\dagger U\Lambda\right)\partial_\tau U^\dagger\right]\right\} \\ =& \frac{1}{4i}\int_0^\beta d\tau \mathrm{Tr}\left\{\delta\hat{Q}\partial_\tau U\Lambda U^\dagger\hat{Q} - \delta\hat{Q}\hat{Q}U\Lambda\partial_\tau U^\dagger\right\} \\ =& \frac{1}{4i}\int_0^\beta d\tau \mathrm{Tr}\left\{\hat{Q}\delta\hat{Q}\partial_\tau U\Lambda U^\dagger + \hat{Q}\delta\hat{Q}U\Lambda\partial_\tau U^\dagger\right\} \\ =& \frac{1}{4i}\int_0^\beta d\tau \mathrm{Tr}\left\{\hat{Q}\delta\hat{Q}\left(\partial_\tau U\Lambda U^\dagger + U\Lambda\partial_\tau U^\dagger\right)\right\} \\ =& \frac{1}{4i}\int_0^\beta d\tau \mathrm{Tr}\{\hat{Q}\delta\hat{Q}\partial_\tau\hat{Q}\}. \end{aligned} \tag{4.139}$$

Then Berry's phase reads:

$$-in_c \int dx \frac{\delta\omega}{\delta\hat{N}}(x)\hat{L}(x) = \frac{n_c}{4}\int_0^\beta d\tau \int dx \,\mathrm{Tr}\big[\hat{L}(x,\tau)\hat{N}(x,\tau)\partial_\tau\hat{N}(x,\tau)\big] \quad (4.140)$$

and the action (4.126) is:

$$S_E = \frac{Jn_c^2 a}{2N}\int_0^\beta d\tau \int dx \,\mathrm{Tr}\left[\hat{L}^2 - 2\hat{L}\left(\frac{1-\gamma}{2}\partial_x\hat{N} + \frac{N}{4Jn_c a}\hat{N}\partial_\tau\hat{N}\right) + \frac{1-\gamma}{2}(\partial_x\hat{N})^2\right]. \quad (4.141)$$

Notice that we can complete the square inside the trace:

$$\begin{aligned}
&\mathrm{Tr}\left[\hat{L}^2 - 2\hat{L}\left(\frac{1-\gamma}{2}\partial_x\hat{N} + \frac{N}{4Jn_c a}\hat{N}\partial_\tau\hat{N}\right)\right] \\
&= \mathrm{Tr}\left[\left(\hat{L} - \frac{1-\gamma}{2}\partial_x\hat{N} - \frac{N}{4Jn_c a}\hat{N}\partial_\tau\hat{N}\right)^2\right] \\
&- \mathrm{Tr}\left[\frac{(1-\gamma)^2}{4}(\partial_x\hat{N})^2 + \frac{N^2}{16J^2n_c^2a^2}(\partial_\tau\hat{N})^2 - \frac{(1-\gamma)N}{4Jn_c a}\hat{N}\partial_\tau\hat{N}\partial_x\hat{N}\right]
\end{aligned} \quad (4.142)$$

leaving us with a Gaussian integral that makes it possible to integrate out the field $\hat{L}$:

$$\begin{aligned}
S_E = &\frac{Jn_c^2 a}{2N}\int_0^\beta d\tau \int dx \,\mathrm{Tr}\left[\frac{(1-\gamma^2)}{4}(\partial_x\hat{N})^2 + \frac{N^2}{16J^2n_c^2a^2}(\partial_\tau\hat{N})^2\right] \\
&+ i\frac{(1-\gamma)\pi n_c}{8\pi i}\int_0^\beta d\tau \int dx \,\mathrm{Tr}\big[\hat{N}\partial_\tau\hat{N}\partial_x\hat{N}\big].
\end{aligned} \quad (4.143)$$

Now we define:

$$\begin{aligned}
g &= \frac{4}{n_c\sqrt{1-\gamma^2}} \\
v_s &= \frac{2Jn_c a}{N}\sqrt{1-\gamma^2} \\
\theta &= \pi n_c(1-\gamma)
\end{aligned} \quad (4.144)$$

in order to make evident the Lagrangian of the $U(N)/U(m)\times U(N-m)$ Non-Linear Sigma Model which we eventually find, with the additional topological term:

$$\mathcal{L}_{NL\sigma M} = \frac{1}{2g}\left(\frac{1}{2}\mathrm{Tr}\left[v_s(\partial_x\hat{N})^2 + \frac{1}{v_s}(\partial_\tau\hat{N})^2\right]\right) + i\frac{\theta}{4\pi}\left(-\frac{i}{2}\mathrm{Tr}\big[\hat{N}\partial_\tau\hat{N}\partial_x\hat{N}\big]\right) \quad (4.145)$$

where:

$$\Theta(\hat{N}) = \frac{1}{4\pi}\int d\tau \int dx \left(-\frac{i}{2}\mathrm{Tr}\big[\hat{N}\partial_\tau\hat{N}\partial_x\hat{N}\big]\right) \quad (4.146)$$

is always an integer. In appendix D we show that the O(3) case we are already familiar with is indeed recovered when $N = 2$ and $\gamma = 0$.

4.4.4 Comments on the theoretical predictions

Let us first consider further the $N = 2$ case. If the assumed semiclassical approximation could be still considered correct down to $s = 1$, or equivalently down to $n_c = 2$, then we would expect a critical system, i.e. a phase transition, at $2\pi(1-\gamma) = (2k+1)\pi$ where k is an integer [40]. There is only a point that gives a critical value for γ in the interval $[0,1]$, that is $\gamma = 0.5$ for $k = 0$. Despite that, we found a critical value of $\gamma \approx 0.25$, that is exactly half the prediction based on the semilclassical limit. Analogous results have been found in [49, 41, 20]. Moreover it seems that also for $s = 3/2, 2$ the field theoretical predictions are not in agreement with numerical results [23, 50]. We may conclude that the semiclassical approximation is able to capture the main qualitative features of the model, correctly predicting the existence of a phase transition, but it does not give a reliable estimate of the critical points, at least for the lowest value of s.
The case $N = 3$ is trickier, as we know very little about non-linear sigma models with topological terms. It may be worth then to study this case from another perspective.

CP^{N-1} models and the effect of the topological term

Recall that both our cases of interest corresponds to $m = 1$, so the effective field theory we get, discarding the topological term, is a $U(N)/U(N-1) \times U(1)$ non-linear sigma model, which corresponds to another well known model, i.e. the CP^{N-1} model. These models represent a generalization of the O(3) non-linear sigma model as they share several features as asymptotically freedom, instantons solutions and so on [34]. If we parametrize the matrix field $\hat{N}$ as follows [35]:

$$\hat{N}^{\beta}_{\alpha}(\tau, x) = -\delta^{\beta}_{\alpha} + 2z^{*}_{\alpha}(\tau, x) z^{\beta}(\tau, x) \tag{4.147}$$

where $\mathbf{z} = (z^1, z^2, \ldots, z^N)$ is a N-component complex vector field, which satisfy $\mathbf{z}^{\dagger}\mathbf{z} = 1$, then the action of the non-linear sigma model can be expressed as:

$$\begin{aligned} S =& \frac{2}{g} \int d^2x \left[\partial_\mu \mathbf{z}^{\dagger} \partial_\mu \mathbf{z} - (\mathbf{z}^{\dagger} \partial_\mu \mathbf{z})^{\dagger} (\mathbf{z}^{\dagger} \partial_\mu \mathbf{z}) \right] \\ =& \frac{2}{g} \sum_{\alpha} \int d^2x \left[\left| \partial_\mu z^{\alpha} \right|^2 - \left| z^{*}_{\alpha} \partial_\mu z^{\alpha} \right|^2 \right]. \end{aligned} \tag{4.148}$$

and we get the action of the CP^{N-1} model. Here $\partial_\mu = \partial_{\tau', x}$ where we have redefined the time coordinate as $\tau' = v_s \tau$. This model has a local $U(1)$ gauge invariance, indeed if we redefine locally the phase of the fields z^{α}:

$$z^{\alpha}(\tau', x) \to z^{\alpha}(\tau', x) e^{i\phi(\tau', x)} \tag{4.149}$$

then the Lagrangian remains invariant. We can thus introduce an auxiliary gauge field A_μ in terms of the field $\mathbf{z}$:

$$A_\mu = -\frac{i}{2}\left[\mathbf{z}^\dagger \partial_\mu \mathbf{z} - \partial_\mu \mathbf{z}^\dagger \mathbf{z}\right] \tag{4.150}$$

and re-express the action as:

$$S = \frac{2}{g}\int dx^2 \left[\partial_\mu \mathbf{z}^\dagger \partial_\mu \mathbf{z} - (A_\mu)^2\right]. \tag{4.151}$$

This gauge field correctly transform under a U(1) gauge transformation as $A_\mu \to A_\mu + \partial_\mu \phi$.
Moreover it can be easily shown that with the parametrization (4.147) the topological term (4.146) becomes:

$$\Theta = \frac{1}{2\pi i}\int dx^2 \epsilon_{\mu\nu}\partial_\mu \mathbf{z}^\dagger \partial_\nu \mathbf{z}. \tag{4.152}$$

The importance of this term depends again on value of the angle $\theta = n_c\pi(1-\gamma)$, given that the topological term (4.146) is always an integer. It can be shown that in the large N limit ($N \sim n_c$) and for $\theta = (2k+1)\pi$, $k \in \mathbb{Z}$, the CP^{N-1} model with topological term gives a two-fold degeneracy of the ground state [36]. On the other hand, for $\theta = 2k\pi$, the ground state is expected to be non-degenerate. Recall that we are interested in the specific case $N = 3$ and $n_c = 1$ and even though we are far from both the large n_c and large N limits, it seems that these results are in agreement with the expected degeneracy of the SU(3) Heisenberg model given by $\gamma = 0$, and the non-degeneracy of the dimer state given by $\gamma = 1$. Analytical predictions for intermediate values of θ are not available, but from our numerical simulations it is clear that no critical points are expected and that the non-degeneracy of the ground state has to remain intact for every value of $\theta \neq (2k+1)\pi$.

Conclusions

In this work we have shown that is possible to define and use correctly new non-local order parameters in order to detect the topological phases of a one-dimensional spin system. It is evident how the matrix product states have helped us especially in the analytical evaluation of these quantities, but also in the general understanding of how and why the expectation values of certain non-local operators are sensitive to topological order. From the MPS representation of a ground state we can easily extract a lot of information about the phase the state is in, indeed we have seen how to completely characterize the different SPT phases looking at how the symmetries act on the "un-physical" level of the matrices. When the exact MPS representation is unknown we can still use numerical algorithms, as the one used here [19], to get the matrices of the MPS with good approximation.
We have used these numerical methods also to test our analytical results. First of all we have checked that the values of the different non-local order parameters were coherent with our exact calculations. We found indeed no discrepancies. Secondly we have tried to locate the transition points from the Haldane phase to the dimer phase of the bilinear-biquadratic model with bond alternation. Although our results are qualitatively in agreement with theoretical predictions when we let only the β parameter to vary, keeping $\gamma = 0$, the exact location of this transition point could not be inferred due to very limited computing power. On the other hand varying the parity-breaking parameter γ while keeping $\beta = 0$ has given us a nice location of the transition point. It is undoubtedly around $\gamma \approx 0.25$. We have already discuss that this value is in disagreement with the field theoretical predictions based on the semiclassical limit, but it consistent with several other works. We are led to conclude that the predictions obtained within the semiclassical limit cannot be extended down to lower spins. Again there are several works showing these discrepancies also for $s = 3/2$ and $s = 2$. We initially thought to recover the correct localization of the transition point by naively re-normalizing the spin s to $s + 1$ in $\theta = 2\pi s(1 - \gamma)$, given that this kind of corrections are not uncommon when in semiclassical approximations the quantum nature of the spin is taken into account more carefully. Anyway this fix would have introduced another transition at $\gamma = 3/4$, but there is no trace of such a transition in our simulations. On the other hand the field theoretical predictions give the correct number of transitions expected in the interval $[0, 1]$ in which γ varies.

Appendix A

Spin waves theory: a closer look

A.1 From real space to momentum space Hamiltonian

To begin with we show how to get the momentum space Hamiltonian (1.14) from the corresponding real space Hamiltonian (1.12):

$$H \approx -\frac{Jzs^2N}{2} + \frac{Js}{2}\sum_{\langle ij\rangle}\left(a_i a_j + a_i^\dagger a_j^\dagger + a_i^\dagger a_i + a_j^\dagger a_j\right). \tag{A.1}$$

Considering the following Fourier transform:

$$\begin{aligned} a_{\mathbf{k}} &= \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\cdot\mathbf{j}} a_j \\ a_j &= \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{j}} a_{\mathbf{k}} \end{aligned} \tag{A.2}$$

each term in (A.1) can be expressed as:

$$\begin{aligned} \sum_{\langle ij\rangle} a_j^\dagger a_j &= \frac{1}{N}\sum_{\langle ij\rangle}\sum_{\mathbf{k}\mathbf{k}'} e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{j}} a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} \\ &= \frac{z}{N}\sum_j\sum_{\mathbf{k}\mathbf{k}'} e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{j}} a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} \\ &= z\sum_{\mathbf{k}\mathbf{k}'} \delta_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} \\ &= z\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \end{aligned} \tag{A.3}$$

$$\begin{aligned}
\sum_{\langle ij\rangle} a_i a_j &= \frac{1}{N}\sum_{\langle ij\rangle}\sum_{\mathbf{k}\mathbf{k}'} e^{-i\mathbf{k}\cdot\mathbf{i}-i\mathbf{k}'\cdot\mathbf{j}} a_{\mathbf{k}'} a_{\mathbf{k}} \\
&= \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\sum_{j}\sum_{\eta} e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{j}-i\mathbf{k}\cdot\eta} a_{\mathbf{k}'} a_{\mathbf{k}} \\
&= \sum_{\mathbf{k}\mathbf{k}'}\sum_{\eta} e^{-i\mathbf{k}\cdot\eta}\delta_{\mathbf{k},-\mathbf{k}'} a_{\mathbf{k}'} a_{\mathbf{k}} \\
&= \sum_{\mathbf{k}}\sum_{\eta} e^{-i\mathbf{k}\cdot\eta} a_{\mathbf{k}} a_{-\mathbf{k}} \\
&= z\sum_{\mathbf{k}} \gamma_{\mathbf{k}} a_{\mathbf{k}} a_{-\mathbf{k}}
\end{aligned} \tag{A.4}$$

$$\begin{aligned}
\sum_{\langle ij\rangle} a_i^\dagger a_j^\dagger &= \frac{1}{N}\sum_{\langle ij\rangle}\sum_{\mathbf{k}\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{i}+i\mathbf{k}'\cdot\mathbf{j}} a_{\mathbf{k}'}^\dagger a_{\mathbf{k}}^\dagger \\
&= \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\sum_{j}\sum_{\eta} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{j}+i\mathbf{k}\cdot\eta} a_{\mathbf{k}'}^\dagger a_{\mathbf{k}}^\dagger \\
&= \sum_{\mathbf{k}\mathbf{k}'}\sum_{\eta} e^{i\mathbf{k}\cdot\eta}\delta_{\mathbf{k},-\mathbf{k}'} a_{\mathbf{k}'}^\dagger a_{\mathbf{k}}^\dagger \\
&= \sum_{\mathbf{k}}\sum_{\eta} e^{i\mathbf{k}\cdot\eta} a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger \\
&= z\sum_{\mathbf{k}} \gamma_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger
\end{aligned} \tag{A.5}$$

hence giving (1.14):

$$H \approx -\frac{Jzs^2N}{2} + Jsz\sum_{\mathbf{k}}\left[a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{\gamma_{\mathbf{k}}}{2}\left(a_{\mathbf{k}}a_{-\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger\right)\right]. \tag{A.6}$$

A.2 Diagonalizing the Hamiltonian: the Bogoliubov Transformation

In order to diagonalize this Hamiltonian we apply the following Bogoliubov transformation:

$$\begin{aligned}
\alpha_{\mathbf{k}} &= \cosh(\theta_{\mathbf{k}})a_{\mathbf{k}} - \sinh(\theta_{\mathbf{k}})a_{-\mathbf{k}}^\dagger \\
a_{\mathbf{k}} &= \cosh(\theta_{\mathbf{k}})\alpha_{\mathbf{k}} + \sinh(\theta_{\mathbf{k}})\alpha_{-\mathbf{k}}^\dagger
\end{aligned} \tag{A.7}$$

where $\theta_{\mathbf{k}}$ is a real parameter and even under the exchange $\mathbf{k} \to -\mathbf{k}$. Such a transformation is canonical since the correct commutation relation between these new bosonic operators are satisfied:

$$\begin{aligned}
\left[\alpha_{\mathbf{k}}, \alpha_{\mathbf{k}'}^\dagger\right] &= \delta_{\mathbf{k},\mathbf{k}'} \\
\left[\alpha_{\mathbf{k}}, \alpha_{\mathbf{k}'}\right] &= \left[\alpha_{\mathbf{k}}^\dagger, \alpha_{\mathbf{k}'}^\dagger\right] = 0
\end{aligned} \tag{A.8}$$

We can now express (A.6) in terms of these new α-bosons:

$$\begin{aligned}
\sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} &= \sum_{\mathbf{k}} \left[\cosh(2\theta_{\mathbf{k}}) \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + \frac{1}{2} \sinh(2\theta_{\mathbf{k}}) (\alpha_{\mathbf{k}}^{\dagger} \alpha_{-\mathbf{k}}^{\dagger} + \alpha_{\mathbf{k}} \alpha_{-\mathbf{k}}) + \sinh^2(\theta_{\mathbf{k}}) \right] \\
\sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}}{2} a_{\mathbf{k}} a_{-\mathbf{k}} &= \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}}{2} \left[\cosh^2(\theta_{\mathbf{k}}) \alpha_{\mathbf{k}} \alpha_{-\mathbf{k}} + \sinh^2(\theta_{\mathbf{k}}) \alpha_{\mathbf{k}}^{\dagger} \alpha_{-\mathbf{k}}^{\dagger} + \sinh(2\theta_{\mathbf{k}}) \left(\alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + \frac{1}{2} \right) \right] \\
\sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}}{2} a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} &= \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}}{2} \left[\cosh^2(\theta_{\mathbf{k}}) \alpha_{\mathbf{k}}^{\dagger} \alpha_{-\mathbf{k}}^{\dagger} + \sinh^2(\theta_{\mathbf{k}}) \alpha_{\mathbf{k}} \alpha_{-\mathbf{k}} + \sinh(2\theta_{\mathbf{k}}) \left(\alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + \frac{1}{2} \right) \right].
\end{aligned} \tag{A.9}$$

Putting all together we get the following:

$$\begin{aligned}
H \approx & -\frac{Jzs^2 N}{2} + Jsz \sum_{\mathbf{k}} [\alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \left(\cosh(2\theta_{\mathbf{k}}) + \gamma_{\mathbf{k}} \sinh(2\theta_{\mathbf{k}}) \right) \\
& + \frac{1}{2} (\alpha_{\mathbf{k}}^{\dagger} \alpha_{-\mathbf{k}}^{\dagger} + \alpha_{\mathbf{k}} \alpha_{-\mathbf{k}}) \left(\sinh(2\theta_{\mathbf{k}}) + \gamma_{\mathbf{k}} \cosh(2\theta_{\mathbf{k}}) \right) \\
& + \sinh^2(\theta_{\mathbf{k}})]
\end{aligned} \tag{A.10}$$

which is in diagonal form if $\theta_{\mathbf{k}}$ is chosen such that:

$$\tanh(2\theta_{\mathbf{k}}) = -\gamma_{\mathbf{k}}. \tag{A.11}$$

Eventually we get (1.19):

$$H \approx -\frac{JNz}{2} s(s+1) + \sum_{\mathbf{k}} \left(\alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + \frac{1}{2} \right) \omega_{\mathbf{k}} \tag{A.12}$$

where

$$\omega_{\mathbf{k}} = Jsz \sqrt{1 - {\gamma_{\mathbf{k}}}^2} \tag{A.13}$$

is the energy of the excitations. This energy vanishes linearly for $\mathbf{k} \approx \mathbf{0}$ and $\mathbf{k} \approx \boldsymbol{\pi}$, indeed for small $\mathbf{k}$:

$$\begin{aligned}
\gamma_{\mathbf{k}} &= \frac{1}{z} \sum_{\boldsymbol{\eta}} e^{i\mathbf{k}\cdot\boldsymbol{\eta}} \\
&= \frac{1}{z} \sum_{\boldsymbol{\eta}} \left[1 + i\mathbf{k}\cdot\boldsymbol{\eta} - \frac{1}{2} (\mathbf{k}\cdot\boldsymbol{\eta})^2 + \mathcal{O}(|\mathbf{k}|^4) \right] \\
&= 1 - \frac{1}{2z} \sum_{\boldsymbol{\eta}} (\mathbf{k}\cdot\boldsymbol{\eta})^2 + \mathcal{O}(|\mathbf{k}|^4) \\
&= 1 - \frac{1}{z} |\mathbf{k}|^2 + \mathcal{O}(|\mathbf{k}|^4)
\end{aligned} \tag{A.14}$$

thus:

$$\omega_{\mathbf{k}} \approx Js\sqrt{2z} |\mathbf{k}| \tag{A.15}$$

while if $\mathbf{k} = \boldsymbol{\pi} + \mathbf{k'}$ and $\mathbf{k'} \approx \mathbf{0}$:

$$\begin{aligned}\gamma_{\mathbf{k}} = \gamma_{\boldsymbol{\pi}+\mathbf{k'}} &= \frac{1}{z}\sum_{\boldsymbol{\eta}} e^{i\mathbf{k'}\cdot\boldsymbol{\eta}+i\boldsymbol{\pi}\cdot\boldsymbol{\eta}} \\ &= -\frac{1}{z}\sum_{\boldsymbol{\eta}}\left[1 + i\mathbf{k'}\cdot\boldsymbol{\eta} - \frac{1}{2}(\mathbf{k'}\cdot\boldsymbol{\eta})^2 + \mathcal{O}(|\mathbf{k'}|^4)\right] \\ &= 1 - \frac{1}{2z}\sum_{\boldsymbol{\eta}}(\mathbf{k'}\cdot\boldsymbol{\eta})^2 + \mathcal{O}(|\mathbf{k'}|^4) \\ &= 1 - \frac{1}{z}|\mathbf{k'}|^2 + \mathcal{O}(|\mathbf{k'}|^4)\end{aligned} \tag{A.16}$$

thus:

$$\omega_{\mathbf{k}} \approx Js\sqrt{2z}|\mathbf{k'}| = Js\sqrt{2z}|\mathbf{k} - \boldsymbol{\pi}|. \tag{A.17}$$

A.3 Correction to the staggered magnetization

The order parameter that detects antiferromagnetic order is the staggered magnetization (1.23):

$$m^s = \frac{1}{N}\left(\sum_i S_i^z - \sum_j S_j^z\right) \tag{A.18}$$

which in a classical Néel state has its maximum value of $m^s = s$. The quantum corrections to this value can be evaluated as:

$$\begin{aligned}\Delta m^s = \langle m^s - s\rangle &= -\frac{1}{N}\langle\sum_i a_i^\dagger a_i\rangle = -\frac{1}{N}\langle\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\rangle \\ &= -\frac{1}{N}\langle\sum_{\mathbf{k}}\cosh^2(\theta_{\mathbf{k}})\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} + \sinh^2(\theta_{\mathbf{k}})\alpha_{-\mathbf{k}}\alpha_{-\mathbf{k}}^\dagger + \cosh(\theta_{\mathbf{k}})\sinh(\theta_{\mathbf{k}})(\alpha_{\mathbf{k}}^\dagger\alpha_{-\mathbf{k}}^\dagger + \alpha_{-\mathbf{k}}\alpha_{\mathbf{k}})\rangle \\ &= -\frac{1}{N}\sum_{\mathbf{k}}\langle\sinh^2(\theta_{\mathbf{k}})\alpha_{-\mathbf{k}}\alpha_{-\mathbf{k}}^\dagger\rangle \\ &= -\frac{1}{N}\sum_{\mathbf{k}}\sinh^2(\theta_{\mathbf{k}}) \\ &= -\frac{1}{2N}\sum_{\mathbf{k}}\left(\frac{1}{\sqrt{1-\gamma_{\mathbf{k}}^2}} - 1\right).\end{aligned} \tag{A.19}$$

In the continuum limit $\mathbf{k}$ is a continuous variable and the summation can be substituted with an integral and the correction Δm^s reads:

$$\Delta m^s = -\frac{1}{2}\int\frac{d^d\mathbf{k}}{(2\pi)^d}\left(\frac{1}{\sqrt{1-\gamma_{\mathbf{k}}^2}} - 1\right). \tag{A.20}$$

The value of this integral is expected to be finite for $d > 1$, as it contains no singularities, but when $d = 1$ the correction becomes divergent at $k \approx 0, \pi$ as:

$$\Delta m^s \approx -\int \frac{dk}{2\pi} \frac{1}{2k} = -\infty. \tag{A.21}$$

Appendix B

Matrix Product States from Singular Value Decomposition

Any rectangular $m \times n$ matrix A can be decomposed as [39]:

$$A = USV^\dagger \tag{B.1}$$

where

- U is a $m \times \chi$ matrix such that $U^\dagger U = \mathbb{I}_{\chi\times\chi}$;
- S is a $\chi \times \chi$ diagonal matrix, with non-zero positive entries called *singular values*;
- $V^\dagger$ is a $\chi \times n$ matrix such that $V^\dagger V = \mathbb{I}_{\chi\times\chi}$.

Thus χ is the number of singular values, also called the *Schmidt rank* of A, and it is always $\chi \leq \min(m, n)$.
If we consider a generic quantum state $|\psi\rangle$ on a chain of length L:

$$|\psi\rangle = \sum_{i_1\dots i_L} c_{i_1\dots i_L} |i_1 \dots i_L\rangle \tag{B.2}$$

where the local state space $|i_k\rangle$ is d-dimensional, then the tensor $c_{i_1\dots i_L}$ can be thought as a $d \times d^{L-1}$ matrix and we can apply the singular value decomposition:

$$c_{i_1 i_2\dots i_L} = c_{i_1, i_2\dots i_L} = \sum_{\alpha_2} U^{[1]}_{i_1,\alpha_2} S^{[1]}_{\alpha_2,\alpha_2} V^{\dagger[1]}_{\alpha_2, i_2\dots i_L} \qquad \alpha_2 = 1, \dots \chi_2. \tag{B.3}$$

where now $U^{[1]}_{i_1,\alpha_2}$ and $V^{\dagger[1]}_{\alpha_2,i_2\dots i_L}$ are respectively $d \times \chi_2$ and $\chi_2 \times d^{L-1}$ matrices.
For every possible value of the index i_1 we define a row vector $A^{[1]}_{i_1}$ with components:

$$(A^{[1]}_{i_1})^{\alpha_2} = U^{[1]}_{i_1,\alpha_2}. \tag{B.4}$$

Moreover we define a new $\chi_2 d \times d^{L-2}$ matrix as:

$$c_{\alpha_2 i_2, i_3\dots i_L} = S^{[1]}_{\alpha_2,\alpha_2} V^{\dagger[1]}_{\alpha_2, i_2\dots i_L} \tag{B.5}$$

thus (B.3) can be now expressed as:

$$c_{i_1 i_2 \dots i_L} = \sum_{\alpha_2} (A^{[1]}_{i_1})^{\alpha_2} c_{\alpha_2 i_2, i_3 \dots i_L}. \tag{B.6}$$

We now decompose the matrix $c_{\alpha_2 i_2, (i_3 \dots i_L)}$:

$$c_{\alpha_2 i_2, i_3 \dots i_L} = \sum_{\alpha_3} U^{[2]}_{\alpha_2 i_2, \alpha_3} S^{[2]}_{\alpha_3, \alpha_3} V^{\dagger [2]}_{\alpha_3, i_3 \dots i_L} \qquad \alpha_3 = 1, \dots \chi_3. \tag{B.7}$$

Again we can define for every i_2 a $\chi_2 \times \chi_3$ matrix $A^{[2]}_{i_2}$ with elements:

$$(A^{[2]}_{i_2})^{\alpha_2 \alpha_3} = U^{[2]}_{\alpha_2 i_2, \alpha_3}. \tag{B.8}$$

and a new $\chi_3 d \times d^{L-3}$ matrix:

$$c_{\alpha_3 i_3, i_4 \dots i_L} = S^{[2]}_{\alpha_3, \alpha_3} V^{\dagger [2]}_{\alpha_3, i_3 \dots i_L} \tag{B.9}$$

so to express (B.6) as:

$$c_{i_1 i_2 \dots i_L} = \sum_{\alpha_2 \alpha_3} (A^{[1]}_{i_1})^{\alpha_2} (A^{[2]}_{i_2})^{\alpha_2 \alpha_3} c_{\alpha_3 i_3, i_4 \dots i_L}. \tag{B.10}$$

It is now clear how to iterate this decomposition until we get a $\chi_L d \times 1$ matrix $c_{\alpha_L i_L}$, which for every i_L gives a column vector $A^{[L]}_{i_L}$ with components:

$$(A^{[L]}_{i_L})^{\alpha_L} = c_{\alpha_L i_L}. \tag{B.11}$$

Eventually $c_{i_1 i_2 \dots i_{L-1} i_L}$ in (B.2) reads:

$$c_{i_1 i_2 \dots i_{L-1} i_L} = \sum_{\alpha_2 \dots \alpha_{L-1}} (A^{[1]}_{i_1})^{\alpha_2} (A^{[2]}_{i_2})^{\alpha_2 \alpha_3} \dots (A^{[L-1]}_{i_{L-1}})^{\alpha_{L-1} \alpha_L} (A^{[L]}_{i_L})^{\alpha_L}, \tag{B.12}$$

or equivalently:

$$c_{i_1 i_2 \dots i_{L-1} i_L} = A^{[1]}_{i_1} A^{[2]}_{i_2} \dots A^{[L-1]}_{i_{L-1}} A^{[L]}_{i_L} \tag{B.13}$$

where the matrix multiplication is understood. Thus the matrices $A^{[k]}_{i_k}$ form the MPS representation of the state $|\psi\rangle$.
Notice that each χ_k is bounded to be $\chi_k \leq \min(d^{k-1}, d^{L-k+1})$, thus the bond dimension χ of the MPS, i.e. $\chi = \max_k \chi_k$, is $\chi \leq d^{\frac{L}{2}}$.

Appendix C

SU(3) symmetry of the biquadratic model

In § 2.1 we mentioned that some points of the bilinear-biquadratic class of Hamiltonians (2.1) (2.27) have a larger SU(3) symmetry. Here we want to explicitly show this for a particular point, the purely biquadratic model (2.12):

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

which correspond to $\beta = \infty$ and $J > 0$ in (2.1) or to $\theta = \frac{\pi}{2}$ in (2.27). Specifically we will show how to map this spin-1 model onto the antiferromagnetic SU(3) Heisenberg model with fundamental and anti-fundamental representations on alternated sites, that is:

$$\bar{H} = J \sum_i \boldsymbol{\lambda}_{2i-1} \cdot \bar{\boldsymbol{\lambda}}_{2i} + J \sum_i \bar{\boldsymbol{\lambda}}_{2i} \cdot \boldsymbol{\lambda}_{2i+1} \tag{C.2}$$

where $\boldsymbol{\lambda}$ ($\bar{\boldsymbol{\lambda}}$) represent the SU(3) "spin" operator, i.e. a vector with the 8 generators of SU(3) in the fundamental (anti-fundamental) representation as components. These generators can be expressed in terms of the Gell-Mann matrices:

$$\begin{aligned}
\lambda^1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \lambda^2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \lambda^3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
\lambda^4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} & \lambda^5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} & \lambda^6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\
\lambda^7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} & \lambda^8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}
\end{aligned} \tag{C.3}$$

where $\boldsymbol{\lambda}^\alpha = \lambda^\alpha$ and $\bar{\boldsymbol{\lambda}}^\alpha = -(\lambda^\alpha)^*$, $\alpha = 1, \ldots, 8$. Having the explicit representation of the generators of SU(3) in terms of the Gell-Mann matrices, it is easy to check that the following commutation and anticommutation relations are

satisfied:

$$\begin{aligned}\left[\lambda^\alpha, \lambda^\beta\right] &= 2if^{\alpha\beta\gamma}\lambda^\gamma \\ \{\lambda^\alpha, \lambda^\beta\} &= \frac{4}{3}\delta^{\alpha\beta}\mathbb{I} + 2d^{\alpha\beta\gamma}\lambda^\gamma\end{aligned} \tag{C.4}$$

where the non-null $f^{\alpha\beta\gamma}$ and $d^{\alpha\beta\gamma}$ are:[1]

$$\begin{aligned}&f^{123} = 1, \quad f^{147} = -f^{156} = f^{246} = f^{257} = f^{345} = -f^{367} = \frac{1}{2}, \quad f^{458} = f^{678} = \frac{\sqrt{3}}{2} \\ &d^{118} = d^{228} = d^{338} = -d^{888} = \frac{1}{3} \\ &d^{146} = d^{157} = -d^{247} = d^{256} = d^{344} = d^{355} = -d^{366} = -d^{377} = \frac{1}{2} \\ &d^{448} = d^{558} = d^{668} = d^{778} = -\frac{1}{2\sqrt{3}}.\end{aligned} \tag{C.5}$$

Now we notice that both the Gell-Mann matrices λ^α and the spin-1 SU(2) spin operators S^α are 3×3 matrices, so we ask ourself if there is a basis in which the spin operators S^α can be expressed in terms of the Gell-Mann matrices λ^α. Indeed a possible choice is:

$$S^x = \lambda^7 \qquad S^y = -\lambda^5 \qquad S^z = \lambda^2. \tag{C.6}$$

and using (C.5) we can see that the SU(2) commutation relations are correctly satisfied:

$$[\lambda^7, (-\lambda^5)] = i\lambda^2 \qquad [(-\lambda^5), \lambda^2] = i\lambda^7 \qquad [\lambda^2, \lambda^7] = -i\lambda^5. \tag{C.7}$$

So now we can explicitly show the correspondence between the SU(2) and SU(3) model.
To begin with we can straightforwardly express the bilinear term as:

$$\mathbf{S}_i \cdot \mathbf{S}_{i+1} = S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z = \lambda_i^7 \lambda_{i+1}^7 + \lambda_i^5 \lambda_{i+1}^5 + \lambda_i^2 \lambda_{i+1}^2. \tag{C.8}$$

We are interested in the biquadratic term, so we have to evaluate the square of the previous expression:

$$\begin{aligned}(\lambda_i^7 \lambda_{i+1}^7 + \lambda_i^5 \lambda_{i+1}^5 + \lambda_i^2 \lambda_{i+1}^2)^2 =& (\lambda_i^7)^2 (\lambda_{i+1}^7)^2 + (\lambda_i^5)^2 (\lambda_{i+1}^5)^2 + (\lambda_i^2)^2 (\lambda_{i+1}^2)^2 \\ &+ \lambda_i^5 \lambda_i^7 \lambda_{i+1}^5 \lambda_{i+1}^7 + \lambda_i^7 \lambda_i^5 \lambda_{i+1}^7 \lambda_{i+1}^5 \\ &+ \lambda_i^5 \lambda_i^2 \lambda_{i+1}^5 \lambda_{i+1}^2 + \lambda_i^2 \lambda_i^5 \lambda_{i+1}^2 \lambda_{i+1}^5 \\ &+ \lambda_i^7 \lambda_i^2 \lambda_{i+1}^7 \lambda_{i+1}^2 + \lambda_i^2 \lambda_i^7 \lambda_{i+1}^2 \lambda_{i+1}^7.\end{aligned} \tag{C.9}$$

[1] all the other non-zero coefficients can be found by permutation of the indices, taking into account that the indices of $f^{\alpha\beta\gamma}$ are completely antisymmetric while the indeces of $d^{\alpha\beta\gamma}$ are symmetric

We can use the anticommutation relation (C.4) to find:

$$\begin{aligned}(\lambda^7)^2 &= \frac{1}{2}\{\lambda^7,\lambda^7\} = \frac{2}{3}\mathbb{I} - \frac{1}{2}\lambda^3 - \frac{1}{2\sqrt{3}}\lambda^8;\\ (\lambda^5)^2 &= \frac{1}{2}\{\lambda^5,\lambda^5\} = \frac{2}{3}\mathbb{I} + \frac{1}{2}\lambda^3 - \frac{1}{2\sqrt{3}}\lambda^8;\\ (\lambda^2)^2 &= \frac{1}{2}\{\lambda^2,\lambda^2\} = \frac{2}{3}\mathbb{I} + \frac{1}{\sqrt{3}}\lambda^8.\end{aligned} \tag{C.10}$$

Thus the first three terms in the right hand side of (C.9) give:

$$(\lambda_i^7)^2(\lambda_{i+1}^7)^2 + (\lambda_i^5)^2(\lambda_{i+1}^5)^2 + (\lambda_i^2)^2(\lambda_{i+1}^2)^2 = \frac{4}{3}\mathbb{I} + \frac{1}{2}\lambda_i^3\lambda_{i+1}^3 + \frac{1}{2}\lambda_i^8\lambda_{i+1}^8. \tag{C.11}$$

If we exploit also the commutation relation (C.4) then we find:

$$\begin{aligned}\lambda^5\lambda^7 &= \frac{1}{2}\{\lambda^5,\lambda^7\} + \frac{1}{2}\left[\lambda^5,\lambda^7\right] = \frac{1}{2}(\lambda^1 + i\lambda^2)\\ \lambda^7\lambda^5 &= \frac{1}{2}\{\lambda^7,\lambda^5\} + \frac{1}{2}\left[\lambda^7,\lambda^5\right] = \frac{1}{2}(\lambda^1 - i\lambda^2)\\ \lambda^5\lambda^2 &= \frac{1}{2}\{\lambda^5,\lambda^2\} + \frac{1}{2}\left[\lambda^5,\lambda^2\right] = \frac{1}{2}(\lambda^6 - i\lambda^7)\\ \lambda^2\lambda^5 &= \frac{1}{2}\{\lambda^2,\lambda^5\} + \frac{1}{2}\left[\lambda^2,\lambda^5\right] = \frac{1}{2}(\lambda^6 + i\lambda^7)\\ \lambda^7\lambda^2 &= \frac{1}{2}\{\lambda^7,\lambda^2\} + \frac{1}{2}\left[\lambda^7,\lambda^2\right] = -\frac{1}{2}(\lambda^4 - i\lambda^5)\\ \lambda^2\lambda^7 &= \frac{1}{2}\{\lambda^2,\lambda^7\} + \frac{1}{2}\left[\lambda^2,\lambda^7\right] = -\frac{1}{2}(\lambda^4 + i\lambda^5).\end{aligned} \tag{C.12}$$

Hence the remaining terms in (C.9) read:

$$\begin{aligned}\lambda_i^5\lambda_i^7\lambda_{i+1}^5\lambda_{i+1}^7 + \lambda_i^7\lambda_i^5\lambda_{i+1}^7\lambda_{i+1}^5 &= \frac{1}{2}\left(\lambda_i^1\lambda_{i+1}^1 - \lambda_i^2\lambda_{i+1}^2\right)\\ \lambda_i^5\lambda_i^2\lambda_{i+1}^5\lambda_{i+1}^2 + \lambda_i^2\lambda_i^5\lambda_{i+1}^2\lambda_{i+1}^5 &= \frac{1}{2}\left(\lambda_i^6\lambda_{i+1}^6 - \lambda_i^7\lambda_{i+1}^7\right)\\ \lambda_i^7\lambda_i^2\lambda_{i+1}^7\lambda_{i+1}^2 + \lambda_i^7\lambda_i^2\lambda_{i+1}^7\lambda_{i+1}^2 &= \frac{1}{2}\left(\lambda_i^4\lambda_{i+1}^4 - \lambda_i^5\lambda_{i+1}^5\right).\end{aligned} \tag{C.13}$$

Then we eventually get:

$$\begin{aligned}(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2 = \frac{4}{3}\mathbb{I} &+ \frac{1}{2}\left(\lambda_i^1\lambda_{i+1}^1 + \lambda_i^3\lambda_{i+1}^3 + \lambda_i^4\lambda_{i+1}^4 + \lambda_i^6\lambda_{i+1}^6 + \lambda_i^8\lambda_{i+1}^8\right)\\ &- \frac{1}{2}\left(\lambda_i^2\lambda_{i+1}^2 + \lambda_i^5\lambda_{i+1}^5 + \lambda_i^7\lambda_{i+1}^7\right).\end{aligned} \tag{C.14}$$

Now we can use the relation $\bar{\lambda^\alpha} = -(\lambda^\alpha)^*$ on the site, for instance, $i+1$ in order to get the final form of the previous expression:

$$(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2 = \frac{4}{3}\mathbb{I} - \frac{1}{2}\boldsymbol{\lambda}_i\cdot\bar{\boldsymbol{\lambda}}_{i+1}. \tag{C.15}$$

Therefore:

$$H_{bq} = -\frac{4}{3}L + \frac{1}{2}\bar{H} \tag{C.16}$$

where L is the length of the chain. It is now clear the equivalence between the two models.
Furthermore from (C.8) and (C.14) it is trivial to show that also the point $\theta = -\frac{\pi}{4}$ in (2.27) has SU(3) symmetry and specifically corresponds to the antiferromagnetic SU(3) Heisenberg model with fundamental representations on every site:

$$\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 = \frac{4}{3}\mathbb{I} + \frac{1}{2}\boldsymbol{\lambda}_i \cdot \boldsymbol{\lambda}_{i+1}. \tag{C.17}$$

Appendix D

Derivation of the O(3) Non-linear Sigma Model from the general $U(N)/U(N-m)\times U(m)$ case

Let us check that when $N=2$ and $\gamma=0$ we get back the O(3) NLσM (1.71) from (4.145). First of all the constants (4.144) becomes:

$$\begin{aligned} g =& \frac{2}{s} \\ v_s =& 2Jsa \\ \theta =& 2\pi s \end{aligned} \tag{D.1}$$

which are exactly the same we found in chapter 1. The components of the matrix $\hat{N}$ are:

$$\hat{N} = \begin{pmatrix} n^z & n^- \\ n^+ & -n^z \end{pmatrix} \tag{D.2}$$

thus

$$\begin{aligned} -\frac{i}{2}\operatorname{Tr}\left[\hat{N}\partial_\tau\hat{N}\partial_x\hat{N}\right] &= -\frac{i}{2}[n^z(\partial_\tau n^-\partial_x n^+ - \partial_\tau n^+\partial_x n^-) \\ &+ n^+(\partial_\tau n^z\partial_x n^- - \partial_\tau n^-\partial_x n^z) \\ &+ n^-(\partial_\tau n^+\partial_x n^z - \partial_\tau n^z\partial_x n^+)] \\ &= -\frac{i}{2}[2in^z(\partial_\tau\mathbf{n}\times\partial_x\mathbf{n})^z \\ &+ in^+(\partial_\tau\mathbf{n}\times\partial_x\mathbf{n})^- \\ &+ in^-(\partial_\tau\mathbf{n}\times\partial_x\mathbf{n})^+] \\ &= \mathbf{n}\cdot\partial_\tau\mathbf{n}\times\partial_x\mathbf{n} \end{aligned} \tag{D.3}$$

where we used the following identities:

$$\begin{aligned} &\mathbf{a}\cdot\mathbf{b} = \frac{1}{2}(a^+b^- + a^-b^+) + a^zb^z; \\ &\mathbf{a}\times\mathbf{b} = i\left[(a^zb^+ - a^+b^z)\mathbf{e}^+ + (a^-b^z - a^zb^-)\mathbf{e}^- + \frac{1}{2}(a^+b^- - a^-b^+)\mathbf{e}^z\right]; \\ &\mathbf{e}^+ = \frac{1}{2}\begin{pmatrix}1 & -i & 0\end{pmatrix} \qquad \mathbf{e}^- = \frac{1}{2}\begin{pmatrix}1 & i & 0\end{pmatrix} \qquad \mathbf{e}^z = \begin{pmatrix}0 & 0 & 1\end{pmatrix}. \end{aligned} \tag{D.4}$$

Similarly for the terms $\mathrm{Tr}\left[(\partial_\alpha \hat{N})^2\right]$, $\alpha = \tau, x$ we find:

$$\frac{1}{2}\,\mathrm{Tr}\Big[(\partial_\alpha \hat{N})^2\Big] = \frac{1}{2}[2(\partial_\alpha n^z)^2 + \partial_\alpha n^+ \partial_\alpha n^- + \partial_\alpha n^+ \partial_\alpha n^-] = (\partial_\alpha \mathbf{n})^2. \qquad \text{(D.5)}$$

Thus we indeed get back the action of the O(3) NLσM (1.71).

Appendix E

Density Matrix Renormalization Group algorithm

In this appendix we want to give a quick review of the Density Matrix Renormalization Group (DMRG) algorithm, introduced in 1992 by Steven R. White [48, 47]. This numerical technique is really efficient in finding the low energy states of one dimensional many-body systems, and gives us the opportunity to better understand the physics behind those systems when analytical methods are not enough or not available. The main problem of many-body systems consists in the exceptionally large dimension of the corresponding Hilbert space $\mathcal{H}$, given that a generic quantum state $|\psi\rangle$ of a spin chain of length L lives in a d^L-dimensional space state, where $d = 2s + 1$ is the dimension of the local state space. Thus the dimension of $\mathcal{H}$ grows exponentially with the length of the system, and the computational cost of any operation which does not take into account any form of approximation becomes impractical very soon. Moreover we recall that we are always more interested in the thermodynamic limit $L \to \infty$ of a system, that is where the exciting physics takes place and many analytical results are rigorously correct. Therefore we need a procedure that provides us an approximate but effective description of a system, which nevertheless recovers all the fundamental physics.

Before we jump into the description of the algorithm it may be worth to explain why it works so well for one-dimensional systems, while it fails in higher dimensions. We want to give here just the idea behind it, without demanding rigorousness and thoroughness, and using some concepts and results of appendix B on MPS and SVD, even though the DMRG method does not need MPS to be defined. Indeed we have shown that any quantum state $|\psi\rangle$ admits a MPS representation that can be found from an iterative application of SVD, and which is characterized by a bond dimension χ. The idea behind the DMRG method, applied to MPS, is to find an approximate representation $|\bar{\psi}\rangle$ for, let us say, the ground state of a system by fixing an upper bound for χ. We recall that χ was given by the highest number of non-zero singular values found during each SVD $\chi = \max_k \chi_k$. This value may not depend on L,[1] giving thus no worries about the exponentially growth

[1] indeed this is what happens for the two states widely used in this thesis, i.e. the AKLT state and the dimer state.

of complexity of the representation, but in general it will depend on L but anyway $\chi \leq d^{\frac{L}{2}}$. In such circumstances an approximation by truncation may be efficient if only a small subset of singular values are considerably different from zero. This is indeed the case if the ground state belongs to a one-dimensional gapped Hamiltonian, where the magnitude of singular values decay exponentially fast [39]. On the other hand higher dimensions systems do not share this special property and DMRG methods become inefficient.

E.1 The algorithm

If we are interested in finding the ground state and the ground state energy of a given Hamiltonian H defined on a finite chain of length L we need to apply two DMRG procedures: first the so-called *infinite-system* DMRG and then the *finite-system* DMRG. The infinite-system DMRG may be independently applied in order to find an approximate solution for systems in the thermodynamic limit, although with not high precision, but it will also serve as a starting point for the finite-system DMRG, thus they have to be both described.

E.1.1 Infinite-system DMRG

To begin with we consider only two finite sub-parts of our one-dimensional chain, that is a so-called *block* $\mathcal{B}_l$ which contain a complete set of m states and have size l, and a single site $\bullet$ which correspondingly is described by d states and has size 1. Normally, in the first iteration of this procedure, the initial block is chosen to be one site of the chain as well, thus in that case $m = d$ and $l = 1$. To the block $\mathcal{B}_l$ and the single site $\bullet$ correspond two Hamiltonians, $H_{\mathcal{B}_l}$ and $H_\bullet$, which are represented respectively by a $m \times m$ and a $d \times d$ matrix, while the interactions between the block and the single site are represented by a $md \times md$ matrix $H_{\mathcal{B}_l \leftrightarrow \bullet}$. Obviously the form of these matrices depends on the original Hamiltonian describing the system.
Now we form a so-called *superblock* adding to the previous block+site ($\mathcal{B}_l \bullet$), also called the *system*, a mirrored copy of itself ($\bullet \mathcal{B}_l^R$), also called the *universe*, thus forming a system block+site+site+block ($\mathcal{B}_l \bullet \bullet \mathcal{B}_l^R$) of size $2l + 2$. If we introduce an interaction term $H_{\bullet \leftrightarrow \bullet}$ between the middle sites then the Hamiltonian of the superblock reads:

$$H_{SB} = H_{\mathcal{B}_l} + H_{\mathcal{B}_l \leftrightarrow \bullet} + H_\bullet + H_{\bullet \leftrightarrow \bullet} + H_\bullet + H_{\bullet \leftrightarrow \mathcal{B}_l^R} + H_{\mathcal{B}_l^R}. \tag{E.1}$$

From the notation of the previous expression it may seem that we are summing matrices with different dimensions, but instead it is tacitly assumed that each term already contains as many copies of the identity operator $\mathbb{I}$ to suitably augment the dimension of the matrices. For instance the first term $H_{\mathcal{B}_l}$, which was defined as a $m \times m$ matrix, is instead redefined as:

$$H_{\mathcal{B}_l} \rightarrow H_{\mathcal{B}_l} \otimes \mathbb{I}_d \otimes \mathbb{I}_d \otimes \mathbb{I}_m \tag{E.2}$$

such that the dimension of $H_{\mathcal{B}_l}$ matches now the required dimension of H_{SB}, that is $m^2d^2 \times m^2d^2$.
The superblock Hamiltonian H_{SB}, stored in memory in sparse form, can now be diagonalized, using different standard methods as Davidson or Lanczos algorithms, in order to find the *target state* $|\psi\rangle$, which in our case is the ground state. This vector lives in a m^2d^2-dimensional state space, and if we introduce two set of $m \cdot d$ complete states $|i\rangle$ and $|j\rangle$ for the system $\mathcal{B}_l \bullet$ and the universe $\bullet\mathcal{B}_l^R$ respectively, then we can express the target state as:

$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle . \tag{E.3}$$

Now it comes into play the approximation procedure of the DMRG, i.e. we want to find a new basis $|u^\alpha\rangle$, which contains at most χ vectors thus $\alpha = 1, \cdots, \chi$, that may substitute the basis $|i\rangle$ for the system $\mathcal{B}_l \bullet$. Obviously this introduce an approximation because if $m < \chi$ then the new basis cannot form a complete set. The new state $|\bar{\psi}\rangle$ reads:

$$\begin{aligned} |\bar{\psi}\rangle &= \sum_{\alpha,j} a_{\alpha j} |u^\alpha\rangle |j\rangle \\ &= \sum_{\alpha=1}^{\chi} a_\alpha |u^\alpha\rangle |v^\alpha\rangle \end{aligned} \tag{E.4}$$

where $|u^\alpha\rangle = \sum_i u_i^\alpha |i\rangle$ and $|v^\alpha\rangle = \sum_j N_\alpha a_{\alpha j} |j\rangle$, with N_α chosen such that $\sum_j \left|v_j^\alpha\right| = 1$. It represents a good approximation for $|\psi\rangle$ if:

$$||\psi\rangle - |\bar{\psi}\rangle|^2 \tag{E.5}$$

is small. In order to understand how to make this difference small we use the SVD for $|\psi\rangle$ to decompose it in a form similar to (E.4). Indeed applying the SVD (see appendix B) to the $md \times md$ matrix ψ_{ij} in (E.2) we get:

$$\begin{aligned} \psi_{ij} = (USV^\dagger)_{ij} &= \sum_{\alpha=1}^{\tilde{\chi}} U_{i,\alpha} S_{\alpha,\alpha} (V^\dagger)_{\alpha,j} \\ &= \sum_{\alpha=1}^{\tilde{\chi}} \lambda_\alpha U_{i,\alpha} (V^\dagger)_{\alpha,j} \end{aligned} \tag{E.6}$$

where $\tilde{\chi} \leq md$ is the Schimdt rank of ψ_{ij} and λ_α are the corresponding non-zero singular values. Thus:

$$|\psi\rangle = \sum_{\alpha=1}^{\tilde{\chi}} \lambda_\alpha |U^\alpha\rangle |V^\alpha\rangle \tag{E.7}$$

where $|U^\alpha\rangle = \sum_i U_{i,\alpha} |i\rangle$ and $|V^\alpha\rangle = \sum_j (V^\dagger)_{\alpha,j} |j\rangle$. It is now clear that an approximation for $|\psi\rangle$ can be easily attained if we discard the smaller singular values λ_α, and moreover we exactly get the state $|\bar{\psi}\rangle$ if we retain only the χ

largest of them, identifying thus:

$$a_\alpha = \lambda_\alpha \qquad |u^\alpha\rangle = |U^\alpha\rangle \qquad |v^\alpha\rangle = |V^\alpha\rangle \qquad \text{for } \alpha = 1, \dots, \chi. \tag{E.8}$$

In order to find the χ largest singular values λ_α and the corresponding states $|u^\alpha\rangle$ we introduce the *density matrix* ρ:

$$\rho = \mathrm{Tr}_U[|\psi\rangle\langle\psi|] = \sum_j \langle j|\psi\rangle\langle\psi|j\rangle = \sum_{ii'}\sum_j \psi^*_{ij}\psi_{i'j}|i\rangle\langle i'|. \tag{E.9}$$

Using (E.6) we find that:

$$\rho = \psi\psi^\dagger = US^2U^\dagger \tag{E.10}$$

thus the square of the singular values λ_α and the states $|u^\alpha\rangle$ are respectively the χ largest eigenvalues and the corresponding eigenvectors of the density matrix ρ.
We have now achieved an effective representation of the system $\mathcal{B}_l \bullet$ in terms of only χ states which we now identify with a new block $\mathcal{B}_{l+1}$ of size $l+1$ and with $m = \chi$. The block Hamiltonian $H_{\mathcal{B}_{l+1}}$ can be found using the $\chi \times md$ matrix O:

$$H_{\mathcal{B}_{l+1}} = OH_{\mathcal{B}_l \bullet}O^\dagger \tag{E.11}$$

where $O_{\alpha,i} = u^\alpha_i$ and:

$$H_{\mathcal{B}_l \bullet} = H_{\mathcal{B}_l} + H_{\mathcal{B}_l \leftrightarrow \bullet} + H_\bullet. \tag{E.12}$$

From this new block $\mathcal{B}_{l+1}$ we can define a new superblock $\mathcal{B}_{l+1} \bullet\bullet \mathcal{B}^R_{l+1}$ of size $2l+4$ and repeat all the previous steps until convergence is reached or, if a finite-system DMRG will follow, until we get a superblock of size L, that is after $L/2 - 1$ steps assuming L even and the starting size of $\mathcal{B}_l$ to be $l = 1$. In the latter case we need also to store in memory each block $\mathcal{B}_l$, from $\mathcal{B}_1$ to $\mathcal{B}_{L/2-1}$, and the corresponding block Hamiltonians $H_{\mathcal{B}_l}$ and interaction terms $H_{\mathcal{B}_l \leftrightarrow \bullet}$.

E.1.2 Finite-system DMRG

As we have already said, the finite-system DMRG needs the first $L/2 - 1$ blocks $\mathcal{B}_l$ of the infinite-system DMRG as a starting point. Moreover the block $\mathcal{B}_{L/2}$ is straightforwardly formed getting together $\mathcal{B}_{L/2-1}$ and a single site $\bullet$. From here we form a new superblock of size L using the block $\mathcal{B}_{L/2}$, two single sites $\bullet\bullet$ and the mirrored block $\mathcal{B}^R_{L/2-2}$: $\mathcal{B}_{L/2} \bullet\bullet \mathcal{B}^R_{L/2-2}$. Following the procedures seen in the previous section we get a new block $\mathcal{B}_{L/2+1}$ of size $l = L/2 + 1$ which we store in memory. We repeat these steps starting always from a superblock of size L of the form $\mathcal{B}_l \bullet\bullet \mathcal{B}_{L-l-2}$, until we get to $\mathcal{B}_{L-3} \bullet\bullet \mathcal{B}_1$. At this point in memory we have $L-3$ blocks, which we are now using for the second iteration of this finite-system DMRG procedure.
In the first step of this second iteration we form the superblock $\mathcal{B}_1 \bullet\bullet \mathcal{B}^R_{L-3}$. Notice that the first block $\mathcal{B}_1$ is know exactly as it corresponds to a single site,

while the mirrored block $\mathcal{B}^R_{L-3}$ is known from the previous iteration. Once again, diagonalizing the Hamiltonian of the system $\mathcal{B}_1\bullet$ we eventually find the block $\mathcal{B}_2$ which we store in memory in place of the previous $\mathcal{B}_2$. We repeat these steps to obtain the new blocks $\mathcal{B}_l$ from $\mathcal{B}_1$ to $\mathcal{B}_{L-3}$. At the end of the second iteration we have a new set of $L-3$ blocks, which we may use for the next one. During the very last iteration we do not replace all the $L-3$ blocks from the previous iteration, but we stop once we have replaced only the blocks from $\mathcal{B}_1$ to $\mathcal{B}_{L/2-1}$. Finally we can use the wave function of the superblock $\mathcal{B}_{L/2-1}\bullet\bullet\mathcal{B}^R_{L/2-1}$ which effectively represents the original system of size L to evaluate its energy, the correlation functions, the non-local order parameters and so on.

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