# Towards quantum glasses

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# TOWARDS QUANTUM GLASSES: DISORDER IN TOPOLOGICAL FRUSTRATED QUANTUM SYSTEMS

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# PREMA KVANTNIM STAKLIMA: NERED U TOPOLOŠKI FRUSTRIRANIM KVANTNIM SUSTAVIMA

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Master Thesis

# Towards quantum glasses: disorder in topological frustrated quantum systems

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*Majci Suzani i ocu Denisu, za sve, jer za išta manje ne bi bilo dovoljno.*

# Prema kvantnim staklima: nered u topološki frustriranim kvantnim sustavima

## Sažetak

Jednodimenzionalni XY model u transverzalnom magnetskom polju predstavlja prototip egzaktno rješivog kvantnog sustava s netrivijalnim faznim dijagramom kojega karakteriziraju dva kvantna fazna prijelaza na temperaturi nula. Koristeći Jordan-Wignerovu transformaciju, ovaj model se uvijek može preslikati u sustav slobodnih fermiona.

U ovom se radu fokusiramo na zatvoreni XY lanac bez vanjskog magnetskog polja i sa neparnim brojem spinova, odnosno sustav koji je podložan frustraciji u slučaju dominantne antiferomagnetske interakcije—nemogućnosti istovremenog minimiziranja globalnog Hamiltonijana i svih lokalnih. Za ovaj sustav je demonstrirano da pokazuje zanimljiva svojstva ovisno o vrijednosti parametra anizotropije $\phi$ koji određuje relativnu magnitudu i predznak interakcija u $x$ i $y$ smjeru. Uz to, ovisno o vrijednosti tog parametra, razlikujemo tri faze u kojima se sustav može naći: uređenu $(1.)$, mezoskopsku $(2.)$ i nesrazmjernu $(3.)$ temeljem dosad pokazanih rezultata.

Nakon pronalaska svojstvenih stanja i spektra modela koristeći JW transformaciju i Bogoljubovljevu rotaciju, okrećemo se računanju korelacijskih funkcija jednog (magnetizacija) i dvaju operatora i to za statički i dinamički vremenski okvir. Dinamički okvir je posljedica globalne promjene parametra $\phi$ u trenutku $t = 0$.

U statičkom režimu $t = 0$, referiramo se na poznate asimptotske rezultate i diskutiramo slaganje s izrazima do kojih smo došli. Nastavno na to, koristeći dinamičke izraze koje smo dobili rješavanjem problema vremenske evolucije za XY model, istražujemo valjanost *principa dekompozicije nakupina* za $6$ evolucija koje počinju u nekoj od prve dvije faze. Dolazimo do nekoliko zanimljivih rezultata, posebno postojanja mezoskopskog ponašanja CD za razmjerno velike brojeve spinova. Konačno, diskutiramo brzine trnjenja DN na temelju fizikalnih argumenata i naglašavamo da je analiza evolucija koje započinju u trećoj fazi zahtjevnija zbog narušenja translacijske invarijantnosti sustava te stoga ostavljena za predstojeći članak.

Ključne riječi: $1$D XY model, degenerirana osnovna stanja, spinski lanac, frustracija, princip dekompozicije nakupina

# Towards quantum glasses: disorder in topological frustrated quantum systems


## Abstract

The one-dimensional XY model in a transverse field is a prototypical exactly solvable quantum system with nontrivial phase diagram, characterised by two different quantum phase transitions, i.e. ones at temperature zero. Using the Jordan-Wigner transformation, the model can always be mapped into a system of free fermions.

In the thesis, we focus on the closed XY chain without external magnetic field and with odd number of spins, conducive to the phenomenon of *frustration* in case of the dominant antiferromagnetic interaction, i.e. the inability of minimising all of the local interactions simultaneously. This system was shown to exhibit interesting properties depending on the value of the anisotropy parameter $\phi$ determining the relative magnitude and sign of the $x$ and $y$ direction interactions. Also depending on this value, we make distinction between three phases, denoted *ordered* $(1)$, *mesoscopic* $(2)$ and *incommensurate* $(3)$ based on the previously obtained results for each.

After solving the XY model for its ground states and spectra via the Jordan-Wigner transformation and Bogoliubov rotation, we focus on calculating the one- and two-point static and dynamic correlation functions after the system has undergone a global quench at $t = 0$, only changing its anisotropy parameter $\phi$. In the $t = 0$ limit, we discuss the agreement of our results with known analytic limiting behaviour. Furthermore, using the dynamic expressions calculated through solving the time-evolution problem for the XY model, we explore the validity of the *cluster decomposition hypothesis* for all evolutions starting in one of the first two phases. In this way, several interesting results are obtained, namely the emergence of mesoscopic behaviour in the long-time regime for several evolutions and also a usual exponential decay of the cluster decomposition for the remaining ones. We discuss the rates of decay and emphasise that the evolutions starting in the third phase require additional subtlety to be analysed properly due to the breaking of translational invariance and are thus left for an upcoming paper.



Keywords: 1D XY model, degenerate ground states, spin chain, frustration, cluster decomposition hypothesis

# Contents

# 1 Introduction and motivation

It is well known that the vast majority of the most striking aspects and results of modern physics lies in the study of complex systems. Their eponymous attribute, while providing a plethora of novel and interesting phenomena, simultaneously represents a substantial difficulty since most of the relevant problems are extremely difficult or even impossible to solve exactly or otherwise. Obviously, this has granted more than enough incentive to physicists and other scientists to develop an enormous toolbox used to attack said phenomena in a variety of ways. Consequences of this progress could hardly be more dramatic, both in the sense of expansion of our collective knowledge, but also in everyday use of technology we can fortunately take for granted in the current era.

One of the most prominent among such advances in course of the previous century is indeed "the creation of quantum mechanics"[1] and despite its somewhat traumatic youth and the inconvenient fact that it is still not fully understood in many respects even today, QM has given birth to several extremely useful frameworks[2] inside which one can analyse different aspects of modern physical systems.

Well established among these frameworks is the quantum many-body theory that allows treating quantum systems with macroscopic number of particles. The fact that this type of treatment is problematic even in classical mechanics renders the formalism that more remarkable.

Let us now motivate the system we will explore with two additional concepts, the first of three being the aforementioned many-body theory.

We start with a question of what is a *quantum phase transition*? Returning to classical physics, we know that the classical phase transitions are determined by their critical temperature and a relevant correlation length that becomes divergent at that critical temperature: arbitrarily little change is still felt throughout the significant portion of the system, corresponding to our everyday intuition as well. How would one go about translating this into the quantum regime? As it turns out, quantum systems exhibit more versatile types of change. First off, the quantum phase transitions are happening at zero temperature[3]—to induce this type of a change, we alter the

[1] One W.K. Heisenberg was awarded a Nobel prize with this lauding description in 1932.

[2] Many-body theory, quantum field theory, renormalisation group, etc.

[3] Shortly, classical phase transitions occur due to thermal fluctuations at finite temperature and quantum ones due to quantum fluctuations at zero temperature.

values of some of the Hamiltonian parameters. We also know empirically that such phase transitions are indeed as exotic as they sound, as per superconductor-insulator transition, Mott insulation, Ising-nematic ordering of the Fermi liquid [1], etc. Mott insulator transition, for example, happens at zero temperature and is not a result of usual energy-entropy competition driving the classical phase transitions, but rather an energy-energy competition that is decided by changing the value of, e.g. lattice interaction strength.

A convenient way to represent such transitions is using a *phase diagram*, i.e. a set of curves in the space of dimension corresponding to number of the parameters of the Hamiltonian that are able to change. For example, standard example in the classical physics is the phase diagram of water, dependent on temperature, volume and pressure. As we have stated, quantum phase transitions occur at zero temperature and thus coordinates in the phase diagram will be the parameters of the Hamiltonian, instead of, e.g. temperature.

As a third point, let us consider an important concept deeply rooted in our present work and the works we will be referencing, i.e. the phenomenon of *frustration*, final part of our picture.

Informally, frustration[4] corresponds to the inability of simultaneous minimisation of the global Hamiltonian and all the local ones, usually due to competing interactions. Classic example of frustration is a system of three spins arranged in a $2$D triangular configuration and antiferromagnetic interaction between each pair, as depicted in Figure 1.1. Wishing to minimise the total energy of the system, one could choose any of the two spins to be antiparallel so their local interaction is minimal, so let us choose spins $1$ and $2$, as in said figure. It is easy to see that this corresponds to the global minimum as well, regardless of the third spin. However, since the two spins are opposite, one of them will be parallel to the third spin (in our case spin $1$ is parallel to spin $3$) and thus their interaction will not be minimal, i.e. global energy minimum does not correspond to sum of the local minima. Based on this discussion, one can immediately see that the spin chain in our model is frustrated for every odd $N > 1$, i.e. if we start from arbitrary spin and align every subsequent spin by alternating between up and down direction, we see that when we arrive to the final

[4]To begin our short discussion on frustrations, we note that an enormous body of work has been done on them and instruct the reader to consult the relevant literature [2–8].

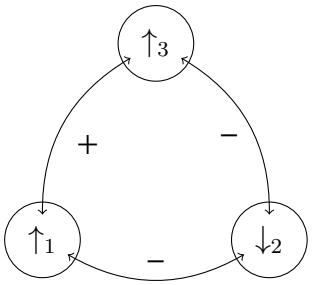



Figure 1.1: Frustrated system of three spins in triangular 2D configuration. There is no way of orienting the spins so that all of the local interactions are minimal.

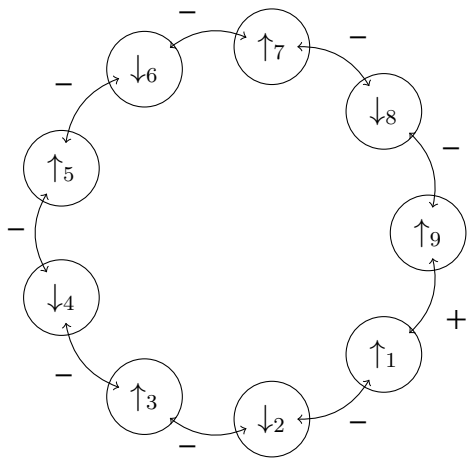



Figure 1.2: Frustrated system of nine spins in 2D configuration. There is no way of orienting the spins so that all of the local interactions are minimal, however we note that the amount of frustration is constant, i.e. there is only one nonminimal interaction regardless of the number of spins, as long as it is odd.

interaction, it ought to be between the aligned spins, i.e. not a minimum, as can be seen in the Figure 1.2. We also notice that, regardless of the system size for odd spin number, this effect remains only between two spins (one interaction) and thus corresponds to *weak* (nonextensive) *frustration*.

Classically, we note that the nonminimised interaction can be placed between any two spins and thus the system is $2N$ degenerate, where $N$ is the spins number. Since the system is doubly degenerate for even $N$ (order the spins as we have described above to get the first ground state, then flip them all for the second), we see that for large $N$, i.e. thermodynamic limit, there is a massive increase/decrease in degeneracy as one adds one by one spin to the chain, i.e. the frustration effect is generally of *nonperturbative* nature.

We now wish to connect the three concepts we have introduced: many-body theory, (nontrivial) quantum phase diagram and frustration. To this end, let us present the *XY model* for the spin chain of length $N$, i.e. a generalisation of the 1D quantum

Ising model with additional interaction along the axis (say $y$) orthogonal to the one in Ising model (say $x$) and with the magnetic field along the third direction (say $z$). First off, this model is in general given by the Hamiltonian that is elementary enough to be exactly solvable using the many-body formalism, i.e. it permits a straightforward diagonalisation. Second, despite its apparent simplicity, this model admits a highly nontrivial quantum phase diagram[5]. Precisely, if we write its Hamiltonian in terms of three parameters[6]: interaction strength $J$, anisotropy parameter $\gamma$ and magnetic field $h$:

$$H = \frac{J}{2}\sum_{j=1}^{N}\left[\left(\frac{1+\gamma}{2}\right)\sigma_j^x\sigma_{j+1}^x + \left(\frac{1-\gamma}{2}\right)\sigma_j^y\sigma_{j+1}^y + h\sigma_j^z\right] , \tag{1.1}$$

with $\sigma^\mu$, $\mu \in x, y, z$ customarily denoting the Pauli matrices. Also note that the sum is over all the spin sites in the system. Setting $J = -1$, one notices that the Hamiltonian is symmetric under the exchange $\gamma \rightsquigarrow -\gamma$ since this leads to the exchange $x \leftrightarrow y$ and exchange $h \rightsquigarrow -h$ corresponds to reflecting all of the spins with respect to the $xy$ plane. Thus, for the phase diagram in the $(\gamma, h)$ space we can only focus on the upper right quadrant $\gamma, h \geq 0$ since the other three are related by symmetries. Phase diagram of the XY model is given in Figure 1.3. We note that the two wavy lines represent the critical segments and that the quantum phase transitions correspond to crossing them. First one is at $\gamma = 0$. Upon crossing this line, one can see that the terms in Hamiltonian (1.1) change their relative magnitude, while keeping their signs. In this way, the dominant interaction changes and thus the (non)vanishing order parameter[7] switches from $x$ to $y$ and viceversa for another direction of crossing. On the other hand, when crossing the $h = 1$ line, one crosses between the phase in which the ground state is nondegenerate and the one in which it is doubly degenerate (particularly, it is doubly degenerate for $h < 1$).

The phase diagram of the XY model is not directly relevant to our present work, but due to its importance the author not only decided to include its extremely short description, but also boldly state that every physicist should at least once take a

[5]It is arguably the simplest model to exhibit two quantum phase transitions.

[6]We will soon introduce another notation and remove two of the parameters since that will be the model of interest to us, however for completeness and historical reasons [9] we present the basic properties of the general XY model as well.

[7]This order parameter is magnetisation in, e.g. $x$ direction defined as an expectation value of the $\sigma^x$ operator in the ground state.

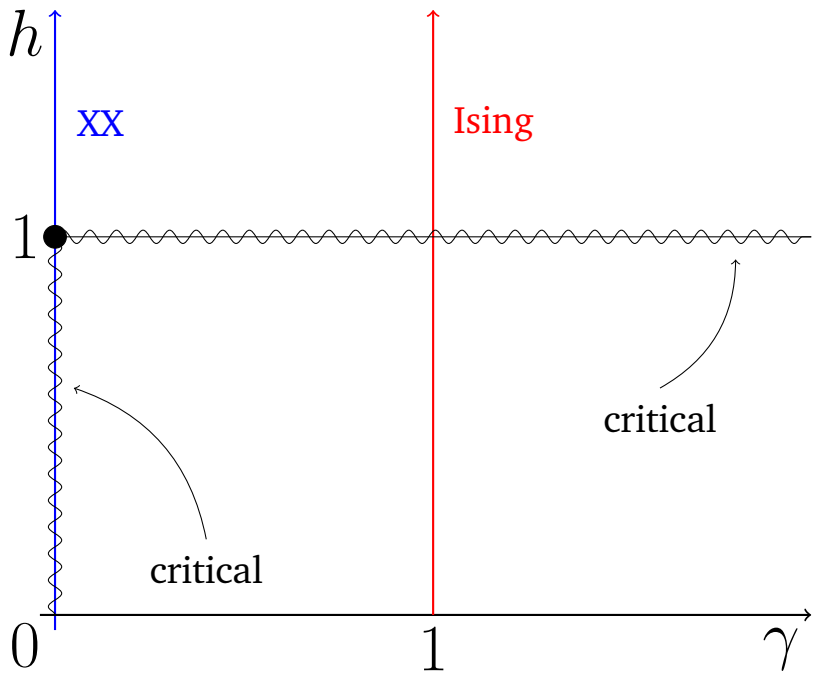



Figure 1.3: Phase diagram for the XY model in magnetic field $h$ and with anisotropy parameter $\gamma$. There are two critical segments denoted by the wavy lines, i.e. the one at $\gamma = 0$ and the other at $h = 1$. The point $(\gamma, h) = (0, 1)$ at which the two critical segments intersect is called the bi-critical point. Furthermore, we see that for $\gamma = 0$ the model reduces to the 1D XX model (blue line) and for $\gamma = 1$ the regular quantum Ising model (red line).

detailed look into its derivation and consequences, for education both in physics and history.

Since we have discussed the nontriviality of the XY model phase diagram, we move to the third point, i.e. the connection between the XY model and frustration. To this end, we will introduce another form of the Hamiltonian (1.1) by making two changes. Anisotropy parameter $\gamma$ will be replaced by the anisotropy parameter $\phi$ that will take range of angular variable. In this way, we can keep track only of the relative signs and magnitudes of the $x$ and $y$ direction interaction since this will be the only data of importance. Furthermore, the magnetic field $h$ is set to zero. Thus, the Hamiltonian in this convenient form becomes:

$$H = \sum_{j=1}^{N} \left[ \cos\phi \; \sigma_j^x \sigma_{j+1}^x + \sin\phi \; \sigma_j^y \sigma_{j+1}^y \right] \quad , \tag{1.2}$$

where $\sigma$ operators again evidently denote the Pauli matrices for spin operators and the anisotropy is provided by the parameter $\phi$. As announced, since there is no global constant in the Hamiltonian, we can see that only the relative sign and magnitude of

the two interactions will be of interest. Also note that, had we retained the magnetic field in $z$ direction, choosing $\phi = \pi/4$ or $\phi = 3\pi/4$ would reduce $H$ to the XX model and choosing $\phi = k\pi/2$ for $k \in \{0, 1, 2, 3\}$ to the Ising model. One should note the correspondence with particular values of $\gamma$ in Figure 1.3 in these limits. To further connect this new notation with the phase diagram in Figure 1.3, we note that crossing $\phi = \pi/4$ or $\phi = 3\pi/4$ will serve the same purpose as crossing the $\gamma = 0$ line, i.e. it will keep the signs of the interactions, while taking their relative magnitude across the value $1$.

Further still, it is easily seen from (1.2) that shifting[8] $\phi$ by $\pi/2$ interchanges $x$ and $y$ interactions and based on this and the periodicity of the parameter, we conclude that it is sufficient to restrict oneself to one half of the unit circle. This is what we will indeed do and consequently distinguish between three different phases of our system:

- The first phase, in which $\phi \in \langle -3\pi/4, -\pi/4\rangle$ we demarcate as the *ordered phase* based on the magnetisation along the $y$ axis for periodic boundary conditions and odd number of spin sites [10].

- The second one, in which $\phi \in \langle -\pi/4, 0\rangle$ we denote as the *mesoscopic phase* since in it appears an algebraically decaying ferromagnetic magnetisation in $x$ direction[9], again for the periodic boundary conditions and odd site number [10].

- Finally, the third phase, i.e. $\phi \in \langle 0, \pi/4\rangle$ we name *incommensurate phase* after the novel type of antiferromagnetic order was observed (again for periodic boundary conditions and odd spin number); one that spontaneously breaks translational invariance and is modulated in an incommensurate way [11].

For the three phases we will occasionally use the abbreviations $1$O, $2$M and $3$I, respectively.

From their short descriptions, one can immediately see that in each of the phases it was emphasised that the spin system has periodic boundary conditions, i.e. it corresponds to a closed chain and also that the number of spins in the chain was odd.

[8] One should convince oneself that this is equivalent to the exchange $\gamma \rightsquigarrow -\gamma$.

[9] Since the interaction in $x$ direction is antiferromagnetic, one would expect for magnetisation to be staggered.

As one can recall from our discussion complementary to Figure 1.2, these conditions correspond to the spin chain with frustrated boundary conditions. We underline the fact that, as was explained in detail in previous works [10–12], there are several layers in which the frustrated boundary conditions and the type of interaction affect the system properties. In the first phase, the system displays what we termed the frustrated boundary conditions, but since the interaction is ferromagnetic, the system is not frustrated since there are no competing dominant antiferromagnetic interactions[10]. However, the odd number of spins is necessary since in that case there is degeneracy and thus a nonvanishing order parameter. In the case of even spin number, the ground state would not be degenerate and thus said order parameter would have nonvanishing value only in the thermodynamic limit in which the ground states coincide. Thus, we will ocassionally refer to this phase as the *unfrustrated phase*. On the contrary, in the third and the second phase the frustration is absolutely essential to emergence of the interesting phenomena we pointed out. Opening the chain (so it does not exhibit periodic boundary conditions), considering the chain with even number of spins or switching the dominant interaction from antiferromagnetic to ferromagnetic eradicates these behaviours.

Also, introducing some terminology, requirement of odd spin number and the periodicity of the chain can be condensed into one term—*frustrated boundary conditions*.

Thus, a nontrivial phase diagram, along with its exact solvability[11] and its remarkable behaviour under frustrated boundary conditions render the one-dimensional[12] XY model[13] a pertinent one, both in terms of its educational relevance and research applicability [10, 13–15].

Having introduced the frustration and the three distinct phases, we emphasise that it will be of great importance for us to be able calculate one- and two-point correlation functions. However, one-point correlations are difficult to access directly, mainly due to the fact that our diagonalisation process will separate the Hamiltonian

[10]Recall that our toy model in Figure 1.2 assumed the antiferromagnetic interaction between adjacents spins.

[11]In general, XY model with interaction strength, anisotropy parameter and magnetic field is exactly solvable when at least one of the three parameters is equal to zero.

[12]A somewhat more general advantage of considering 1D systems is, besides a wide range of exact results, the fact that many methods, especially powerful approximate ones have been developed for these systems and have been well understood for decades.

[13]Of course, as previously stated and quantified in (1.2), the magnetic field in our work will henceforth be set to zero.

into two distinct terms, each one with different parity along the $z$ direction[14] and thus the ground states of the system obtained by our solving procedure have definite parity along the $z$-axis and are mutually orthogonal. This in turn means that the expectation values of $\sigma^x$ and $\sigma^y$ necessarily vanish[15] in those states since their action changes the $z$-parity of the ground state.

However, since the Hamiltonian is degenerate in all three phases, there is a way to construct the states with definite $x$ and $y$ parities as well [10, 11]. Using this idea, one can obtain the expectation values of interest directly and this is indeed what we will do in present work.

One way of trying to circumvent the aforementioned difficulty is using the *cluster decomposition hypothesis* (CDH in the following), i.e. the idea that:

$$\lim_{r\to\infty}\left[\left\langle\sigma_j^\mu\sigma_{j+r}^\mu\right\rangle-\left\langle\sigma_j^\mu\right\rangle\left\langle\sigma_{j+r}^\mu\right\rangle\right]=0\,, \tag{1.3}$$

with $\mu$ denoting the direction ($x$, $y$, or $z$). Essentially, it conjectures that the two-point correlations between different sites can be evaluated as independent expectation values in the limit of their diverging distance. In this context, divergence implies that the two sites are separated as far as possible, i.e. that they are at antipodal points in the closed spin chain of diverging total length. In addition, there is subtlety in this behaviour since it is also interesting to see what type of approach of the two terms in $(1.3)$ is and thus at which values of the chain lengths does it start to be a reasonable approximation.

First problem with the CDH is the fact that the proper procedure of taking the limit is not always immediately evident. For example, let us denote the separation of the two sites in question by $r$, as in (1.3) and the (odd) number of spins by $N$. Then the expressions such as $r/N$ can be evaluated in two ways[16]. One could either take the limit of diverging $N$ first, in which case the expression tends to zero, or one could take $r$ to be the distance between antipodal sites, i.e. $r=(N\pm1)/2$, and in this case one is left with a leading term of $1/N$. In previous works [10], this difference has been shown to yield differing results for magnetisation in certain direction and it thus

[14]Parity operators will be defined later; they correspond to products of spin matrices of certain direction over all the spin sites in the system.

[15]To play the role of an order parameter, i.e. to signal the rise of a macroscopic order, an operator must violate at least one of the symmetries system of the system.

[16]This ambiguity emerges when there is an algebraic decay of correlation functions and not for an exponential one [15].

implies a certain ambiguity in the CDH approach. Therefore, it is of great use to be able to access said magnetisations directly. Besides this, there is no general proof for the CDH at the time of writing of this thesis, although it has been shown that it holds in static conditions for gapless systems [16], as was found in previous work [10] and also confirmed by our analysis at $t = 0$.

Regarding the present work and its objective, we wish to generalise these results to the case of dynamically evolving XY model (specifically after a global quench[17] at $t = 0$) and explore the validity of the CDH. Furthermore, not only will we be considering its behaviour inside different time regimes and for thermodynamic limit of diverging spin chain length, but also the functional dependence of its decay, i.e. how fast do the terms converge to their limiting values with increasing chain length.

First we discuss the dependence of CDH on the number of spin sites in the static case, i.e. at $t = 0$ and show that it corresponds to previous results [10]. After this, we consider two regimes of the time evolution of the CDH, specifically very short and very long times. In this way, we obtain enough points for the long time regime and average them out to check the CDH at long times as a function of the number of spin sites. In each case, the two spin sites we consider correspond to antipodal points in the chain, i.e. $1$ and $r = (N + 1)/2$. We also note that in the first two phases, one can take any two sites, as long as they are antipodal, but in the third, these expression depend on the site choice, i.e. translational invariance does not hold anymore, as will be seen from analytic expressions. This is one of the reasons why only the evolutions starting in first two phases were considered in the present work, although we note that there is no such problem when evolving *into* the third phase, as will be discussed in Chapter $4$[18].

This succinctly described process is actually carried out in several steps. We begin by solving the XY model in Chapter $2$ by means of the Jordan-Wigner transformation, followed by a Fourier transform into the momentum space and finishing with diagonalisation using the Bogoliubov rotation. In Chapter $3$, we calculate the static (for pedagogical purposes) and dynamic two-point correlation functions for all three

[17] Quench of a system is usually defined as an instant change of some of the Hamiltonian parameters [17, 18]. We focus on changing the parameter $\phi$ and we do so globally, i.e. the interaction remains uniform along the chain. In this way, as discussed in the section on symmetry properties of the model, the system retains all of its initial symmetries and thus the form of the spectrum and similar properties as well.

[18] Discussion of evolutions starting in the third phase requires additional subtlety and is thus left for an upcoming paper.

spatial directions and phases, corresponding to the first term in (1.3). For the second term in this expression, we turn to calculating the dynamic magnetisations, i.e. one-point expectation values and emphasise the use of the ground states with well-defined parities along each spatial direction; this is done in Chapter $4$. Finally, in Chapter $5$ all of the results are discussed in a systematic way.

We also note that several appendices are referenced at natural points throughout the calculations and discussions, each included either to facilitate intuitive understanding of the methodology and physics of the process or as an overview of additional results that would unnecessarily clutter the body of the thesis.

In the end, besides reiterating the importance of the problem we are considering based on the presence of CDH in general use, we remark that the spin chains such as the ones we consider can be designed and realised experimentally as well. This is due to the rapid development of experimental techniques in recent times, especially manipulation of cold atoms [19] which introduce the possibility of constructing essentially arbitrary spatial configuration and interaction between the spins.

# 2 Solving the XY model

## *2.1 Introduction*

The first solution to the XY model was presented by Lieb, Schultz and Mattis in 1961 [9] with the aim of investigating the effect of anisotropy in the Heisenberg model, i.e. the one in which the strength of interaction is not necessarily the same in the $x$ and $y$ direction, also with the $z$ axis interaction omitted. This was later expanded by Barouch and McCoy in series of seminal papers on the general statistical properties and associated quantities of interest (most notably spin correlation functions and magnetisations) for the XY model [20] with external magnetic field in the transverse direction which is set to zero in our analysis. Besides this, other quantities such as nonelementary correlators, entropies and out-of-equilibrium properties were obtained as well [21–24], although these are not directly relevant to our present work.

Rough outline of our approach to solving the XY model will be to use the Jordan–Wigner transformation to turn the spin system into a fermionic one and after a Fourier transform, use Bogolioubov rotation to diagonalise it. During this approach, we mostly follow [13]. But before solving the model, we provide a detailed look into the symmetry properties of the model so that the steps in solving it can be appreciated in full.

## *2.2 Symmetry properties of the XY model*

As announced, we begin our analysis by discussing the importance of symmetry in the XY model.

To do so, we reiterate the corresponding Hamiltonian (1.2):

$$H = \sum_{j=1}^{N} \left[ \cos\phi \; \sigma_j^x \sigma_{j+1}^x + \sin\phi \; \sigma_j^y \sigma_{j+1}^y \right] \quad , \tag{2.1}$$

with $\phi$ denoting relative strength and sign of interactions in the $x$ and $y$ directions, the only information regarding interaction of interest to present work. This was the case in some of the previous papers as well [10, 11], since both the destruction of local order and occurence of phase transitions were consequences of said relative

strength and sign. Furthermore, variable $j$ runs over spin sites, the total number of which is $N$.

First obvious symmetry of the system is the invariance under spatial translations if we choose to work with the closed spin chain[19], meaning that the spins at sites $j = 1$ and $j = N$ are adjacent. We choose the basis of the $N$-spin Hilbert space to consist of kets of the form:

$$|\psi\rangle = \bigotimes_{j=1}^{N} \left(\sigma_j^-\right)^{n_j} |\uparrow_j\rangle \quad , \tag{2.2}$$

with $|\uparrow_j\rangle$ defined to acquire a vain $+1$ factor when acted upon with $\sigma_j^z$ and $n_1, n_2, ..., n_N$ taking values of either $0$ or $1$. The raising and lowering operators are defined as usual:

$$\sigma_j^{\pm} = \frac{1}{2}\left[\sigma_j^x \pm \imath\sigma_j^y\right] \quad . \tag{2.3}$$

The *translation operator* $T$ can then be introduced in a natural way:

$$T\,|\psi\rangle = \bigotimes_{j=1}^{N} \left(\sigma_j^-\right)^{n_{j+1}} |\uparrow_j\rangle \quad , \tag{2.4}$$

with identification for the closed chain $n_{N+j} \equiv n_j$. First important property of this operator is unitarity, which is evident from its defining relation since $\langle T^\dagger T\rangle = 1$ holds for all the basis vectors and hence for all the vectors in the Hilbert space:

$$T^\dagger T = \mathbb{1} \ , \tag{2.5}$$

which can also be interpreted as the operator $T^\dagger$ providing translation in the opposite direction of that of operator $T$. Furthermore, since there are $N$ spins in the chain, it is evident that $N$ successive applications of the translation operator should leave the system invariant (idempotence of order $N$), i.e.:

$$T^N = \mathbb{1} \ , \tag{2.6}$$

from which it is immediately seen that its eigenvalues are the $N$-th roots of unity, i.e.

[19] We will indeed choose to do so since, as was announced in the Introduction, the closed spin chains with odd $N$ exhibits *frustration*.

$e^{\imath q}$ with

$$q \in \left\{ -\frac{N-1}{N}\pi,\ ...,\ -\frac{2}{N}\pi,\ 0,\ \frac{2}{N}\pi,\ ...,\ \frac{N-1}{N}\pi \right\} \ . \tag{2.7}$$

To mathematically state the translational invariance of the system, we write the spin operators as external products of the basis states to immediately observe that they are translated by action of $T$ and its inverse:

$$T^\dagger \sigma_j^\mu T = \sigma_{j+1}^\mu \ , \quad \mu = x, y, z \ , \tag{2.8}$$

where $\sigma_{N+j}^\mu = \sigma_j^\mu$ as before. Now it is seen that the translation operator commutes with the Hamiltonian of the system (1.2):

$$\big[T, H\big] = 0 \ , \tag{2.9}$$

which is the formal formulation of its translational invariance.

We proceed by defining the *parity operator* along the $z$ axis

$$\Pi^z \coloneqq \bigotimes_{j=1}^{N} \Big(1 - 2c_j^\dagger c_j\Big) = \bigotimes_{j=1}^{N} \sigma_j^z \ . \tag{2.10}$$

To make sense of its name, observe that it represents the product of all the spin orientations along the $z$ axis in the system at hand and it is therefore equal to $-1$ when the number of down spins (along the $z$ axis) is odd and $+1$ otherwise.

From (2.8) we see that, exploiting (2.5) repeatedly, the translation operator commutes with the parity operator along the $z$ axis as well. Furthermore, since the former relation is valid for all three axes, we conclude that it will commute with the parity operators along all three spatial directions:

$$\big[T, \Pi^\mu\big] = 0 \ , \quad \mu = x, y, z \ , \tag{2.11}$$

with the *parity operator* along the axis $\mu$ defined as expected:

$$\Pi^\mu \coloneqq \bigotimes_{j=1}^{N} \sigma_j^\mu \ . \tag{2.12}$$

The parity operators along all three spatial axes commute with the Hamiltonian

(1.2) as well:

$$\left[\Pi^{\mu}, H\right] = 0 \ , \quad \mu = x, y, z \ . \tag{2.13}$$

This is seen easily from (anti)commutation relations for Pauli matrices, i.e.:

$$\left[\sigma_j^{\mu}, \sigma_j^{\nu}\right] = 2\imath\epsilon^{\mu\nu\rho}\sigma_j^{\rho} \ \text{ and } \ \left\{\sigma_j^{\mu}, \sigma_j^{\nu}\right\} = 2\delta^{\mu\nu}\mathbb{1} \ . \tag{2.14}$$

Intuitively, each term in Hamiltonian flips (up to a factor) two spins at a time, thus preserving the parity.

We remark that (2.13) would cease to be valid along certain axes upon introducing, e.g. the magnetic field along said axes. Models of this kind are analysed in works such as [20].

Another relevant property of the parity operators are their mutual (anti)commutation relations which rely on the fact that the number of spins in the chain $N$ is odd, i.e. that the system displays the frustrated boundary conditions. First note that for equal $\mu$ and $\nu$ it holds that

$$\mu = \nu : \quad \{\Pi^{\mu}, \Pi^{\nu}\} = 2\left(\bigotimes_{j=1}^{N}\sigma_j^{\mu}\right)^2 = 2 \tag{2.15}$$

and

$$\mu = \nu : \quad [\Pi^{\mu}, \Pi^{\nu}] = 0 \tag{2.16}$$

since squares of Pauli matrices are equal to unity and also the operators on different sites commute since they belong to different Hilbert spaces. Furthermore, for $\mu$ and $\nu$ different we obtain:

$$\begin{aligned} \mu \neq \nu : \quad \{\Pi^{\mu}, \Pi^{\nu}\} &= \left(\bigotimes_{j=1}^{N}\sigma_j^{\mu}\right) \otimes \left(\bigotimes_{j=1}^{N}\sigma_j^{\nu}\right) + \left(\bigotimes_{j=1}^{N}\sigma_j^{\nu}\right) \otimes \left(\bigotimes_{j=1}^{N}\sigma_j^{\mu}\right) \\ &= (\sigma_1^{\mu}\sigma_1^{\nu}) \cdots (\sigma_N^{\mu}\sigma_N^{\nu}) + (\sigma_1^{\nu}\sigma_1^{\mu}) \cdots (\sigma_N^{\nu}\sigma_N^{\mu}) \\ &= \left[1 + (-1)^N\right] (\sigma_1^{\mu}\sigma_1^{\nu}) \cdots (\sigma_N^{\mu}\sigma_N^{\nu}) \\ &= 0 \ , \end{aligned} \tag{2.17}$$

where we have exchanged the $\mu$ and $\nu$ operators in the second row to get to the third one, with each exchange introducing a factor of $-1$. To obtain the final row, we have used the fact that the number of spins $N$ is odd.

We can obtain the final commutation relation in a similar manner if we use the previous calculation with the $-$ sign in the square brackets to obtain:

$$\begin{aligned}\mu \neq \nu: \quad [\Pi^\mu, \Pi^\nu] =& 2\left(\sigma_1^\mu \sigma_1^\nu\right) \cdots \left(\sigma_N^\mu \sigma_N^\nu\right) \\ =& \{\text{use the relation: } \sigma^\mu \sigma^\nu = \delta_{\mu,\nu} \mathbb{1} + \imath \epsilon_{\mu\nu\rho} \sigma^\rho\} \\ =& 2\left(\epsilon_{\mu\nu\rho}\right)^N \imath^N \left(\sigma_1^\rho \cdots \sigma_N^\rho\right) \\ =& 2\imath\epsilon_{\mu\nu\rho} \left(-1\right)^{\frac{N-1}{2}} \Pi^\rho \ ,\end{aligned} \tag{2.18}$$

where we have used the property of Levi-Civita symbol $\epsilon^N = \epsilon$ since it only takes on values of $\pm 1$ and $0$ and the fact that $N$ is odd, i.e. of form $N = 2k+1,\ k \in \mathbb{Z}$ for the penultimate row. The final row is obtained by recognising the definition of the parity operator (7.5).

All of the (anti)commutation relations can now be condensed in the following two relations:

$$\{\Pi^\mu, \Pi^\nu\} = 2\delta_{\mu,\nu} \tag{2.19}$$

and

$$[\Pi^\mu, \Pi^\nu] = 2\imath\epsilon_{\mu\nu\rho} \left(-1\right)^{\frac{N-1}{2}} \Pi^\rho \ , \tag{2.20}$$

with $\mu, \nu, \rho = x, y, z$.

The fact that the different parity operators commute with the Hamiltonian of the system, but not with each other implies the existence of degeneracies. This is a known quantum mechanical result [25] and also easily seen since a generic eigenstate of the Hamiltonian and the same state when acted upon with, e.g. $\Pi^x$ will have different parities along the $z$ axis, but the same energy, implying the existence of at least twofold degeneracy. We will discuss the importance of this degeneracy in a moment.

Furthermore, we see that, because of the degeneracy and the fact that parity operators commute with the Hamiltonian, one can in general construct a linear combination of the states that will be eigenstate of the Hamiltonian, but not of the parity operator along the $z$ axis[20]. Thus, we see that the initial[21] $\mathbb{Z}_2$ symmetry is broken.

Another relevant symmetry of the system is upon mirror imaging with respect to

[20] Indeed, we will construct such states.

[21] This symmetry corresponds to the model being invariant under flipping of all the spins, as can easily be seen from its Hamiltonian since the spin products come in pairs.

arbitrary spin site. If we consider again a spin chain with $N$ sites for odd $N$, we can see that the mirroring of the $j$th site with respect to the $k$th site is obtained[22] by the transformation $j \rightsquigarrow 2k-j$. Using this fact, we can write the defining equation for the *mirror operator* with respect to the $k$th site $M_k$ through its action on the basis kets (2.2)

$$M_j \left|\psi\right\rangle = \bigotimes_{l=1}^{N} \left(\sigma_l^-\right)^{n_{2j-l}} \left|\uparrow_l\right\rangle \ . \tag{2.21}$$

As with the translation operator, we deduce the unitarity of the mirror operator:

$$M_j^\dagger M_j = \mathbb{1} \ , \quad \forall j \tag{2.22}$$

and the idempotence of order $2$ since applying the mirroring an even amount of times leaves the system invariant:

$$M_j^2 = \mathbb{1} \ , \quad \forall j \ , \tag{2.23}$$

implying that its only eigenvalues are $\pm 1$. Along this, from the previous two equations it is seen that the mirror operator $M_j$ is Hermitian as well, i.e.:

$$M_j^\dagger = M_j \ . \tag{2.24}$$

Mirror operators on different spin sites are related by the translation operator:

$$T^\dagger M_j T = M_{j+1} \ , \quad \forall j \ , \tag{2.25}$$

as is seen in a manner analogous to (2.8). This last equation allows us to express the mirror operators with respect to all the sites if only one of them is known. We will exploit this fact in the end of this chapter to prove a convenient result for mirror operator action on ground states of the system.

Finally, we note that the mirror operator obviously does not change the parity of the system along any direction since it only permutes the sites and the parity is given by their product, which is a commutative operation:

$$\left[M_j, \Pi^\mu\right] = 0 \ , \ \mu = x, y, z \ . \tag{2.26}$$

[22] If $j < k$ we can interpret this transformation as first going to the $k$th site which is the center of reflection and then subsequent $k-j$ steps from it, i.e. at the same distance at which the $j$th site was before, only in the opposite direction. For $j > k$ the line of reasoning is similar.

Having finished the discussion on mirror and translation operators, we return shortly to the parity operators to emphasise one additional point which we will rely on regularly in the following chapters. This is related to the fact that the ground states of the system always come in pairs, at least one for each parity. However, there is a more transparent (and somewhat obvious) way of deducing this fact. As per (2.13), we know that the Hamiltonian commutes with the parity operators along all three axes. Howewer, by (2.19), as we have discussed, the parity operators mutually anticommute and this implies the existence of degenerate eigenstates. Then, taking into account that, e.g. the parity operator $\Pi^x$ commutes with the Hamiltonian as well, a certain eigenstate of the Hamiltonian will remain an eigenstate when acted upon by $\Pi^x$ (or $\Pi^y$). However, because the number of spins in the chains we will consider $N$ is odd, $\Pi^{x,y}$ will change their $z$ parity, as is seen through an elementary action of Pauli matrices for $x$ and $y$ directions on the eigenstates of the $z$ parity operator. It will turn out that it is of great convenience to use only the state from one sector and express the other one as the first, but acted upon by one of these parity operators since we will be able to relatively easily write the parity operators in terms of string of operators whose expectation values are analytically calculable. Also, since construction of the states with definite parities in the directions other than $z$ allows us to access certain quantities of interest directly as was demonstrated in [10] and [11], we have also obtained a way of checking whether or not the cluster decomposition hypothesis is valid in the dynamic case. To this end, we will use the fact that the generator of time evolution, the Hamiltonian, commutes with the parity operators, thus allowing us to carry out calculations in a way that is analogous to the static case. This will also imply that the Hamiltonian retains its original symmetries during its time evolution.

## 2.3 Jordan–Wigner transformation

After discussion on general symmetry properties, we turn to solving the XY model. As was announced in the introduction to this chapter, the first step is the so called Jordan–Wigner transformation which will emerge naturally as an amendment to a naive approach to diagonalisation of the Hamiltonian (1.2).

Upon inserting the raising and lowering operators (2.3) into (1.2), we use the following relation:

$$\sigma_j^x \sigma_{j+1}^x = \left(\sigma_j^+ + \sigma_j^-\right)\left(\sigma_{j+1}^+ + \sigma_{j+1}^-\right) = \sigma_j^+\sigma_{j+1}^+ + \sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+ + \sigma_j^-\sigma_{j+1}^- \tag{2.27}$$

and also an analogous one for the $y$ direction, along with trigonometric relations

$$\begin{aligned} \cos\phi + \sin\phi &= \sqrt{2}\cos\left(\phi - \frac{\pi}{4}\right) \ , \\ \cos\phi - \sin\phi &= -\sqrt{2}\sin\left(\phi - \frac{\pi}{4}\right) \end{aligned} \tag{2.28}$$

to transform the Hamiltonian into

$$H = -\sqrt{2}\sum_{j=1}^{N}\left[\sin\left(\phi - \frac{\pi}{4}\right)\sigma_j^+\sigma_{j+1}^+ - \cos\left(\phi - \frac{\pi}{4}\right)\sigma_j^+\sigma_{j+1}^-\right] + \text{H.c.} \ , \tag{2.29}$$

with H.c. denoting the Hermitian conjugate of the total expression preceding it. Should the H.c. label be inside any type of bracket, it shall denote the Hermitian conjugate of the total expression preceding it inside said bracket. The same will hold for the complex conjugate later on, denoted by c.c.

Having written the Hamiltonian in this manner, we proceed with consulting the properties of spin operators $\sigma_j^\mu$ bearing in mind the already employed (anti)commutation relations for Pauli matrices (2.14):

- $\sigma_j^\pm = \left(\sigma_j^\mp\right)^\dagger$ since $\sigma_j^\mu$ are Hermitian,
- $\left(\sigma_j^\pm\right)^2 = 0$ since $\left(\sigma_j^\mu\right)^2 = \mathbb{1}$ ,
- for spin operators on the same site $\left\{\sigma_j^\pm, \sigma_j^\mp\right\} = 0$ and $\left\{\sigma_j^\pm, \sigma_j^\pm\right\} = \mathbb{1}$ *as per* properties of Pauli matrices,
- for spin operators on different ($j \neq k$) sites $\left[\sigma_j^\pm, \sigma_k^\mp\right] = \left[\sigma_j^\pm, \sigma_k^\pm\right] = 0$ since they are members of independent vector spaces.

It is now evident from the third point that spin operators demonstrate fermionic (in sense of their anticommutation relations) behaviour on the same spin site, but considering the fourth point we see that their behaviour is bosonic on different sites in terms of their commutation relations [25] (fermionic operators anticommute, while bosonic ones commute and this ought to hold both for same and different sites). To diagonalise the Hamiltonian, it is necessary to express it in terms of fully bosonic or fully fermionic operators. A bosonic choice, in form of the Holstein–Primakoff transformation [26] will not be exploited here since, firstly, upon using it, one needs to introduce a strong repulsive interaction to truncate the Hilbert space of states. Secondly, the fermionic states are, because of the Pauli exclusion principle, significantly simpler to construct and endow with further excitations. With this in mind, we choose the Jordan–Wigner (JW) transformation [27] with cost of the system becoming highly nonlocal.

Hence we define a new set of JW creation and annihilation operators in the following manner[23,24]

$$c_j^\dagger \coloneqq \left(\bigotimes_{l=1}^{j-1} \sigma_l^z\right) \otimes \sigma_j^- \quad \text{and} \quad c_j \coloneqq \left(\bigotimes_{l=1}^{j-1} \sigma_l^z\right) \otimes \sigma_j^+ \ . \tag{2.30}$$

It is instructive to ponder the correspondence of the transformed creation operator $c_j^\dagger$ to the annihilation spin operator $\sigma_j^-$ and convince oneself that this choice is physically consistent since the notion of transformed spin states is more of a bookkeeping than a physical one.

Moreover, since $\left(\sigma_j^z\right)^2 = \mathbb{1}$, it holds that:

$$c_j^\dagger c_j = \sigma_j^- \sigma_j^+ \quad \text{and} \quad c_j c_j^\dagger = \sigma_j^+ \sigma_j^- \tag{2.31}$$

from which we can also infer an inverse JW transformation, i.e. from $c_j$ to $\sigma_\mu$ opera-

[23] These operators are sometimes [9] defined with another choice of factors, namely $\exp\left(\imath\pi\sigma_j^+\sigma_j^-\right) = 1 - 2\sigma_j^+\sigma_j^- = -\sigma_j^z \neq \sigma_j^z$ and since $\sigma_j^z$ operators determine the parity (which we will define soon), we defined the transformation using them directly to render subsequent calculations more natural. Note also that it holds $\sigma_j^z = 1 - 2c_j^\dagger c_j$.

[24] The intuitiveness of the JW transformation can be seen the most easily considering action of the spin operator on the fermionic state in occupation number representation—all of these operators commute, i.e. there are no emerging minus signs upon their exchange, which should exist for the fermionic operators. Now one can convince oneself that adding the factors of $z$ projections of all the spins before the site at hand effectively serves so as to add a sign each time our fermionic operator is exchanged with one of those defining the state. E.g. consider the state $|1,0,1,1,0,\cdots\rangle = c_1^\dagger c_3^\dagger c_4^\dagger \cdots |0,0,0,0,0,\cdots\rangle$ and the action of both the spin operator and $c$ operator on it.

tors. Relations in the previous equation imply that the same site fermionic anticommutation relations are satisfied as well:

$$\left\{c_j, c_j^\dagger\right\} = \mathbb{1} \ . \tag{2.32}$$

To verify the consistency of fermionic nature, we are also interested in anticommutation relations when the sites are different ($j \neq k$ and suppose that $j > k$ since H.c. of the following calculation yields the opposite case immediately):

$$\begin{aligned}\left\{c_j, c_l^\dagger\right\} &= \sigma_j^+ \left(\bigotimes_{m=1}^{j-1} \sigma_m^z\right) \left(\bigotimes_{n=1}^{l-1} \sigma_n^z\right) \sigma_l^- + \left(\bigotimes_{m=1}^{j-1} \sigma_m^z\right) \sigma_l^- \sigma_j^+ \left(\bigotimes_{n=1}^{l-1} \sigma_n^z\right) \\ &= \left(\bigotimes_{m=l}^{j-1} \sigma_m^z\right) \left[\sigma_j^+, \sigma_l^-\right] \\ &= 0 \ ,\end{aligned} \tag{2.33}$$

where we have used the JW transformation in the first equation and commutation relations for spin operators and the identity

$$1 - 2\sigma_j^+ \sigma_j^- = -\sigma_j^z \tag{2.34}$$

in the second and the third.

We condense the anticommutation properties (2.32) and (2.33) into a singular equation:

$$\left\{c_j, c_l^\dagger\right\} = \delta_{jl} \ . \tag{2.35}$$

The other anticommutation relations are obtained completely analogously and upon using the commutation properties of Pauli matrices we find that:

$$\{c_j, c_l\} = \left\{c_j^\dagger, c_l^\dagger\right\} = 0 \ . \tag{2.36}$$

It is now evident that JW operators $c_j$ satisfy both the same and different site fermionic anticommutation relations. Finally, we note for completeness that both (2.30) and (2.36) directly imply that their squares are zero:

$$(c_j)^2 = \left(c_j^\dagger\right)^2 = 0 \ , \tag{2.37}$$

as is consistent with Pauli's principle of exclusion. These results demonstrate that the JW operators introduced in (2.30) are indeed fermionic.

Before expressing the Hamiltonian in terms of the JW operators, let us emphasise several important points. First of all, note that relations (2.37) would not hold for bosonic operators and many of the contractions we have been able to make would not hold, so most of the terms would be significantly more complicated. Secondly, initial spin raising and lowering operators corresponded to flipping of physical spin states $|\uparrow\rangle$ and $|\downarrow\rangle$. However, JW particles corresponding to introduced $c_j$ operators are spinless fermions and their two available states correspond to vacant and occupied states.

To obtain the transformed Hamiltonian, we calculate the particular terms in (2.29) using JW transformation and obtain:

$$\begin{aligned} \sigma_j^+\sigma_{j+1}^+ &= -\, c_j c_{j+1} \ , \ j \neq N \\ \sigma_j^+\sigma_{j+1}^- &= -\, c_j c_{j+1}^\dagger \ , \ j \neq N \ . \end{aligned} \tag{2.38}$$

Why have we restricted these equations to $j \neq N$? Peculiarity of the JW transformation is the fact that it breaks the translational invariance of the initial problem (1.2) by singling out a particular initial site ($j = 1$) and thus there are potential inconsistencies when the spin system is closed, i.e. when the first and the $N$th spins interact. We reiterate that the closed *spin chains* with odd number of sites ($N = 2k-1,\ k \in \mathbb{Z}$) will be in the centre of our research since they demonstrate extraordinary properties when subjected to particular boundary conditions and interaction parameter $\phi$ values. With this in mind, we impose cyclicity on our system by requiring that

$$\sigma_{j+N}^\mu \equiv \sigma_j^\mu \tag{2.39}$$

and calculate the remaining Hamiltonian terms explicitly:

$$\begin{aligned} c_N^\dagger c_1^\dagger &= \left( \bigotimes_{j=1}^{N-1} \sigma_j^z \right) \sigma_N^- \sigma_1^- = \\ &= -\left( \bigotimes_{j=1}^{N} \sigma_j^z \right) \sigma_N^- \sigma_1^- = \\ &= -\Pi^z \sigma_N^- \sigma_1^- \end{aligned} \tag{2.40}$$

upon recalling (2.10) and, analogously:

$$c_N^\dagger c_1 = -\Pi^z \sigma_N^- \sigma_1^+ \ . \tag{2.41}$$

We are now able to write the Hamiltonian explicitly in terms of JW fermions (along with exchange of the written part in (2.29) and its H.c.):

$$\begin{aligned} H = -\sqrt{2}\Bigg[\sum_{j=1}^{N}\Big[\sin\Big(\phi-\frac{\pi}{4}\Big)\, c_j^\dagger c_{j+1}^\dagger - \cos\Big(\phi-\frac{\pi}{4}\Big)\, c_j^\dagger c_{j+1}\Big] + \\ +\Pi^z\sqrt{2}\Big[\sin\Big(\phi-\frac{\pi}{4}\Big)\, c_N^\dagger c_1^\dagger - \cos\Big(\phi-\frac{\pi}{4}\Big)\, c_N^\dagger c_1\Big]\Bigg] + \text{H.c.} \end{aligned} \tag{2.42}$$

To advance towards the eigenstates and eigenvalues of $H$, we recall from the preceding section that $\Pi^z$ commutes with the Hamiltonian, i.e.:

$$\big[\Pi^z, H\big] = 0 \tag{2.43}$$

and point out that this relation can also be seen from (2.42) since neither the BCS terms nor the number operator terms alter the total parity of the system.

Consequently, since Hamiltonian and the $z$ parity operator commute, they admit a complete set of common eigenstates. These eigenstates are divided by the latter into two sectors, one corresponding to each of its eigenvalues $\pm 1$. In terms of JW operators[25] representation of the parity operator, eigenvalue $\Pi^z = -1$ corresponds to states with odd number of JW fermions and $\Pi^z = +1$ to states with an even one.

Given the two parity sectors, we must deduce how to consistently connect the boundary JW terms on our closed spin chain. Mathematically, it is seen from (2.42) that interaction consistency implies that

$$\begin{aligned} &\Pi^z = +1 \implies c_{j+N}^+ = -c_j^+ \text{ (anti-periodic b.c.; even number of JW particles)}, \\ &\Pi^z = -1 \implies c_{j+N}^+ = c_j^+ \text{ (periodic b.c.; odd number of JW particles)}. \end{aligned} \tag{2.44}$$

Notice the introduction of $\pm$ marks to imply the type of boundary conditions (b.c.)

[25] We emphasise that JW particles and their number should not be confused with the number of sites $N$. Also, positivity of eigenvalue of the JW operator implies that a certain position is vacated by a JW fermion, while that of the spin operator regards the upward orientation of spin on the same site.

in use. We can interpret these conditions in a more physically transparent way. Due to a highly nonlocal mapping, JW operators further from the beginning site at $j = 1$ (in the direction of increasing $j$) will pick up more and more phase factors which cancel out in Hamiltonian terms (e.g. in (2.38)) unless we complete a path around the chain—this phase is then given by the total parity operator which is independent from the first site choice and thus persists as a phase factor (e.g. in (2.40) and (2.41)).

With the aforementioned sector separation in mind, we separate the Hamiltonian as well, using two projectors that in sum project on the total Hilbert space:

$$H = \left(\frac{1+\Pi^z}{2}\right) H^+ \left(\frac{1+\Pi^z}{2}\right) + \left(\frac{1-\Pi^z}{2}\right) H^- \left(\frac{1-\Pi^z}{2}\right) \ . \tag{2.45}$$

Introducing the boundary conditions (2.44), we see that both $H^\pm$ can be written in a compact form:

$$H^\pm = -\sqrt{2}\sum_{j=1}^{N}\left[\sin\left(\phi-\frac{\pi}{4}\right) c_j^{\pm\dagger} c_{j+1}^{\pm\dagger} - \cos\left(\phi-\frac{\pi}{4}\right) c_j^{\pm\dagger} c_{j+1}^{\pm}\right] + \text{H.c.} \tag{2.46}$$

Although the form of both Hamiltonians is expectedly (remember our mathematical argument for b.c.) the same, it is important to note that the Fock spaces that their eigenstates span are distinct.

## *2.4 Fourier transform of the Hamiltonian in JW form*

The next step towards the solution is transforming $H$ into the momentum[26] (Fourier) space while taking b.c. into account. We define a symmetric discrete Fourier transform (FT) as follows[27]:

$$c_j^\pm = \frac{1}{\sqrt{N}}\sum_q e^{\imath qj} b_q \quad \leftrightarrow \quad b_q = \frac{1}{\sqrt{N}}\sum_j e^{-\imath qj} c_j^\pm \ . \tag{2.47}$$

[26] A Fourier transform is useful when solving certain classes of condensed matter Hamiltonians such as the one of the XY model since the differences between operators are replaced with simple phase factors.

[27] We could have added a factor of $\exp(\imath\pi/4)$ in the FT definition to render the subsequent step, Bogoliubov rotation, a true $O(2)$ rotation. However, we chose a symmetric version of the FT since it will make future calculations and referencing the papers more natural. For the former, consult [13].

The $b_q$ operators are fermionic[28] as well, as we demonstrate in Appendix A. Furthermore, observe that the Fourier transform implies that $c^{\pm}_{j+N} = e^{\imath qj} c^{\pm}_j$ and thus for periodic b.c. it holds that

$$q \in \Gamma^+ = \left\{ -\frac{N-2}{N}\pi,\ ...,\ -\frac{1}{N}\pi,\ \frac{1}{N}\pi,\ ...,\ \frac{N-2}{N}\pi,\ \pi \right\} \ , \tag{2.48}$$

while for anti-periodic b.c. it holds that[29]

$$q \in \Gamma^- = \left\{ -\frac{N-1}{N}\pi,\ ...,\ -\frac{2}{N}\pi,\ 0,\ \frac{2}{N}\pi,\ ...,\ \frac{N-1}{N}\pi \right\} \ , \tag{2.49}$$

as is seen from (2.44). It is important to note that the $b$ operators have no $\pm$ sector reference, since the information on parity sector restrictions is conveyed by the allowed $q$ values. Also, only the $0$ and $\pi$ modes have no negative counterparts—these modes will be fundamental in forthcoming calculations.

Having defined the values which the modes $q$ can assume, we can state a more precise form of our FT:

$$c^{\pm}_j = \frac{1}{\sqrt{N}} \sum_{q \in \Gamma^{\pm}} e^{\imath qj} b_q \quad \leftrightarrow \quad b_q = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-\imath qj} c^{\pm}_j \ . \tag{2.50}$$

We are now ready to calculate the Hamiltonian terms explicitly:

$$\begin{aligned} \sum_{j=1}^{N} c^{\pm\dagger}_j c^{\pm\dagger}_{j+1} &= \sum_{j=1}^{N} \left( \frac{1}{\sqrt{N}} \sum_{q \in \Gamma^{\pm}} e^{-\imath qj} b^{\dagger}_q \right) \left( \frac{1}{\sqrt{N}} \sum_{k \in \Gamma^{\pm}} e^{-\imath k(j+1)} b^{\dagger}_k \right) \\ &= \frac{1}{N} \sum_{q,k \in \Gamma^{\pm}} b^{\dagger}_q b^{\dagger}_k e^{-\imath k} \sum_{j=1}^{N} e^{-\imath j(q+k)} \\ &= \sum_{q \in \Gamma^{\pm}} e^{\imath q} b^{\dagger}_q b^{\dagger}_{-q} \end{aligned} \tag{2.51}$$

upon using the FT expression (7.15) in the first equation and the delta function identity $\sum\limits_{j=1}^{N} \exp\left(-\imath j(q+k)\right) = N\delta_{q,-k}$ in the third one. Completely analogously, the

[28] Note that this can be deduced from the symmetry of the Fourier transform as well.

[29] Recall that this range of values of modes emerged in (2.7) and that they correspond to roots of unity.

second term is obtained as well:

$$\sum_{j=1}^{N} c_j^{\pm\dagger} c_{j+1}^{\pm} = \sum_{q\in\Gamma^{\pm}} e^{\imath q} b_q^{\dagger} b_q \ . \tag{2.52}$$

Inserting these into (2.46) and using the symmetry properties of trigonometric functions as well as the fact that the center of mass of a homogenous regular polygon defined by $N$th roots of unity lies at the origin of the complex plane (specifically $\sum_{q\in\Gamma^{\pm}} \cos q = 0$), we write the Hamiltonian in a convenient matrix form:

$$H^{\pm} = \sum_{q\in\Gamma^{\pm}} \begin{pmatrix} b_q^{\dagger} & b_{-q} \end{pmatrix} \begin{bmatrix} C_{q,\phi} & -\imath S_{q,\phi} \\ \imath S_{q,\phi} & -C_{q,\phi} \end{bmatrix} \begin{pmatrix} b_q \\ b_{-q}^{\dagger} \end{pmatrix} \tag{2.53}$$

upon introducing abbreviations

$$C_{q,\phi} = \sqrt{2}\cos\left(\phi - \frac{\pi}{4}\right)\cos q \quad \text{and} \quad S_{q,\phi} = \sqrt{2}\sin\left(\phi - \frac{\pi}{4}\right)\sin q \ . \tag{2.54}$$

The initial problem of diagonalising $H^{\pm}$ has reduced to diagonalising the matrices in (2.53), all having the same general form. We diagonalise each of them by the method of Bogoliubov rotation [28], discussed in the forthcoming section.

## *2.5 Bogoliubov rotation*

Noting the equality between matrix elements in (2.53) and following the diagonalisation in Appendix B, we define the *Bogoliubov angle* $\theta_q$ as follows:

$$\theta_q \coloneqq \arctan \frac{|e^{\imath 2q}\cos\phi + \sin\phi| - [\cos\phi + \sin\phi]\cos q}{[\cos\phi - \sin\phi]\sin q} \quad \text{for} \quad q \neq 0, \pi \ . \tag{2.55}$$

This choice of this definition is discussed in said appendix and is due to the fact that we expect the sine and cosine of $\theta_q$ to behave in a natural way[30], i.e.:

$$\cos\theta_{-q} = \cos\theta_q \quad \text{and} \quad \sin\theta_{-q} = -\sin\theta_q \tag{2.56}$$

and also lest we have troubles with multiple-valued quantities (note that definitions in terms of trigonometric functions of $2\theta_q$ are inherently ambiguous when seeking

[30] Notice also that $\sin\theta_q$ and $\cos\theta_q$ are defined uniquely by (2.55).

$\theta_q$).

We hold off the discussion of $q = 0$ and $\pi$ modes for now and proceed to apply the standard procedure of diagonalising a matrix of form (2.53), although it is useful to note that said matrix is diagonal for these two modes and hence there is no need for Bogoliubov rotation. We also remark that this method is more of an algebraic one, since it is essentially a problem of diagonalising a form quadratic in fermionic operators. Most elementary, by requiring that the linear combinations of $b$ operators yield a new quadratic form with vanishing nondiagonal (mixed) terms [9], we obtain that the desired transformation into operators $a$ in terms of which the Hamiltonian is diagonal is given by:

$$\begin{pmatrix} a_q \\ a^\dagger_{-q} \end{pmatrix} = \begin{bmatrix} \cos\theta_q & \imath \sin\theta_q \\ \imath \sin\theta_q & \cos\theta_q \end{bmatrix} \begin{pmatrix} b_q \\ b^\dagger_{-q} \end{pmatrix} \quad \text{for} \quad q \neq 0, \pi \ . \tag{2.57}$$

The appropriateness of this transformation can be seen in yet another way—write $\cos(2\theta_q)$ and $\sin(2\theta_q)$ in terms of $C_{q,\phi}$ and $S_{q,\phi}$ and then interpret the transformation as rotation[31,32] of the Hamiltonian into the diagonal form, accomplished by wedging it between the rotation matrix and its inverse. Also note that, consistent with this argument, is the fact that the angle in transformation matrix (2.57) is $\theta_q$, while the matrix elements of (2.53) are, by virtue of (2.54), those of angles $2\theta_q$.

Since operators $a_q$ are given as linear combinations of the JW fermions which are themselves obtained by transforming spin operator, the excitations of the system will in general be quasiparticles, i.e. collective phenomena. It is shown in Appendix A that the $a_q$ operators are fermionic as well. Furthermore, it is important to remark that the general $a^\dagger_{-q}$ can be obtained directly from the expression for $a_q$ in (2.57) and that it is consistent with (2.56), as it ought to be.

Exploiting (2.57), as well as anticommutation relations for operators $a_q$ obtained from those for operators $b_q$, Hamiltonian (2.53) finally becomes:

$$H^\pm = \sum_{q \in \Gamma^\pm} \epsilon(q) \left[ a^\dagger_q a_q - \frac{1}{2} \right] \quad \text{for} \quad q \neq 0, \pi \quad \text{and} \quad \epsilon(q) = 2\sqrt{1 + \sin(2\phi)\cos(2q)} \ . \tag{2.58}$$

As a useful consistency control, in Appendix A we rewrite (2.58) to obtain the ex-

[31] Another convincing property of this matrix is the fact that its determinant is 1.

[32] It is also seen that the following transformation is consistent with rotation by redefining the sine in the Hamiltonian matrix (2.53) to be real.

pression (15) from [10] and observe that the two are equal.

Let us now turn to discussing the $q = 0, \pi$ modes which were excluded from our expressions each time.

We start by noting that the dispersion in (2.58) is manifestly nonegative. However, if we turn back to the unrotated Hamiltonian (2.53), by direct calculation (with nondiagonal terms vanishing) we see that the correct expressions for the energies of $0$ and $\pi$ modes are given by:

$$\epsilon^{\text{corr}}(0) = -\epsilon^{\text{corr}}(\pi) = 2\sqrt{2}\cos\left(\phi - \frac{\pi}{4}\right) = 2\left[\cos\phi + \sin\phi\right] \ , \tag{2.59}$$

both of which can obviously assume negative values, depending on the parameter $\phi$. Having shown the potential negativeness of the energies of these modes, it is instructive and also necessary for future calculations to elucidate where and how has our method of Bogoliubov rotation failed. To see this, we use the defining relation for the Bogoliubov angle (2.55) to calculate its value for the $0$ mode. Inserting $q = 0$ explicitly into said equation, we obtain for $\phi \in \langle -\pi/4, \pi/4\rangle$ a seemingly undefined relation $0/0$ since it holds that $|\cos\phi + \sin\phi| = \cos\phi + \sin\phi$. However, upon exploiting the L' Hospital's rule once, it is seen that in this range we obtain the zero value for the Bogoliubov angle. Conversely, for the parameter range $\phi \in \langle -\pi/2, -\pi/4\rangle$ we obtain a nonzero expression in the numerator, while the expression in the denominator tends to zero so the Bogoliubov angle is calculated to be that of $\arctan$ of infinity, which is $\pi/2$. These results can be written in the following manner:

$$\theta_0 = \begin{cases} \frac{\pi}{2} \ ; \ \ \phi \in \langle -\frac{\pi}{2}, -\frac{\pi}{4}\rangle \ , \\ 0 \ ; \ \ \phi \in \langle -\frac{\pi}{4}, 0\rangle \ , \\ 0 \ ; \ \ \phi \in \langle 0, \frac{\pi}{4}\rangle \ . \end{cases} \tag{2.60}$$

Analogous calculation for the $\pi$ mode yields:

$$\theta_\pi = \begin{cases} 0 \ ; \ \ \phi \in \langle -\frac{\pi}{2}, -\frac{\pi}{4}\rangle \ , \\ \frac{\pi}{2} \ ; \ \ \phi \in \langle -\frac{\pi}{4}, 0\rangle \ , \\ \frac{\pi}{2} \ ; \ \ \phi \in \langle 0, \frac{\pi}{4}\rangle \ . \end{cases} \tag{2.61}$$

Turning back to (2.53), as already mentioned, we see that in $q = 0$ and $q = \pi$ cases the matrix is diagonal so it should not be rotated. However, consulting (2.57), (2.60) and (2.61), it is seen that for some parameter $\phi$ ranges, there will be unwanted rotations when using the notation introduced for Bogoliubov rotation. This implies that, when carrying out calculations with general Bogoliubov angles later on, it will be necessary to exclude the faulty angles explicitly. We will denote these angles with standard $\theta_q$ symbol and the correct ones as $\theta^{\text{corr}}_{0,\pi} = 0\ ,\ \ \forall q,\ \phi$.

## *2.6 Ground states and spectra of the system*

Studying the ground states of the XY model for three different parameter $\phi$ ranges, we will see that they correspond to three different types of thermodynamic behaviour.

### 2.6.1 First (ordered)—1O phase

The first distinct kind of ground states is obtained when the parameter $\phi$ takes on values in the interval $\langle -\pi/2, -\pi/4\rangle$, a phase we have denoted ordered (1O) due to the presence of order parameter (magnetisation) at $t = 0$, as was explained in the Introduction. From (2.59) we observe that:

$$\epsilon^{\text{corr}}(0) < 0 \quad \text{and} \quad \epsilon^{\text{corr}}(\pi) > 0 \tag{2.62}$$

and from (7.14) it is seen that the negative energy $0$ mode belongs to the odd parity sector. Upon remembering the parity constraints in (2.44), we construct the ground states for each parity sectors taking into account that even (odd) sector must have an even (odd) number of JW fermions and that all the modes have positive energies besides the $0$ one, as seen from (2.62). This means that the minimum energy will correspond to no JW particles in the even sector, but since there ought to be an odd number of them in the odd sector, we construct the ground state by adding the lightest possible excitation, that of a $0$ mode. Then the ground states for each of the sectors are:

$$\text{even: } |g^+\rangle = |0^+\rangle \ \text{ and } \ \text{odd: } |g^-\rangle = a_0^\dagger\,|0^-\rangle\ \ , \tag{2.63}$$

with $|0^\pm\rangle$ denoting the quasiparticle vacua corresponding to each parity sector defined in a natural way by demanding that they yield zero when acted upon by their

respective annihilation operators:

$$a_{q\in\Gamma^{\pm}}\left|0^{\pm}\right\rangle = 0 \ . \tag{2.64}$$

Analogously to a standard BCS derivation, it can be shown that these vacua[33] are given explicitly by:

$$\left|0^{\pm}\right\rangle = \bigotimes_{0<q<\pi;\ q\in\Gamma^{\pm}} \left[\cos\theta_q - \imath \sin\theta_q \ b_q^{\dagger} b_{-q}^{\dagger}\right] \left|0\right\rangle \ . \tag{2.65}$$

with $\left|0\right\rangle$ denoting the JW fermion vacuum determined by

$$b_q \left|0\right\rangle = 0 \quad \forall q \ . \tag{2.66}$$

One can also convince oneself of expressions (2.65) by acting upon them with $a_q$ operators explicitly.

We proceed with calculating the ground state energies. We do so by acting upon ground states wave functions (2.65) with the Hamiltonian (2.58), but taking (2.59) into account. In this way, we obtain for the even parity sector:

$$H^{+}\left|g^{+}\right\rangle = \sum_{q\in\Gamma^{+}} \epsilon(q) \left[a_q^{\dagger} a_q - \frac{1}{2}\right] \left|0^{+}\right\rangle = -\frac{1}{2} \sum_{q\in\Gamma^{+}} \epsilon(q) \left|0^{+}\right\rangle \implies E_0^{+} = -\frac{1}{2} \sum_{q\in\Gamma^{-}} \epsilon\left(q + \frac{\pi}{N}\right) \ . \tag{2.67}$$

It is important to notice the sum over the $\Gamma^{-}$ sector, which we have obtained from sum over $\Gamma^{+}$ sector by shifting the argument of the dispersion by $\pi/N$ (cf. (7.13) and (7.14)). This is done so as to allow to easily take the thermodynamic limit $N \to \infty$ later on.

Calculation for the odd parity sector is a tad more subtle since the $0$ mode has negative energy (as shown in (2.59)) and thus has to be explicitly corrected in the sum in (2.58) so that the correct Hamiltonian is:

$$H^{-} = \epsilon^{\text{corr}}(0) \left[a_0^{\dagger} a_0 - \frac{1}{2}\right] + \sum_{q\in\Gamma^{-}\setminus\{0\}} \epsilon(q) \left[a_q^{\dagger} a_q - \frac{1}{2}\right] \ . \tag{2.68}$$

[33] Notice that the products in these wave functions are only over the positive modes of respective parity sectors. This has to do with the fact that the Hamiltonian (2.58) can be written as two times the same expression (each nondiagonal matrix in the sum corresponds to the subspace of $q$ and $-q$ modes simultaneously), but factored only over positive modes with terms corresponding to $0$ and $\pi$ modes being added explicitly later on since they have no negative counterparts (the corresponding matrices are diagonal).

Its action on the odd parity ground state is then given by:

$$H^- \left|g^-\right\rangle = \epsilon^{\text{corr}}(0) \left[a_0^\dagger a_0 - \frac{1}{2}\right] a_0^\dagger \left|0^-\right\rangle + \sum_{q\in\Gamma^-\setminus\{0\}} \epsilon(q) \left[a_q^\dagger a_q - \frac{1}{2}\right] a_0^\dagger \left|0^-\right\rangle \ , \tag{2.69}$$

inside of which we use the anticommutation relations for $a$ operators (A.5) in the first term:

$$\left[a_0^\dagger a_0 - \frac{1}{2}\right] a_0^\dagger \left|0^-\right\rangle = a_0^\dagger \left[\left\{a_0, a_0^\dagger\right\} - a_0^\dagger a_0\right] \left|0^-\right\rangle - \frac{1}{2} a_0^\dagger \left|0^-\right\rangle = \frac{1}{2} a_0^\dagger \left|0^-\right\rangle \ , \tag{2.70}$$

which upon reinserting into (2.69) and using (2.64) yields:

$$\begin{aligned} H^- \left|g^-\right\rangle =& \frac{1}{2}\left[\epsilon^{\text{corr}}(0) - \sum_{q\in\Gamma^-\setminus\{0\}} \epsilon(q)\right] \left|g^-\right\rangle = \frac{1}{2}\left[-\epsilon(0) - \sum_{q\in\Gamma^-\setminus\{0\}} \epsilon(q)\right] \left|g^-\right\rangle \\ =& -\frac{1}{2}\sum_{q\in\Gamma^-} \epsilon(q) \left|g^-\right\rangle \implies E_0^- = -\frac{1}{2}\sum_{q\in\Gamma^-} \epsilon(q) \ . \end{aligned} \tag{2.71}$$

It is of paramount importance to notice from (2.67) and the previous expression that the two ground-state energies, each corresponding to respective parity sector, are degenerate[34] for odd $N$ and thus the general ground-state wave function is their linear combination.

Regarding the spectrum of the system, in the $\phi$ range we are currently discussing $\phi \in \langle -\pi/2, -\pi/4\rangle$ we see from (2.59) that:

$$\epsilon^{\text{corr}}(0) \in \langle -2, 0\rangle \ \text{ and } \ \epsilon^{\text{corr}}(\pi) \in \langle 0, 2\rangle \tag{2.72}$$

and also that for the rest of the spectrum it holds that

$$\epsilon(q \neq 0, \pi) = 2\sqrt{1 + 2\sin(2\phi)\cos(2q)} \geq 2\sqrt{1 + 2\sin(2\phi)\cos(2\pi)} \tag{2.73}$$

and since the $0$ mode has the lowest energy and the rest of the spectrum has energy greater or equal to that of the $\pi$ mode, we conclude that there exist a gap in the spectrum of the system, as depicted in Fig. 2.1. It is worth noting that this gap in the spectrum persists in the thermodynamic limit since no energies can be negative and the $0$ mode energy does not shift toward $0$ as $N \to \infty$.

[34] For an another perspective on the degeneracy (a deeper physical one), consult [29].

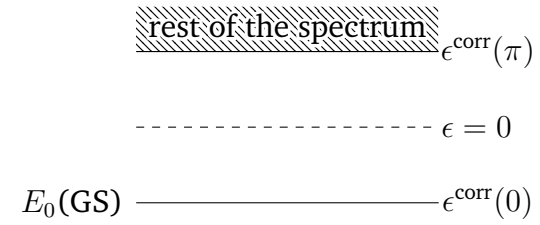



Figure 2.1: Spectrum of the system for $\phi \in \langle -\pi/2, -\pi/4 \rangle$ with relevant energies labeled, along with the one of ground state (GS). Note that the continuousness of the spectrum above a certain energy is present only in the thermodynamic limit and also that the energy of the ground state is given with respect to the quasiparticle vacuum energy.

### 2.6.2 Second (mesoscopic)—2M phase

In the mesoscopic phase, the parameter $\phi$ takes on values in the interval $\langle -\pi/4, 0 \rangle$. From (2.59) we observe that:

$$\epsilon^{\text{corr}}(0) > 0 \quad \text{and} \quad \epsilon^{\text{corr}}(\pi) < 0 \tag{2.74}$$

and from (7.13) it is seen that the negative energy mode $\pi$ belongs to the even parity sector. As in the previous section, we refer to the parity constraints in (2.44) and construct the ground states for each parity sector, taking into account that even (odd) sector must have and even (odd) number of JW fermions and that all the modes besides the $\pi$ one have positive energies. This will imply that it would be energetically favourable to excite the $\pi$ mode in the even parity sector, however, there must be an even number of particles in it and the inequality in (2.73) implies that their energy will be greater in absolute value than that of a $\pi$ mode, so the minimal energy configuration for the even parity sector is that of no particles. Regarding the odd parity sector, the lowest energy excitation will be the $0$ mode (albeit of positive energy) and thus the ground states for each of the sectors are as before:

$$\text{even: } |g^+\rangle = |0^+\rangle \;\; \text{and} \;\; \text{odd: } |g^-\rangle = a_0^\dagger |0^-\rangle \;\; , \tag{2.75}$$

but with a significant difference in the spectrum which is observed after using (2.59) to obtain:

$$\epsilon^{\text{corr}}(0) \in \langle 0, 2 \rangle \;\; \text{and} \;\; \epsilon^{\text{corr}}(\pi) \in \langle -2, 0 \rangle \;\; . \tag{2.76}$$

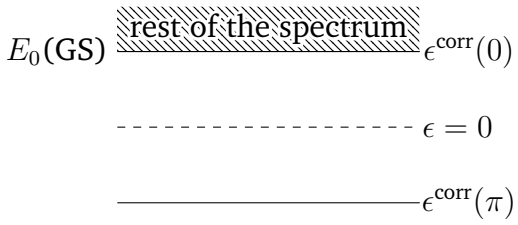



Figure 2.2: Spectrum of the system for $\phi \in \langle -\pi/2, -\pi/4 \rangle$ with relevant energies labeled, along with the one of ground state (GS). Note that the continuousness of the spectrum above a certain energy is present only in the thermodynamic limit and also that the energy of the ground state is given with respect to the quasiparticle vacuum energy.

The spectrum in this phase is gapless since the energies above the ground state form a continuous range in the thermodynamic limit, as is depicted in Fig. 2.2. We also remark that the two ground states are again degenerate, completely analogously to the analysis in the preceding section for the first phase—this is evident since the ground states are of the same form so the derivations leading up to (2.67) and (2.71) are identical.

To recapitulate, we have shown that in the first two phases a twofold degeneracy is present in the ground state of the system with the same energies in both phases. However, the essential difference lies within the existence of spectrum gap in the first and lack thereof in the latter.

We also point out the effect of frustration—the negative energy mode has moved into the even parity sector and thus cannot be excited alone. This makes the lowest possible energy higher than what it would be were there no parity constraints.

### 2.6.3 Third (incommensurate)—3I phase

We conclude the calculation of ground state wavefunctions and spectra with the third phase. In it, the parameter $\phi$ takes on values in the interval $\langle 0, \pi/4 \rangle$. As we have noted, the ground states in the first two phases are doubly degenerate—we have also explicitly shown in (2.73) that the rest of the spectrum energies are greater than those of $0$ and $\pi$ modes. This conclusion hinged on the fact that for all $\phi \in \langle -\pi/2, 0 \rangle$ it holds that $\sin(2\phi) < 0$. However, in the third phase, the last inequality obviously does not hold and thus the ground state(s) will be different than in FM and FM-AFM phases. Let us find them.

We first recall (2.59) and see that in the current phase it holds that:

$$\epsilon^{\text{corr}}(0) > 0 \quad \text{and} \quad \epsilon^{\text{corr}}(\pi) < 0 \quad , \tag{2.77}$$

i.e. the $\pi$ mode still has the lowest possible energy in the system. However, new minima emerge with energies less than that of the $0$ mode—from (2.58) we see that these would in general correspond to $\pm\pi/2$ modes. Since these are not present among the allowed modes except in the thermodynamic limit, we see that the modes closest to them depend on the remainder of $N$ when divided by $4$. In the even sector, we denote them with $\pm p' \in \Gamma^+$ , given by:

$$p' = \begin{cases} \frac{\pi}{2}\left(1 + \frac{1}{N}\right) \ ; \ \ N \bmod 4 = 1 \ , \\ \frac{\pi}{2}\left(1 - \frac{1}{N}\right) \ ; \ \ N \bmod 4 = 3 \end{cases} \tag{2.78}$$

and in the odd sector with $\pm p \in \Gamma^-$ , given by:

$$p = \begin{cases} \frac{\pi}{2}\left(1 - \frac{1}{N}\right) \ ; \ \ N \bmod 4 = 1 \ , \\ \frac{\pi}{2}\left(1 + \frac{1}{N}\right) \ ; \ \ N \bmod 4 = 3 \ . \end{cases} \tag{2.79}$$

Having these minimum energy modes in mind, we proceed to construct the ground states in each sector. Since the $\pi$ mode belongs to the even sector and its energy is negative, we see that we can construct the ground state starting with the quasiparticle vacuum and adding both $\pi$ and one of the $\pm p'$ modes since absolute values of their energies are less than that of the $\pi$ mode and thus the states

$$|\pm p'\rangle = a^\dagger_{\pm p'} a^\dagger_\pi \, |0^+\rangle \tag{2.80}$$

will have less energy than the $|0^+\rangle$ quasiparticle vacuum state. Analogously, to construct the ground state in the odd sector, we have to add at least one JW particle and thus we choose those with minimum energies to obtain the following two ground states:

$$|\pm p\rangle = a^\dagger_{\pm p} \, |0^-\rangle \ . \tag{2.81}$$

We now proceed to calculate the associated energies of the four obtained states by

acting with Hamiltonian (2.58) upon them:

$$H^+ |\pm p'\rangle = \sum_{q\in\Gamma^+\setminus\{\pi,\pm p'\}} \epsilon(q) \left[a_q^\dagger a_q - \frac{1}{2}\right] a_{\pm p'}^\dagger a_\pi^\dagger |0^+\rangle + \\ + \epsilon(\pm p') \left[a_{\pm p'}^\dagger a_{\pm p'} - \frac{1}{2}\right] a_{\pm p'}^\dagger a_\pi^\dagger |0^+\rangle + \epsilon^{\text{corr}}(\pi) \left[a_\pi^\dagger a_\pi - \frac{1}{2}\right] a_{\pm p'}^\dagger a_\pi^\dagger |0^+\rangle \ . \tag{2.82}$$

As for (2.71), we use the anticommutation relations for operators $a$ and the fact that $a_{q\in\Gamma^\pm} |0^\pm\rangle = 0$ to obtain:

$$H^+ |\pm p'\rangle = \left[-\frac{1}{2} \sum_{q\in\Gamma^+\setminus\{\pi,\pm p'\}} \epsilon(q) + \frac{1}{2}\epsilon(p') + \frac{1}{2}\epsilon^{\text{corr}}(\pi)\right] |\pm p'\rangle \tag{2.83}$$

and after remembering that $\epsilon^{\text{corr}}(\pi)$ is negative, we add it to the sum and arrive at:

$$E_0^+(\pm p') = -\frac{1}{2} \sum_{q\in\Gamma^+\setminus\{\pm p'\}} \epsilon(q) + \frac{1}{2}\epsilon(\pm p') \ , \tag{2.84}$$

where we note for clarity that $\pm p$ in the sum does not imply that both terms are excluded, but rather only one of them.

Regarding the odd sector and the $|\pm p\rangle$ states, we obtain the similar expression completely analogously:

$$E_0^-(\pm p) = -\frac{1}{2} \sum_{q\in\Gamma^+\setminus\{\pm p\}} \epsilon(q) + \frac{1}{2}\epsilon(\pm p) \ , \tag{2.85}$$

where we again note that $\pm p'$ in the sum does not imply that both terms are excluded, but rather only one of them.

We now observe that, besides the obvious double degeneracies both in the even and odd sector, there is also a general quadruple degeneracy between all four states since simple trigonometric arguments demonstrate that energies in (2.84) and (2.85) are the same. Thus the ground state in the AFM phase is in general quadruply degenerate and a linear combination of all four states $|\pm p'\rangle$ and $|\pm p\rangle$, with spectrum depicted in Fig. 2.3. Hereby the process of calculation of ground states and spectra is concluded for all three phases, i.e. parameter $\phi$ ranges.

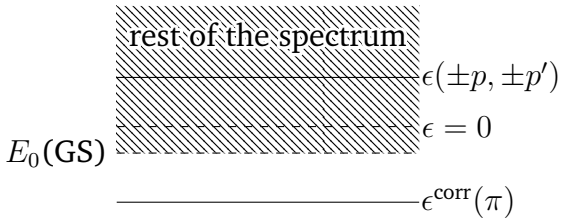



Figure 2.3: Spectrum of the system for $\phi \in \langle 0, \pi/4 \rangle$ with relevant energies labeled, along with the one of ground state (GS). Note that the continuousness of the spectrum above a certain energy is present only in the thermodynamic limit and also that energies are given with respect to the quasiparticle vacuum energy.

## *2.7 Symmetries revisited*

Having obtained the spectra of the XY model for all three phases of interest and having introduced three types of operators along the way ($c_j$, $b_q$ and $a_q$), we return to point out two additional results to be used later to calculate the correlation functions and magnetisations.

### 2.7.1 One translation theorem

The eigenstates of the translation operator (2.4) are the states of form

$$b^\dagger_{q_1} b^\dagger_{q_2} \cdots b^\dagger_{q_m} |0\rangle \quad , \tag{2.86}$$

with $m$ odd and $q_1, q_2, ..., q_m \in \Gamma^-$. Their eigenvalues are $\exp\left[\imath \sum_{j=1}^m q_j\right]$, i.e.:

$$T\left(b^\dagger_{q_1} b^\dagger_{q_2} \cdots b^\dagger_{q_m} |0\rangle\right) = \exp\left[\imath \sum_{j=1}^m q_j\right] \left(b^\dagger_{q_1} b^\dagger_{q_2} \cdots b^\dagger_{q_m} |0\rangle\right) \quad . \tag{2.87}$$

The proof of this relation will be omitted since it is given in detail in [11] and is also similar to the forthcoming proof regarding the mirror operator which we will write out in detail. We instruct the reader to consult the following derivation for an argument on why this relation holds for the $a$ operators as well, only with the ground states being the quasiparticle vacua.

### 2.7.2 One mirroring theorem

As we have stated in the section on symmetry properties of the XY model, relation (2.25) is useful since, if it is possible to find some result of interest for mirroring with

respect to one spin site, it allows us to relate it to all the other sites as well. This is indeed possible to do for the operator $M_N$ acting on a general state of JW fermions:

$$M_N \left( a^\dagger_{q_1} a^\dagger_{q_2} \cdots a^\dagger_{q_m} |0^-\rangle \right) = a^\dagger_{-q_m} a^\dagger_{-q_{m-1}} \cdots a^\dagger_{-q_1} |0^-\rangle \quad . \tag{2.88}$$

We now prove this relation and emphasize once again that the proof of (2.87) is analogous and given in detail [11].

To begin, let us remember that we want to obtain the relation in terms of $a$ operators, but if we observe that

$$\begin{aligned} a^\dagger_q |0^-\rangle &\propto \left[ \cos\theta_q b^\dagger_q - \imath \sin\theta_q b_{-q} \right] \left[ \cos\theta_q - \imath \sin\theta_q b^\dagger_q b^\dagger_{-q} \right] |0\rangle \\ &= \left[ \cos^2\theta_q + \sin^2\theta_1 \right] b^\dagger_q |0\rangle = b^\dagger_q |0\rangle \end{aligned} \tag{2.89}$$

upon using (2.57) and (2.65), we conclude that we can prove an analogous relation for the $b$ operators and the $|0\rangle$ vacuum rather than start with the quasiparticle vacuum and then need to do an additional transformation in the proof. Thus, we introduce the notation for an ordered product of $m$ raising operators $b^\dagger$:

$$\left( \prod_{j=1}^{m} b^\dagger_{q_j} \right) |0\rangle \coloneqq b^\dagger_{q_1} b^\dagger_{q_2} \cdots b^\dagger_{q_m} |0\rangle \quad . \tag{2.90}$$

Our goal is to arrive at the spin operators since the basis (2.2) in which the action of the mirror operator is known is of those operators. To this end, we first turn to the $c$ operators via the Fourier transform (7.15):

$$\begin{aligned} \left( \prod_{j=1}^{m} b^\dagger_{q_j} \right) |0\rangle =& \frac{1}{N^{m/2}} \sum_{j_1=1}^{N} \cdots \sum_{j_m=1}^{N} e^{\imath q_1 j_1} \cdots e^{\imath q_m j_m} c^\dagger_{j_1} \cdots c^\dagger_{j_m} |0\rangle \\ =& \frac{1}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} e^{\imath \sum_{l=1}^{m} q_l j_l} \prod_{n=1}^{m} c^\dagger_{j_n} |0\rangle \quad . \end{aligned} \tag{2.91}$$

Important and soon to be used point to notice from the last expression is the fact that it vanishes unless all $j_l$ are different since the $c_j$ operators are fermionic and thus the Pauli exclusion principle applies.

We turn the $c_j$ operators into spin ones exploiting (2.30), for which the next

example is useful—consider three $c_j$ operators being turned into spin ones:

$$c_1^\dagger c_4^\dagger c_2^\dagger \left|0\right\rangle = -c_1^\dagger c_2^\dagger c_4^\dagger \left|0\right\rangle = -\sigma_1^- \left[\sigma_1^z\right] \sigma_2^- \left[\sigma_1^z \sigma_2^z \sigma_3^z\right] \sigma_4^- \bigotimes_{j=1}^{N} \left|\uparrow_j\right\rangle = -\sigma_1^- \sigma_2^- \sigma_4^- \bigotimes_{j=1}^{N} \left|\uparrow_j\right\rangle \ , \tag{2.92}$$

with the fermionic anticommutation relations used in the first equality, JW transformation (2.30) and the definition of the vacuum states[35] in terms of spin kets in the second and finally the commutation of spin operators for different sites for the last one. The process of bringing all the $\sigma_j^z$ operators to the vacuum state will always be the same when $c_j$ are ordered as in the second expression since they never cross the $\sigma_j^-$ operators of the same site and yield $+1$ when acting on the up spin states $\left|\uparrow\right\rangle$. This implies that the sign of the spin operators will correspond to the permutation that brings the tuple of indices of operators to ascending order, in this case $\{1,4,2\} \rightsquigarrow \{1,2,4\}$ with the $-$ sign. We demarcate this permutation sign with $S\left[\{j_l\}\right]$ and use it to immediately obtain the final expression in (2.91):

$$\frac{1}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} e^{\imath \sum_{l=1}^{m} q_l j_l} \prod_{n=1}^{m} c_{j_n}^\dagger \left|0\right\rangle = \frac{1}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S\left[\{j_l\}\right] e^{\imath \sum_{l=1}^{m} q_l j_l} \bigotimes_{n=1}^{m} \left(\sigma_{j_n}^-\right) \bigotimes_{s=1}^{N} \left|\uparrow_s\right\rangle \ . \tag{2.93}$$

This form of the expression of interest is convenient since we can now easily act with $M_N$ on it, having (2.21) in mind:

$$M_N \left( \prod_{j=1}^{m} b_{q_j}^\dagger \right) \left|0\right\rangle = \frac{1}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S\left[\{j_l\}\right] e^{\imath \sum_{l=1}^{m} q_l j_l} M_N \left( \bigotimes_{n=1}^{m} \left(\sigma_{j_n}^-\right) \bigotimes_{s=1}^{N} \left|\uparrow_s\right\rangle \right) \ . \tag{2.94}$$

Since we intend to act on the spin site index $j_n$ of the $\sigma^-$ operators, we need a transformation inverse to that of (2.21), i.e. the inverse of $j \rightsquigarrow 2N - j$, but this transformation is its own inverse so we need only make exchange $j_n \rightsquigarrow 2N - j_n$ in the previous equation:

$$M_N \left( \prod_{j=1}^{m} b_{q_j}^\dagger \right) \left|0\right\rangle = \frac{1}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S\left[\{j_l\}\right] e^{\imath \sum_{l=1}^{m} q_l j_l} \bigotimes_{n=1}^{m} \left(\sigma_{2N-j_n}^-\right) \bigotimes_{s=1}^{N} \left|\uparrow_s\right\rangle \ . \tag{2.95}$$

We emphasize two points. First off, the choice of the $N$th site for the mirror operator

[35] Note that, since we have related $c_j^\dagger$ with $\sigma_j^-$ in JW transformation (2.30), the vacuum state is a product of up spin states.

$M_N$ is now seen to be appropriate since all the momenta $q$ are in the odd $\Gamma^-$ sector and thus, from (7.14), it holds that $\exp[\pm\imath 2Nq] = 1$ and we can make the following exchange:

$$e^{\imath q_l j_l} = e^{\imath(-2Nq_l)} e^{\imath(-q_l)(-j_l)} = e^{\imath(-q_l)(2N-j_l)} \ . \tag{2.96}$$

Without choosing the $N$th site as the origin of reflection, we would have had lingering phase factors to complicate our discussion. However, as was already mentioned, because of (2.25) we can find the desired expression for the mirror operator on this convenient site and then use the translation operator for the others.

Secondly, since the number of elements $m$ of a tuple $\{j_l\}$ is odd, sign of the permutation $S\{[j_l]\}$ will evidently be the same as $S\{[2N - j_l]\}$ up to a factor of $(-1)^{(m-1)+(m-2)+\cdots+1} = (-1)^{\frac{m(m-1)}{2}}$ (emerging when operators are placed in inverse order) if all of its elements are different than zero (recall that periodicity of the spin chain would imply that the zero index corresponds to the $N$th position in the chain). We now remember the demonstrated fact that all $j_l$ must be different for the expression of interest not to vanish, so at most one term of the form $2N - j_l$ can be zero. Then the normal ordering of $\{j_l\}$ would place that element at the first place and we would need $m - 1$ exchanges of creation operators to put it in its appropriate $N$th place. However, since $m$ is odd, this process does not induce the sign. Along this, the factor in the exponent should be changed as well, but since the expressions for the $0$ or $N$ in exponents both give the factor of $1$, this exchange can be done with no introduction of additional factors as well. These arguments imply that we can write our expression of interest as follows:

$$M_N \left( \prod_{j=1}^{m} b^\dagger_{q_j} \right) |0\rangle = \frac{(-1)^{\frac{m(m-1)}{2}}}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S\left[\{2N - j_l\}\right] e^{\imath \sum_{l=1}^{m}(-q_l)(2N-j_l)} \bigotimes_{n=1}^{m} \left(\sigma^-_{2N-j_n}\right) \bigotimes_{s=1}^{N} |\uparrow_s\rangle \ . \tag{2.97}$$

Since the relative ordering of terms in the exponent and the spin operator product is not relevant, we can equate the indices $l$ and $n$ to obtain:

$$M_N \left( \prod_{j=1}^{m} b^\dagger_{q_j} \right) |0\rangle = \frac{(-1)^{\frac{m(m-1)}{2}}}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S\left[\{2N - j_l\}\right] e^{\imath \sum_{l=1}^{m}(-q_l)(2N-j_l)} \bigotimes_{l=1}^{m} \left(\sigma^-_{2N-j_l}\right) \bigotimes_{s=1}^{N} |\uparrow_s\rangle \ . \tag{2.98}$$

This expression is in the form appropriate for renaming the index $2N - j_l$ as $j_l$ and noticing that, because of the periodicity of the chain, the sums will stay the same and

run through all of the same terms:

$$M_N\left(\prod_{j=1}^{m} b^\dagger_{q_j}\right)|0\rangle = \frac{(-1)^{\frac{m(m-1)}{2}}}{N^{m/2}} \sum_{j_1,\ldots,j_m=1}^{N} S\left[\{j_l\}\right] e^{\imath \sum_{l=1}^{m}(-q_l)j_l} \bigotimes_{l=1}^{m}\left(\sigma^-_{j_l}\right) \bigotimes_{s=1}^{N} |\uparrow_s\rangle \quad . \tag{2.99}$$

We now compare this equation with (2.93) since they have the same form, only with the momenta values negative to obtain:

$$M_N\left(\prod_{j=1}^{m} b^\dagger_{q_j}\right)|0\rangle = (-1)^{\frac{m(m-1)}{2}}\left(\prod_{j=1}^{m} b^\dagger_{-q_j}\right)|0\rangle \quad , \tag{2.100}$$

which, taking into consideration the discussed equivalence of this result for $a$ and $b$ operators and also the fact that the factor in front corresponds to inverting the order of operators, yields the desired expression (2.88):

$$M_N\left(a^\dagger_{q_1} a^\dagger_{q_2} \cdots a^\dagger_{q_m}|0^-\rangle\right) = a^\dagger_{-q_m} a^\dagger_{-q_{m-1}} \cdots a^\dagger_{-q_1}|0^-\rangle \quad . \tag{2.101}$$

Our proof is hereby concluded.

# 3 Correlation functions

## *3.1 Introduction*

Correlation functions[36] are an especially useful way of analysing several properties of a given system. Their use encompasses a broad range in science and technology, from spectral analysis and autocorrelation functions in signal processing [30] to quantum field theory where they are interpreted as propagation amplitudes [31, 32]. The particular ones which will be of importance to our present work are the one- and two-point correlation functions of the spin operators since they will serve as a measure of the order in the system at hand and for evaluating other interesting properties, such as magnetisations. This approach has already been used to identify emergence of interesting types of magnetisations and phase transitions in previous works [10, 11].

## *3.2 Static correlation functions*

Since we have naturally obtained the ground states in the momentum space, we will begin by calculating the particular terms necessary for our end goal, the physically relevant spin correlation functions $\langle \sigma_j^\mu \sigma_k^\mu \rangle$.

Since the process is somewhat lengthy, but straightforward, full calculations will be given for the representative examples and other ones will be cited only. As for motivating our starting point, we cite the result from the succeeding section (3.2.2) to write the spin correlation function in the, e.g. $x$ direction as:

$$\langle \sigma_j^x \sigma_l^x \rangle = (-\imath)^{l-j} \langle B_j A_{j+1} B_{j+1} \cdots A_{l-1} B_{l-1} A_l \rangle = (-\imath)^{l-j} \langle \bigotimes_{m=j}^{l-1} B_m A_{m+1} \rangle \ , \tag{3.1}$$

where $A_j$ and $B_j$ are the *Majorana fermionic operators* and are defined as follow:

$$A_j \coloneqq \left( \bigotimes_{l=1}^{j-1} \sigma_l^z \right) \otimes \sigma_j^x = c_j^\dagger + c_j \quad \text{and} \quad B_j \coloneqq \left( \bigotimes_{l=1}^{j-1} \sigma_l^z \right) \otimes \sigma_j^y = \imath \left( c_j^\dagger - c_j \right) \ . \tag{3.2}$$

As is further discussed in said section, by use of the Wick's theorem, we reduce the problem of finding the correlation functions of form (3.1) to calculating the correla-

[36] The correlation functions and the expectation values of similar type are often denoted shortly as *correlators* in literature.

tion functions of the following three terms:

$$\langle A_j B_l \rangle \ , \ \ \langle A_j A_l \rangle \ \ \text{and} \ \ \langle B_j B_l \rangle \ , \tag{3.3}$$

but since these will by (3.2) in general be sums of terms of the two-operator correlation functions of the $c$ operators, we see that terms of form $\langle c_j c_l \rangle$ are needed. These, on the other hand, can be calculated from $\langle b_q b_k \rangle$ terms by using the Fourier transform (7.15), while $\langle b_q b_k \rangle$ terms can be calculated from the $\langle a_q a_k \rangle$ terms by means of the transformation (2.57). Why have we gone all the way to the $a$ operators? Well, since we will be seeking the correlation functions (expectation values) in the ground states, we need to start from the $a_q$ operators because their[37] action on the ground state wavefunctions is known from (2.64).

Before turning to each of the three phases we note that, because of the identical form of the ground states for the first two, i.e. (2.63) and (2.75), we can evaluate the correlation functions for them simultaneously and only in the end add appropriate corrections to the Bogoliubov angles, as described by (2.60) and (2.61) and the corresponding discussion. By this, we mean that we will write the correct Bogoliubov angles first for the Majorana correlation functions since only they are of direct interest for further calculations. Henceforth, it is explicitly assumed that corrections must be made in other types of correlation functions (expectation values).

### 3.2.1 $1$**O and** $2$**M phases—static Majorana correlation functions**

Since the correlation functions in general differ for the two ground states $|g^{\pm}\rangle$, we evaluate them separately. As announced, we do this in several steps, with *Majorana correlation functions* as the end goal. Begin with the $+$ one and use (2.63) in the first equality, the definition of anticommutator in the second and relations (A.5) and (2.64) in the third:

$$\langle g^+ | \, a_q a_k^\dagger \, | g^+ \rangle = \langle 0^+ | \, a_q a_k^\dagger \, | 0^+ \rangle = \langle 0^+ | \left\{ a_q, a_k^\dagger \right\} - a_k^\dagger a_q \, | 0^+ \rangle = \delta_{q,k} \, \langle 0^+ | 0^+ \rangle = \delta_{q,k} \ . \tag{3.4}$$

[37] Using (2.65) we can work with $b_q$ operators directly. For pedagogical purposes, we will use the longer method first for static correlation functions and then exploit the said more direct method when calculating the dynamic correlation functions so as to demonstrate both of them.

and similarly for the rest of the combinations of $a$ operators:

$$\langle g^+|\, a_q^\dagger a_k\, |g^+\rangle = \langle 0^+|\, a_q^\dagger a_k\, |0^+\rangle = 0\ , \tag{3.5a}$$

$$\langle g^+|\, a_q a_k\, |g^+\rangle = \langle 0^+|\, a_q a_k\, |0^+\rangle = 0\ , \tag{3.5b}$$

$$\langle g^+|\, a_q^\dagger a_k^\dagger\, |g^+\rangle = \langle 0^+|\, a_q^\dagger a_k^\dagger\, |0^+\rangle = 0\ , \tag{3.5c}$$

where we can, beside the referenced expressions, use the fact that there must be the same number of creation and annihilation operators for the correlation function (expectation value) not to vanish. It is also instructive to notice that (3.4) and the first equation in (3.5) are consistent with the anticommutation relations (A.5) for operators $a_q$, while the other two equations in (3.5) are related by a Hermitian conjugate and index exchange.

We continue with expressions for the $|g^-\rangle$ state:

$$\begin{aligned}
\langle g^-|\, a_q a_k^\dagger\, |g^-\rangle &= \langle 0^-|\, a_0 a_q a_k^\dagger a_0^\dagger\, |0^-\rangle \\
&= -\langle 0^-|\, a_q a_0 a_k^\dagger a_0^\dagger\, |0^-\rangle \\
&= -\langle 0^-|\, a_q \left[\left\{a_0, a_k^\dagger\right\} - a_k^\dagger a_0\right] a_0^\dagger\, |0^-\rangle \\
&= -\delta_{0,k}\langle 0^-|\, a_q a_0^\dagger\, |0^-\rangle + \langle 0^-|\, a_q a_k^\dagger a_0 a_0^\dagger\, |0^-\rangle \\
&= -\delta_{0,k}\delta_{q,k} + \delta_{q,k} = \delta_{q,k}\left[1 - \delta_{q,0}\right]\ ,
\end{aligned} \tag{3.6}$$

where we have used the definition of the ground state (2.63) and (2.75) in the first row, the anticommutation relations for $a_q$ operators (A.5) in the second, third and fourth row and the property of orthonormality of fermionic states with different occupation numbers for the final row.

We cite the results for the other three correlation functions in the $|g^-\rangle$ state:

$$\langle g^-|\, a_q^\dagger a_k\, |g^-\rangle = \delta_{q,k}\delta_{q,0}\ , \tag{3.7a}$$

$$\langle g^-|\, a_q a_k\, |g^-\rangle = 0\ , \tag{3.7b}$$

$$\langle g^-|\, a_q^\dagger a_k^\dagger\, |g^-\rangle = 0\ , \tag{3.7c}$$

As before, notice the consistencies between the previous four equations.

As announced in the beginning of this section, we proceed with the correlation functions for $b_q$ operators by exploiting the just obtained correlation functions along

with the transformation (2.57), which we repeat and expand here for convenience:

$$a_q = \cos\theta_q \; b_q + \imath \sin\theta_q \; b^\dagger_{-q} \; , \tag{3.8a}$$

$$a^\dagger_{-q} = \imath \sin\theta_q \; b_q + \cos\theta_q \; b^\dagger_{-q} \tag{3.8b}$$

and also write out its inverse explicitly:

$$b_q = \cos\theta_q \; a_q - \imath \sin\theta_q \; a^\dagger_{-q} \; , \tag{3.9a}$$

$$b^\dagger_{-q} = -\imath \sin\theta_q \; a_q + \cos\theta_q \; a^\dagger_{-q} \; . \tag{3.9b}$$

Using these equations, along with (3.4) and (3.5), we obtain:

$$\begin{aligned} \langle g^+ | \, b_q b^\dagger_k \, | g^+ \rangle &= \langle g^+ | \left[ \cos\theta_q \; a_q - \imath \sin\theta_q \; a^\dagger_{-q} \right] \left[ \imath \sin\theta_k \; a_{-k} + \cos\theta_k \; a^\dagger_k \right] | g^+ \rangle \\ &= \langle g^+ | \cos\theta_q \cos\theta_k \; a_q a^\dagger_k \, | g^+ \rangle \\ &= \frac{1 + \cos(2\theta_q)}{2} \delta_{q,k} \; . \end{aligned} \tag{3.10}$$

Similarly, for the remaining three correlation functions in the $|g^+\rangle$ state we obtain:

$$\langle g^+ | \, b^\dagger_q b_k \, | g^+ \rangle = \frac{1 - \cos(2\theta_q)}{2} \delta_{q,k} \; , \tag{3.11a}$$

$$\langle g^+ | \, b_q b_k \, | g^+ \rangle = \imath \frac{\sin(2\theta_q)}{2} \delta_{q,-k} \; , \tag{3.11b}$$

$$\langle g^+ | \, b^\dagger_q b^\dagger_k \, | g^+ \rangle = \imath \frac{\sin(2\theta_q)}{2} \delta_{q,-k} \; . \tag{3.11c}$$

Notice that the last two equations are connected by a Hermitian conjugate and index exchange. Similarly, sum of (3.10) and the first equation in (3.11) is consistent with the anticommutation relations for $c$ operators (2.35).

We continue with calculations in the $|g^-\rangle$ state and use (3.9), along with (3.6) and (3.7):

$$\begin{aligned} \langle g^- | \, b_q b^\dagger_k \, | g^- \rangle &= \langle g^- | \left[ \cos\theta_q \; a_q - \imath \sin\theta_q \; a^\dagger_{-q} \right] \left[ \imath \sin\theta_k \; a_{-k} + \cos\theta_k \; a^\dagger_k \right] | g^- \rangle \\ &= \langle g^- | \cos\theta_q \cos\theta_k \; a_q a^\dagger_k + \sin\theta_q \sin\theta_k \; a^\dagger_{-q} a_{-k} \, | g^- \rangle \\ &= -\cos(2\theta_0) \delta_{q,k} \delta_{q,0} + \frac{1 + \cos(2\theta_q)}{2} \delta_{q,k} \; . \end{aligned} \tag{3.12}$$

The remaining correlation functions are:

$$\langle g^-|\, b_q^\dagger b_k\, |g^-\rangle = \cos(2\theta_0)\delta_{q,k}\delta_{q,0} + \frac{1-\cos(2\theta_q)}{2}\delta_{q,k}\ , \tag{3.13a}$$

$$\langle g^-|\, b_q b_k\, |g^-\rangle = \imath\frac{\sin(2\theta_q)}{2}\delta_{q,-k}\ , \tag{3.13b}$$

$$\langle g^-|\, b_q^\dagger b_k^\dagger\, |g^-\rangle = \imath\frac{\sin(2\theta_q)}{2}\delta_{q,-k}\ . \tag{3.13c}$$

One should again convince oneself of the internal consistency of these equations, as we have remarked for the $|g^+\rangle$ state.

Having obtained the correlation functions in the Fourier space, we turn back to the coordinate space by means of an inverse Fourier transform (7.15). We begin with the $|g^+\rangle$ state once again:

$$\begin{aligned}
\langle g^+|\, c_j c_l^\dagger\, |g^+\rangle =& \langle g^+|\left(\frac{1}{\sqrt{N}}\sum_{q\in\Gamma^+} e^{\imath qj} b_q\right)\left(\frac{1}{\sqrt{N}}\sum_{k\in\Gamma^+} e^{-\imath kl} b_k^\dagger\right)|g^+\rangle \\
=& \frac{1}{N}\sum_{q,k\in\Gamma^+} e^{\imath(qj-kl)}\,\langle g^+|\, b_q b_k^\dagger\, |g^+\rangle \\
=& \frac{1}{N}\sum_{q,k\in\Gamma^+} e^{\imath(qj-kl)}\frac{1+\cos(2\theta_q)}{2}\delta_{q,k} \\
=& \frac{1}{N}\sum_{q\in\Gamma^+} e^{\imath q(j-l)}\left[\frac{1+\cos(2\theta_q)}{2}\right]\ ,
\end{aligned} \tag{3.14}$$

where we have used (3.12) to obtain the third row. The rest of the correlation functions for the $c$ operators in the $|g^+\rangle$ state are:

$$\langle g^+|\, c_j^\dagger c_l\, |g^+\rangle = \frac{1}{N}\sum_{q\in\Gamma^+} e^{\imath q(j-l)}\left[\frac{1-\cos(2\theta_q)}{2}\right]\ , \tag{3.15a}$$

$$\langle g^+|\, c_j c_l\, |g^+\rangle = \frac{1}{N}\sum_{q\in\Gamma^+} e^{\imath q(j-l)}\left[\imath\frac{\sin(2\theta_q)}{2}\right]\ , \tag{3.15b}$$

$$\langle g^+|\, c_j^\dagger c_l^\dagger\, |g^+\rangle = \frac{1}{N}\sum_{q\in\Gamma^+} e^{\imath q(j-l)}\left[-\imath\frac{\sin(2\theta_q)}{2}\right]\ . \tag{3.15c}$$

Procedure for the $c$ operators in the $|g^-\rangle$ state is completely analogous and yields:

$$\langle g^-|\, c_j c_l^\dagger\, |g^-\rangle = \frac{1}{N}\sum_{q\in\Gamma^-} e^{\imath q(j-l)}\left[\frac{1+\cos(2\theta_q)}{2}\right] - \cos(2\theta_0)\ , \tag{3.16a}$$

$$\langle g^-|\, c_j^\dagger c_l\, |g^-\rangle = \frac{1}{N}\sum_{q\in\Gamma^-} e^{\imath q(j-l)}\left[\frac{1-\cos(2\theta_q)}{2}\right] + \cos(2\theta_0)\ , \tag{3.16b}$$

$$\langle g^-|\, c_j c_l\, |g^-\rangle = \frac{1}{N}\sum_{q\in\Gamma^-} e^{\imath q(j-l)}\left[\imath\frac{\sin(2\theta_q)}{2}\right]\ , \tag{3.16c}$$

$$\langle g^-|\, c_j^\dagger c_l^\dagger\, |g^-\rangle = \frac{1}{N}\sum_{q\in\Gamma^-} e^{\imath q(j-l)}\left[-\imath\frac{\sin(2\theta_q)}{2}\right]\ . \tag{3.16d}$$

upon using (3.9), (3.12) and (3.13), along with properties (2.56). Notice also that the terms including the faulty Bogoliubov angles must be substituted with the correct ones $\theta_0^{\text{corr}}$ in the previous eight equations, as was remarked in the beginning of this section.

To proceed, we find the announced Majorana correlation functions, which are necessary for calculating the physical spin correlation functions. We reiterate the definitions of the Majorana fermionic operators (3.2) here for convenience:

$$A_j \coloneqq \left(\bigotimes_{l=1}^{j-1}\sigma_l^z\right)\otimes\sigma_j^x = c_j^\dagger + c_j \quad \text{and} \quad B_j \coloneqq \left(\bigotimes_{l=1}^{j-1}\sigma_l^z\right)\otimes\sigma_j^y = \imath\left(c_j^\dagger - c_j\right)\ . \tag{3.17}$$

Using the previous two equations, we obtain the first Majorana correlation function for the $|g^+\rangle$ state:

$$\begin{aligned}
\langle g^+|\, A_j B_l\, |g^+\rangle =& \imath\,\langle g^+|\left[c_j^\dagger + c_j\right]\left[c_j^\dagger - c_j\right]|g^+\rangle \\
=& \imath\,\langle g^+|\, c_j^\dagger c_l^\dagger - c_j c_l\, |g^+\rangle + \imath\,\langle g^+|\, c_j c_l^\dagger - c_j^\dagger c_l\, |g^+\rangle \\
=& \frac{1}{N}\sum_{q\in\Gamma^+} e^{\imath q(j-l)}\left[\sin(2\theta_q)\right] + \frac{1}{N}\sum_{q\in\Gamma^+} e^{\imath q(j-l)}\left[\imath\cos(2\theta_q)\right] \\
=& \frac{\imath}{N}\sum_{q\in\Gamma^+} e^{\imath q(j-l)} e^{-\imath 2\theta_q} \\
=& \frac{\imath}{N}\sum_{q\in\Gamma^+} e^{\imath 2\theta_q} e^{-\imath q(j-l)}\ ,
\end{aligned} \tag{3.18}$$

where we have used (3.14) and (3.15) to get from the second to the third row and the property of the Bogoliubov angle (B.8) to get the final equation.

Similar calculation for the $|g^-\rangle$ state yields:

$$\langle g^-|\, A_j B_l\, |g^-\rangle = \frac{\imath}{N}\sum_{q\in\Gamma^-} e^{\imath 2\theta_q} e^{-\imath q(j-l)} - \frac{2\imath}{N}\cos(2\theta_0) \quad . \tag{3.19}$$

We have written the correlation functions for both states since, as we will soon see, they reduce to a more compact form upon introducing the corrections to Bogoliubov angles.

First of all, from (2.60) and (2.61) we see that in the $+$ sector the only potentially faulty angle is that of the $\pi$ mode and in the $1\mathrm{O}$ phase it is correct as it is so we can write:

$$\langle g^+|\, A_j B_l\, |g^+\rangle^{1\mathrm{O,\ corr}} = \frac{\imath}{N}\sum_{q\in\Gamma^+} e^{\imath 2\theta_q} e^{-\imath q(j-l)} \quad . \tag{3.20}$$

In the $2\mathrm{M}$ phase however, we must exclude it, but we wish to keep the form of $\sum_{\Gamma^+}$ because it will make the expression much more elegant and easier to use in calculations:

$$\langle g^+|\, A_j B_l\, |g^+\rangle^{2\mathrm{M,\ corr}} = \frac{\imath}{N}\sum_{q\in\Gamma^+\setminus\{\pi\}} e^{\imath 2\theta_q} e^{-\imath q(j-l)} + \frac{\imath}{N} e^{\imath 2\theta_\pi^{\mathrm{corr}}} e^{-\imath\pi(j-l)} \tag{3.21}$$

and now we add and subtract the incorrect term so that we can retain the original form of the sum:

$$\begin{aligned}
&\langle g^+|A_j B_l\, |g^+\rangle^{2\mathrm{M,\ corr}} \\
&\quad = \frac{\imath}{N}\sum_{q\in\Gamma^+\setminus\{\pi\}} e^{\imath 2\theta_q} e^{-\imath q(j-l)} + \frac{\imath}{N} e^{\imath 2\theta_\pi^{\mathrm{corr}}} e^{-\imath\pi(j-l)} + \frac{\imath}{N} e^{\imath 2\theta_\pi} e^{-\imath\pi(j-l)} - \frac{\imath}{N} e^{\imath 2\theta_\pi} e^{-\imath\pi(j-l)} \\
&\quad = \frac{\imath}{N}\sum_{q\in\Gamma^+} e^{\imath 2\theta_q} e^{-\imath q(j-l)} + \frac{2\imath}{N}(-1)^{j-l} \quad .
\end{aligned} \tag{3.22}$$

Analogous analysis for the $|g^-\rangle$ state, upon noticing that the problematic mode in this sector is the $0$ mode, yields:

$$\langle g^-|\, A_j B_l\, |g^-\rangle^{1\mathrm{O,\ corr}} = \frac{\imath}{N}\sum_{q\in\Gamma^-} e^{\imath 2\theta_q} e^{-\imath q(j-l)} \tag{3.23}$$

and also

$$\langle g^{-}|\, A_j B_l\, |g^{-}\rangle^{\text{2M, corr}} = \frac{\imath}{N}\sum_{q\in\Gamma^{-}} e^{\imath 2\theta_q} e^{-\imath q(j-l)} - \frac{2\imath}{N}\ . \tag{3.24}$$

Results given in (3.20), (3.22), (3.23) and (3.24) can be written in a more concise manner upon defining the function:

$$f_{\phi}^{\pm}(j-l) \coloneqq \begin{cases} 0\ ; \ \ \phi \in \langle -\frac{\pi}{2}, -\frac{\pi}{4}\rangle\ , \\ -(\mp 1)^{j-l+1}\ \ ; \ \ \phi \in \langle -\frac{\pi}{4}, 0\rangle\ . \end{cases} \tag{3.25}$$

Now the Majorana correlation functions for the first two phases phases can be written (omitting the corr denotation) as:

$$\boxed{\langle g^{\pm}|\, A_j B_l\, |g^{\pm}\rangle = \frac{\imath}{N}\sum_{q\in\Gamma^{\pm}} e^{\imath 2\theta_q} e^{-\imath q(j-l)} + \frac{2\imath}{N} f_{\phi}^{\pm}(j-l)}\ . \tag{3.26}$$

In the end of this section, we turn to the more elementary $\langle A_j A_l\rangle$ and $\langle B_j B_l\rangle$ correlation functions. As is easily seen, their final expressions contain no references to Bogoliubov angles so no amendments are needed:

$$\begin{aligned} \langle g^{\pm}|\, A_j A_l\, |g^{\pm}\rangle =& \langle g^{\pm}|\left[c_j^{\dagger} + c_j\right]\left[c_l^{\dagger} + c_l\right]|g^{\pm}\rangle \\ =& \langle g^{\pm}|\, c_j^{\dagger}c_l^{\dagger} + c_j c_l\, |g^{\pm}\rangle + \langle g^{\pm}|\, c_j^{\dagger}c_l + c_j c_l^{\dagger}\, |g^{\pm}\rangle \\ =& \frac{1}{N}\sum_{q\in\Gamma^{\pm}} e^{\imath q(j-l)} \\ =& \delta_{j,l}\ , \end{aligned} \tag{3.27}$$

where we have used (3.2) for the first equality; relations (3.14), (3.15) and (3.16) for the third row and then the delta function relation $\sum_{q\in\Gamma^{\pm}} e^{\imath q(j-l)} = N\delta_{j,l}$ to obtain the final equality.

Similar calculation for the $B_j$ operators yields the same expression and we thus write both of them as:

$$\boxed{\langle g^{\pm}|\, A_j A_l\, |g^{\pm}\rangle = \langle g^{\pm}|\, B_j B_l\, |g^{\pm}\rangle = \delta_{j,l}}\ . \tag{3.28}$$

### 3.2.2 $1$**O and** $2$**M phases—static spin correlation functions**

We now seek to evaluate the physically relevant two-point spin correlation functions which are in general of the form:

$$C^{\mu}_{jl} = \langle \sigma^{\mu}_j \sigma^{\mu}_l \rangle = \langle g^{\pm}| \, \sigma^{\mu}_j \sigma^{\mu}_l \, |g^{\pm}\rangle \quad \mu = x, y, z \ . \tag{3.29}$$

To do this, calculations must be carried out separately for each of the three directions. Let us do so.

Begin with the $x$ direction:

$$\begin{aligned}
C^{xx}_{jl} =& \langle g^{\pm}| \, \sigma^x_j \sigma^x_l \, |g^{\pm}\rangle \\
=& \langle g^{\pm}| \left[\sigma^-_j + \sigma^+_j\right] \left[\sigma^-_l + \sigma^+_l\right] |g^{\pm}\rangle \\
=& \langle g^{\pm}| \left[c^{\dagger}_j + c_j\right] \left(\bigotimes_{m=1}^{j-1} \sigma^z_m\right) \left(\bigotimes_{n=1}^{l-1} \sigma^z_n\right) \left[c^{\dagger}_l + c_l\right] |g^{\pm}\rangle \\
=& \langle g^{\pm}| \left[c^{\dagger}_j + c_j\right] \left[1 - 2c^{\dagger}_j c_j\right] \left(\bigotimes_{m=j+1}^{l-1} \sigma^z_m\right) \left[c^{\dagger}_l + c_l\right] |g^{\pm}\rangle \\
=& \langle g^{\pm}| \left[c^{\dagger}_j - c_j\right] \left(\bigotimes_{m=j+1}^{l-1} \left[c^{\dagger}_m + c_m\right] \left[c^{\dagger}_m - c_m\right]\right) \left[c^{\dagger}_l + c_l\right] |g^{\pm}\rangle \\
=& (-\imath)^{l-j} \, \langle g^{\pm}| \bigotimes_{m=j}^{l-1} B_m A_{m+1} \, |g^{\pm}\rangle \ ,
\end{aligned} \tag{3.30}$$

where we have used (2.3) for the second row, (2.30) for the third,

$$\left[c^{\dagger}_j + c_j\right] \left[1 - 2c^{\dagger}_j c_j\right] = c^{\dagger}_j + c_j - 2\left[1 - c^{\dagger}_j c_j\right] c_j = c^{\dagger}_j - c_j \ , \tag{3.31}$$

$\left(\sigma^z_j\right)^2 = 1$ and

$$\left[c^{\dagger}_m + c_m\right] \left[c^{\dagger}_m - c_m\right] = -c^{\dagger}_m c_m + c_m c^{\dagger}_m = -c^{\dagger}_m c_m + 1 - c^{\dagger}_m c_m = 1 - 2c^{\dagger}_m c_m = \sigma^z_m \tag{3.32}$$

for the fifth row and (3.2) for the last one.

Analogous calculations demonstrate that for the other two directions, i.e. $y$ and

$z$, similar relations for the correlation functions hold:

$$C^{yy}_{jl} = (\imath)^{l-j} \langle g^{\pm}| \bigotimes_{m=j}^{l-1} A_m B_{m+1} |g^{\pm}\rangle \ , \tag{3.33a}$$

$$C^{zz}_{jl} = - \langle g^{\pm}| A_j B_j A_l B_l |g^{\pm}\rangle \ . \tag{3.33b}$$

We now state an extraordinarily useful theorem—Wick's theorem [33]—in copious use both in condensed matter physics and quantum field theory.

**Theorem 1 (Wick's theorem for fermionic operators)** *Let $O_j$ be a linear combination of the fermionic operators $d_l$ and $d_l^\dagger$:*

$$O_j = \sum_l \left[ u_{jl} d_l^\dagger + v_{jl} d_l \right] \ , \tag{3.34}$$

*where $u_{jl}$ and $v_{jl}$ are in general $\in \mathbb{C}$. Then the expectation value of the product of $n$ such operators in their corresponding vacuum state $|0\rangle_d$ defined by*

$$d_j |0\rangle_d = 0 \ , \quad \forall j \tag{3.35}$$

*is a sum over all distinct contractions of pairs, taking into account the permutation sign:*

$$\begin{aligned} &{}_d\langle 0| O_1 O_2 \cdots O_n |0\rangle_d \\ &= \sum_{\substack{k_1<j_1,\ k_2<j_2,\cdots,\ k_n<j_n \\ j_1<j_2<\cdots<j_n}} (-1)^p \ {}_d\langle 0| O_{j_1} O_{k_1} |0\rangle_d \ {}_d\langle 0| O_{j_2} O_{k_2} |0\rangle_d \ \cdots \ {}_d\langle 0| O_{j_n} O_{k_n} |0\rangle_d \ . \end{aligned} \tag{3.36}$$

*The permutation sign $(-1)^p$ is defined as one encountered when permuting the sequence ordered as $1,\ 2, \cdots,\ n$ into $j_1, k_1, \cdots, j_n, k_n$.*

As for important remarks, first note that we have implicitly assumed that $n$ is even in the final sentence of the theorem. This is beacuse the expectation value in (3.36) is zero for odd $n$, as is easily seen since when the number is odd, all the operators except for one can be contracted in pairs, but its expectation value in the ground state will be zero— ${}_d\langle 0| d_j |0\rangle_d = 0$ by definition (3.35) and ${}_d\langle 0| d_j^\dagger |0\rangle_d = 0$ because the different occupation states for fermions are orthonormal (this line of thought is,

of course, valid for the former equation as well). Secondly, the operators for which we will apply the Wick's theorem are the $c$ operators to calculate the expansions such as (3.30) and (3.33). Fourier transform (7.15), along with (2.66), implies that the vacua for $b_q$ and $c_j$ operators are the same:

$$c_j \left|0\right\rangle = 0 \quad \forall j \ . \tag{3.37}$$

We now proceed to write out the expression for the $x$ direction correlation function $C_{jl}^{xx}$, given by (3.30). We see that by the Wick's theorem 1, we will need to evaluate three types of terms:

$$\left\langle A_j B_l \right\rangle \ , \quad \left\langle A_j A_l \right\rangle \quad \text{and} \quad \left\langle B_j B_l \right\rangle \ . \tag{3.38}$$

Since the latter two terms vanish for operators on different sites (indices) by virtue of (3.28), it is seen from (3.30) that the only nonvanishing contractions will be those of form $\langle A_j B_l \rangle$, given by (3.26). Thus, the expression (3.36) can be reduced to such terms, where we now denote the sum as that over all permutations $P$, each of which has a corresponding sign $p$, as defined before:

$$C_{jl}^{xx} = (-\imath)^{l-j} \sum_P (-1)^p \left\langle 0\right| B_j A_{P(j+1)} \left|0\right\rangle \left\langle 0\right| B_{j+1} A_{P(j+2)} \left|0\right\rangle \left\langle 0\right| B_j A_{P(j+1)} \left|0\right\rangle \ \cdots \left\langle 0\right| B_{l-1} A_{P(j)} \left|0\right\rangle \tag{3.39}$$

and the sum is recognised to have the form of the determinant [34]. Upon defining the abbreviations (the second equality is easily seen by using (3.2))

$$G(j-l) \coloneqq -\imath \left\langle g^{\pm}\right| A_j B_l \left|g^{\pm}\right\rangle = \imath \left\langle g^{\pm}\right| B_l A_j \left|g^{\pm}\right\rangle \tag{3.40}$$

this expression takes on the following form:

$$C_{jl}^{xx} = (-1)^r \begin{vmatrix} G(1) & G(0) & G(-1) & \dots & G(2-r) \\ G(2) & G(1) & G(0) & \dots & G(3-r) \\ G(3) & G(2) & G(1) & \dots & G(4-r) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G(r) & G(r-1) & G(r-2) & \dots & G(1) \end{vmatrix} \ , \tag{3.41}$$

where we have defined the distance between the two spin sites of interest $r = l - j$.

We observe that this expression is dependent only on said distance between the sites and thus write it in terms of $r$ only:

$$C^{xx}(r) \coloneqq C^{xx}_{jl} \ , \ \ r = l - j \ . \tag{3.42}$$

Analogous calculation for the $y$ direction yields:

$$C^{yy}(r) \coloneqq C^{yy}_{jl} = (-1)^r \begin{vmatrix} G(-1) & G(-2) & G(-3) & \dots & G(-r) \\ G(0) & G(-1) & G(-2) & \dots & G(1-r) \\ G(1) & G(0) & G(-1) & \dots & G(2-r) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G(r-2) & G(r-3) & G(r-4) & \dots & G(-1) \end{vmatrix} \tag{3.43}$$

upon using $r = l - j$.

The $z$ direction operator has the most elementary form and it is easily seen from the Wick's theorem (3.36) that, upon expanding (3.33), we obtain:

$$C^{zz}(r) \coloneqq C^{zz}_{jl} = \begin{vmatrix} G(0) & G(-r) \\ G(r) & G(0) \end{vmatrix} \ , \tag{3.44}$$

with $r = l - j$, as before.

An astute reader has noticed that all three matrices in (3.41), (3.43) and (3.44) have the special structure in the sense that all of the elements on their left-to-right diagonals have the same values—these matrices are known as *Toeplitz matrices*. Coincidentially, development of the theory of the asymptotic forms of their determinants—*Toeplitz determinants*—has been intimately related to the analysis of the XY and Ising models [20,35] and a vast amount of literature on their properties is accessible. The most useful among them, however, are those of the asymptotic behaviour of their determinants, as used in, e.g. [10]. In the present work (especially the forthcoming section 3.3), we will seek to evaluate the dynamic correlation functions with corresponding deteminants which will in general be extremely tedious or impossible to evaluate or expand by hand or not Toeplitz in their form and we will thus resort to numerical analysis for calculating their determinants for different numbers of spin sites $N$.

### 3.2.3 3I phase—static Majorana correlation functions

We now set out to calculate the Majorana correlation functions for the third phase. As we have discussed in the previous subsection, the most general ground state wavefunction is a linear combination of four states defined in (2.80) and (2.81). In this work, we choose a linear combination of only the two $|\pm p\rangle$ states, as was done in [11]:

$$|u_1, u_2\rangle := u_1 |p\rangle + u_2 |-p\rangle \quad . \tag{3.45}$$

This is partially due to the fact that the $p$ and $-p$ states belong to the same (odd) energy sector and thus the state in the previous equation has a definite parity along the $z$ axis, which will allow[38] us to apply the Wick's theorem.

Furthermore, the states in one sector can be obtained by acting with the parity operators $\Pi^{x,y}$ on the states in the other, if they are the eigenstates of the parity operator along the $z$ axis, which they are by construction. Along this, the restriction to the odd parity sector will be used to identify a special type of behaviour and eliminate the other ones, specifically the most interesting one. Since the process of calculating these functions is conceptually similar to the ones encountered in the previous sections for the first two phases, we only cite the final results of interest here and relegate the rest to the Appendix C which contains all of the intermediary results.

Then the Majorana correlation functions are:

$$\boxed{\langle A_j B_l \rangle_{u_1,u_2} = \frac{\imath}{N} \sum_{q \in \Gamma^-} e^{\imath 2\theta_q} e^{-\imath q(j-l)} - \frac{2\imath}{N} \cos\left[p\,(j-l) - 2\theta_p\right] - \frac{2\imath}{N} \left(u_1^* u_2 e^{-\imath p(j+l)} + \text{c.c.}\right)} \ , \tag{3.46}$$

with c.c. denoting the complex conjugate and $\langle\rangle_{u_1,u_2}$ denoting the expectation value in the $|u_1, u_2\rangle$ state given by (3.45) and also:

$$\boxed{\langle A_j A_l \rangle_{u_1,u_2} = \langle B_j B_l \rangle_{u_1,u_2} = \delta_{j,l} - \frac{2\imath}{N} \left(|u_1|^2 - |u_2|^2\right) \sin\left[p\,(j-l)\right]} \ . \tag{3.47}$$

[38] Recall that, for the Wick's theorem to be applicable, the operators in question ought to have vanishing expectation values. One can convince oneself that this does not hold for a general linear combination of all four states of the third phase.

### 3.2.4 3I phase—static spin correlation functions

As for the first two phases, we calculate the correlation functions for the products of two spin operators along one of the directions. Since these operators are the same for all three phases, we can replicate the results from the previous section up to the point of writing the expectation values in terms of the matrix determinants:

$$\begin{aligned} C_{jl}^{xx} =&(-\imath)^{l-j} \langle u_1, u_2| \bigotimes_{m=j}^{l-1} B_m A_{m+1} |u_1, u_2\rangle \ , \\ C_{jl}^{yy} =&(\imath)^{l-j} \langle u_1, u_2| \bigotimes_{m=j}^{l-1} A_m B_{m+1} |u_1, u_2\rangle \ , \\ C_{jl}^{zz} =&- \langle u_1, u_2| A_j B_j A_l B_l |u_1, u_2\rangle \ , \end{aligned} \tag{3.48}$$

where we have used the expectation values in the most general ground state of the odd parity sector $|u_1, u_2\rangle$ defined in (3.45).

Wishing to write these expectation values in terms of determinants as for the other two phases, we first note that these expressions will not be translationally invariant as the preceding ones since the Majorana correlation function (3.46) depends explicitly on both $j$ and $l$, not only their difference. Because of this, the total matrix will not be of Toeplitz form. Furthermore, consulting (7.35), we see that $\langle AA\rangle$ and $\langle BB\rangle$ will generally not be equal to Kronecker deltas, however, we will set $|u_1| = |u_2| = \frac{1}{\sqrt{2}}$ in later calculations since this choice will maximise the magnetisations we seek to obtain and it is thus appropriate to make this choice here as well, making these two correlation functions translationally invariant. Having all of this in mind, the train of thought for writing the determinants is the same as before (besides the Toeplitz form of matrices):

$$C_{jl}^{xx} = (-1)^{l-j} \begin{vmatrix} H(j+1,j) & H(j+1,j+1) & H(j+1,j+2) & \dots & H(j+1,l-1) \\ H(j+2,j) & H(j+2,j+1) & H(j+2,j+2) & \dots & H(j+2,l-1) \\ H(j+3,j) & H(j+3,j+1) & H(j+3,j+2) & \dots & H(j+3,l-1) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ H(l,j) & H(l,j+1) & H(l,j+2) & \dots & H(l,l-1) \end{vmatrix} , \tag{3.49}$$

with the function $H(j,l)$ defined as follows:

$$H(j,l) \coloneqq -\imath \langle u_1, u_2 | A_j B_l | u_1, u_2 \rangle = \imath \langle u_1, u_2 | B_l A_j | u_1, u_2 \rangle \ , \tag{3.50}$$

with imaginary unit factor in front to render the terms real. Later on, for simplicity we will not use this factor.

Analogous calculation for the $y$ and $z$ directions yields:

$$C_{jl}^{yy} = (-1)^{l-j} \begin{vmatrix} H(j,j+1) & H(j,j+2) & H(j,j+3) & \dots & H(j,l) \\ H(j+1,j+1) & H(j+1,j+2) & H(j+1,j+3) & \dots & H(j+1,l) \\ H(j+2,j+1) & H(j+2,j+2) & H(j+2,j+3) & \dots & H(j+2,l) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ H(l-1,j+1) & H(l-1,j+2) & H(l-1,j+3) & \dots & H(l-1,l) \end{vmatrix} , \tag{3.51}$$

and

$$C_{jl}^{zz} = \begin{vmatrix} H(j,j) & H(j,l) \\ H(l,j) & H(l,l) \end{vmatrix} . \tag{3.52}$$

Note that all three of these matrices would essentially be of the same form as those for the first two phases were their corresponding correlation functions translationally invariant.

## *3.3 Dynamic correlation functions*

Having obtained the static correlation functions, we now turn to the temporal evolution of the XY model, specifically its *dynamic correlation functions*. The particular circumstance which we will consider is that of a *quench* of the Hamiltonian (1.2) parameter[39] $\phi$. The change we will analyse is from $\phi_0$ to $\phi_1$ and in general between the same phase and also the different ones. However, before we begin developing the theory of the dynamic behaviour of the XY model, let us provide a short outline of the process. We start with obtaining the time evolved versions of the ground states for all three phases by emphasising the importance of the $0$ and $\pi$ modes. Here, the fact that their respective Hamiltonians are diagonal will come into play. We will continue with calculating the dynamic Majorana correlation functions and observe that

[39]Recall our discussion given in the section on symmetry properties of the model in which we have remarked that the Hamiltonian will retain its symmetries once it is evolved in time in this way.

the temporal evolution introduces additional terms in each. Finally, we will find the dynamic spin correlation functions in matrix form and see that their form will in general be that of a Pfaffian matrix, a short introduction to which is given in Appendix E.

### 3.3.1 General temporal evolution problem

As was announced while solving the XY model, the fact that its Hamiltonian is separable into subspaces corresponding to $q$ and $-q$ modes simultaneously for each $q$ for which the matrix is nondiagonal (all modes except $0$ and $\pi$) has the factorisation of the vacuum wavefunction over the positive modes $q$ (besides $\pi$) as a direct consequence. From this, we observe that it is possible to evolve the each term in the wave function separately[40].

Taking the aforementioned into consideration, we write the expression for time evolution of the general vacuum states:

$$|\Psi(t)\rangle = \bigotimes_{0<q<\pi;\ q\in\Gamma^{\pm}} |\psi_{q,\phi_1}(t)\rangle = \bigotimes_{0<q<\pi;\ q\in\Gamma^{\pm}} U_{q,\phi_1}(t)\,|\psi_{q,\phi_0}\rangle \ . \tag{3.53}$$

The previous equation implies that the vacuum state of the system was given by product of ground states of the Hamiltonian with parameter $\phi_0$ at the initial moment $t = 0$. At that same moment, quench of the system transformed the Hamiltonian into the one of same form, but with the parameter $\phi_1$. Temporal evolution of each term in the product of states is given by their respective evolution operators $U_{q,\phi_1}(t)$, which are determined from the time evolution differential equation [36]:

$$\imath\frac{\mathrm{d}}{\mathrm{d}t}U_{q,\phi_1}(t) = U_{q,\phi_1}(t)H_{\phi_1,q} \ , \tag{3.54}$$

with $H_{\phi_1,q}$ denoting the Hamiltonian term corresponding to the subspace of $q$ and $-q$ modes. Notice that the $0$ and $\pi$ modes will again demonstrate peculiar behaviour since the chosen basis for the Hamiltonian:

$$|0_q, 0_{-q}\rangle \coloneqq |0_q\rangle\,|0_{-q}\rangle \quad \text{and} \quad |1_q, 1_{-q}\rangle \coloneqq a_q^{\dagger}a_{-q}^{\dagger}\,|0_q, 0_{-q}\rangle \tag{3.55}$$

[40] Formally, this fact corresponds to the time evolution matrix being block diagonal and we are thus able to separate the corresponding blocks according to the subspaces in which they act. The important property is also that the values $q$ of different modes do not depend on the parameter $\phi$, implying that the form of products such as (2.65) will persist even after the system has evolved in time.

is ill defined for these modes[41].

Let us thus solve the equation (3.54) for all modes except $0$ and $\pi$. To do so, expand its matrix form:

$$\imath \begin{bmatrix} \dot{U}^{11}_{q,\phi_1}(t) & \dot{U}^{12}_{q,\phi_1}(t) \\ \dot{U}^{21}_{q,\phi_1}(t) & \dot{U}^{22}_{q,\phi_1}(t) \end{bmatrix} = 2 \begin{bmatrix} U^{11}_{q,\phi_1}(t) & U^{12}_{q,\phi_1}(t) \\ U^{21}_{q,\phi_1}(t) & U^{22}_{q,\phi_1}(t) \end{bmatrix} \begin{bmatrix} C_{q,\phi_1} & -\imath S_{q,\phi_1} \\ \imath S_{q,\phi_1} & -C_{q,\phi_1} \end{bmatrix} \ , \tag{3.56}$$

where the factor of two has emerged since for all the modes $q$ except $0$ and $\pi$ the Hamiltonian term for the $-q$ is the same as the one for $q$, as we have indicated explicitly. The four equations separate into two for $U^{11}$ and $U^{12}$ and two for $U^{21}$ and $U^{22}$. We write out the first two:

$$\begin{aligned} \dot{U}^{11}_{q,\phi_1}(t) &= -2\imath C_{q,\phi_1} U^{11}_{q,\phi_1}(t) + 2S_{q,\phi_1} U^{12}_{q,\phi_1}(t) \ , \\ \dot{U}^{12}_{q,\phi_1}(t) &= -2S_{q,\phi_1} U^{11}_{q,\phi_1}(t) + 2\imath C_{q,\phi_1} U^{12}_{q,\phi_1}(t) \ . \end{aligned} \tag{3.57}$$

These elementary equations are solved, e.g. by differentiating the second with respect to time, inserting into it the expression for $\dot{U}^{11}_{q,\phi_1}$ from the first and then finally rewriting $U^{11}_{q,\phi_1}$ from the second. In this way, we obtain:

$$\ddot{U}^{12}_{q,\phi_1}(t) + \lambda^2_{q,\phi_1} U^{12}_{q,\phi_1}(t) = 0 \ . \tag{3.58}$$

Reinserting this into the two initial differential equations yields the same equation for $U^{11}_{q,\phi_1}$ and those for $U^{22}_{q,\phi_1}$ and $U^{21}_{q,\phi_1}$ follow by symmetry. We must now endow these equations with initial conditions, which are determined from the fact that the evolution matrix at time $t = 0$ is an identity $U_{q,\phi_1}(0) = \mathbb{1}$, i.e.:

$$U^{11}_{q,\phi_1}(0) = U^{22}_{q,\phi_1}(0) = 1 \quad \text{and} \quad U^{12}_{q,\phi_1}(0) = U^{21}_{q,\phi_1}(0) = 0 \tag{3.59}$$

and also from the expression (3.56) upon inserting the equations we have just ob-

[41] Notice that, e.g. $|1_0, 1_0\rangle = 0$ because of the Pauli exclusion principle.

tained:

$$\dot{U}^{11}_{q,\phi_1}(0) = -2\imath C_{q,\phi_1} \ , \tag{3.60a}$$

$$\dot{U}^{12}_{q,\phi_1}(0) = -2S_{q,\phi_1} \ , \tag{3.60b}$$

$$\dot{U}^{21}_{q,\phi_1}(0) = 2S_{q,\phi_1} \ , \tag{3.60c}$$

$$\dot{U}^{22}_{q,\phi_1}(0) = 2\imath C_{q,\phi_1} \ . \tag{3.60d}$$

As is easily shown, the initial conditions altogether imply the solutions for the whole matrix[42] $U$:

$$U^{11}_{q,\phi_1}(t) = \cos\left[\lambda_{q,\phi_1} t\right] - \imath \frac{2C_{q,\phi_1}}{\lambda_{q,\phi_1}} \sin\left[\lambda_{q,\phi_1} t\right] \ , \tag{3.61a}$$

$$U^{12}_{q,\phi_1}(t) = -\frac{2S_{q,\phi_1}}{\lambda_{q,\phi_1}} \sin\left[\lambda_{q,\phi_1} t\right] \ , \tag{3.61b}$$

$$U^{21}_{q,\phi_1}(t) = \frac{2S_{q,\phi_1}}{\lambda_{q,\phi_1}} \sin\left[\lambda_{q,\phi_1} t\right] \ , \tag{3.61c}$$

$$U^{22}_{q,\phi_1}(t) = \cos\left[\lambda_{q,\phi_1} t\right] + \imath \frac{2C_{q,\phi_1}}{\lambda_{q,\phi_1}} \sin\left[\lambda_{q,\phi_1} t\right] \ . \tag{3.61d}$$

Having obtained the evolution operator, we can write the time evolved wavefunctions for all the modes except $0$ and $\pi$:

$$\begin{aligned}
\begin{pmatrix} \widetilde{\alpha}_q(t) \\ \widetilde{\beta}_q(t) \end{pmatrix} =: |\psi_q(t)\rangle = U_{q,\phi_1}(t)\,|\psi_q\rangle &= \begin{bmatrix} U^{11}_{q,\phi_1}(t) & U^{12}_{q,\phi_1}(t) \\ U^{21}_{q,\phi_1}(t) & U^{22}_{q,\phi_1}(t) \end{bmatrix} \begin{pmatrix} \alpha_q \\ \beta_q \end{pmatrix} \\
&= \begin{pmatrix} U^{11}_{q,\phi_1}(t)\alpha_{q,\phi_0} + U^{12}_{q,\phi_1}(t)\beta_{q,\phi_0} \\ U^{21}_{q,\phi_1}(t)\alpha_{q,\phi_0} + U^{22}_{q,\phi_1}(t)\beta_{q,\phi_0} \end{pmatrix} \\
&= \begin{pmatrix} \alpha_{q,\phi_0}\cos\left[\lambda_{q,\phi_1} t\right] + \frac{2}{\lambda_{q,\phi_1}}\left[-\imath C_{q,\phi_1}\alpha_{q,\phi_0} + S_{q,\phi_1}\beta_{q,\phi_0}\right]\sin\left[\lambda_{q,\phi_1} t\right] \\ \beta_{q,\phi_0}\cos\left[\lambda_{q,\phi_1} t\right] + \frac{2}{\lambda_{q,\phi_1}}\left[-S_{q,\phi_1}\alpha_{q,\phi_0} + \imath C_{q,\phi_1}\beta_{q,\phi_0}\right]\sin\left[\lambda_{q,\phi_1} t\right] \end{pmatrix} \ ,
\end{aligned} \tag{3.62}$$

upon introducing the time-dependent wave function coefficients $\widetilde{\alpha}_q(t)$ and $\widetilde{\beta}_q(t)$ which are understood to describe the system during the moment of and after the quenching of the Hamiltonian parameter from $\phi_0$ to $\phi_1$. We have herein exploited the relations (3.61) and (B.10) with (B.11).

Now that the time evolution is solved, it is important to emphasize several notational changes we have made—static coefficients in each mode wave function that

[42] One should convince oneself that the matrix $U$ is unitary for all $q$ and $\phi$, as it should be.

we have denoted with $\alpha_q$ and $\beta_q$ in Appendix B and are essentially sine and cosine of Bogoliubov angle $\theta_q$ per (B.11), now have an additional subscript describing the Hamiltonian parameter $\phi$, explicitly $\alpha_{q,\phi}$ and $\beta_{q,\phi}$. Along this, the same letters with overset tilde will be used to denote said coefficients when evolved in time. It is obvious that we have omitted the reference to parameter on the former lest it clutter the calculations of the static correlation functions. Hence, we will do the same for the latter[43] since the time-dependent coefficients will be used to calculate the dynamic correlation functions.

The previous line of equations demonstrates that the expressions for time-dependent wave function coefficients are cumbersome to work with, so we will identify their one[44] useful property and work with general expression in body of the thesis—this property is behaviour under usual $q \rightsquigarrow -q$ transformation, which can be deduced from (2.54) and (B.11) to be:

$$\widetilde{\alpha}_{-q}(t) = -\widetilde{\alpha}_q(t) \quad \text{and} \quad \widetilde{\beta}_{-q}(t) = \widetilde{\beta}_q(t) \ . \tag{3.63}$$

We now turn to the $0$ and $\pi$ modes. The first important fact to emphasise is that the already used base (3.55)[45] is obviously not appropriate for these modes since for the $0$ mode the expression $|1_0, 1_0\rangle = 0$ because of the Pauli exclusion principle and the $\pi$ mode has no negative counterpart. The appropriate basis for these modes would be that of occupancy or vacancy of each mode. Specifically, for the $0$ mode subspace:

$$|1_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |0_0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.64}$$

and for the $\pi$ mode subspace:

$$|1_\pi\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |0_\pi\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ . \tag{3.65}$$

It is obvious from the form of Hamiltonian (2.58) that it will look the same in this

[43] Also note that omitting the reference to the parameter $\phi$ in the time-dependent coefficients $\widetilde{\alpha}_q(t)$ and $\widetilde{\beta}_q(t)$ is convenient as well since they must respectively reduce to $\alpha_{q,\phi_0}$ and $\beta_{q,\phi_0}$ for $t = 0$ since the interaction parameter is equal to $\phi_0$ at that moment and we thus avoid this potential ambiguity.

[44] Note that these coefficients do not have a particularly convenient form when subjected to complex conjugation.

[45] Or (B.2).

basis (albeit with corrected energies), although it is instructive to obtain this result starting from (2.46) as well:

$$\begin{aligned} H_{0,\phi}|_{\{|1_0,0_0\rangle\}} =& \sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \quad \text{and} \\ H_{\pi,\phi}|_{\{|1_\pi,0_\pi\rangle\}} =& -\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \ , \end{aligned} \tag{3.66}$$

with $H_{q,\phi}$ denoting the term corresponding to the particular mode subspace in sum of form (2.46) or (2.58). Another peculiarity of the $0$ mode is that it is excited in the ground state wavefunctions (2.63) and (2.75). However, because of the independence of different subspaces, this is not that great of an inconvenience since we can work with the $0$ mode subspace separately. This is obviously true for the $\pi$ mode as well. Following the discussion for the other modes and upon realising that the diagonal form of the Hamiltonian terms for these two modes renders the calculations somewhat trivial, we omit writing the solutions to (3.54) and immediately write the evolved wave functions as:

$$|\psi_0(t=0)\rangle = |1_0\rangle \implies |\psi_0(t)\rangle = e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|1_0\rangle \ , \tag{3.67a}$$

$$|\psi_0(t=0)\rangle = |0_0\rangle \implies |\psi_0(t)\rangle = e^{\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|0_0\rangle \ , \tag{3.67b}$$

$$|\psi_\pi(t=0)\rangle = |1_\pi\rangle \implies |\psi_\pi(t)\rangle = e^{\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|1_\pi\rangle \ , \tag{3.67c}$$

$$|\psi_\pi(t=0)\rangle = |0_\pi\rangle \implies |\psi_\pi(t)\rangle = e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|0_\pi\rangle \tag{3.67d}$$

Having these expected simple time evolution factors in mind, we may once again consider the ground state wave functions in the first two phases (2.63) and (2.75). Since the general wavefunctions are the linear combinations of those particular terms, one of which has the $0$ mode excited and the other $\pi$ mode not excited, we see that the time factors originating from said modes will be the same in both cases. Thus, although these terms exist in the full expressions for the time-evolved ground states in

the first two phases:

$$|g^+(t)\rangle = \bigotimes_{0<q<\pi;\ q\in\Gamma^+} \left[\widetilde{\alpha}_q(t)\,|1_q, 1_{-q}\rangle + \widetilde{\beta}_q(t)\,|0_q, 0_{-q}\rangle\right] \otimes e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|0_\pi\rangle \quad , \tag{3.68a}$$

$$|g^-(t)\rangle = \bigotimes_{0<q<\pi;\ q\in\Gamma^-} \left[\widetilde{\alpha}_q(t)\,|1_q, 1_{-q}\rangle + \widetilde{\beta}_q(t)\,|0_q, 0_{-q}\rangle\right] \otimes e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|1_0\rangle \quad , \tag{3.68b}$$

we are able to extract and furthermore omit them on the account of arbitrariness of the global phase factor of the wave function.

Analysing the temporal evolution in the third phase is somewhat elementary now that we have derived most of the relations for the previous two phases. First off, when considering the ground states (2.80) and (2.81), we see that the ones in the even sector have the $\pi$ mode excited while for those in the odd sector the $0$ mode is not. Considering (3.67), we thus conclude that once again these potentially problematic modes will induce only an irrelevant global phase factor when evolved in time. Furthermore, if we consider the states in the odd parity sector (since they are of the simpler form for this; compare this fact to the previous two phases), one of the $\pm p$ modes is excited in those states so we need to account for this in the time evolution. To obtain a tad more illuminating form of these terms, we act on the vacuum states (2.65) with the creation operators while using (3.8):

$$\begin{aligned}
&a_p^\dagger \left[\cos\theta_p\,|0_p, 0_{-p}\rangle - \imath\sin\theta_p\,|1_p, 1_{-p}\rangle\right] \\
&= \left[\cos\theta_p b_p^\dagger - \imath\sin\theta_p b_{-p}\right]\left[\cos\theta_p\,|0_p, 0_{-p}\rangle - \imath\sin\theta_p\,|1_p, 1_{-p}\rangle\right] \\
&= \left[\cos^2\theta_p + \sin^2\theta_p\right]|1_p, 0_{-p}\rangle \\
&= |1_p, 0_{-p}\rangle
\end{aligned} \tag{3.69}$$

and similarly for its negative counterpart:

$$a_{-p}^\dagger \left[\cos\theta_p\,|0_p, 0_{-p}\rangle - \imath\sin\theta_p\,|1_p, 1_{-p}\rangle\right] = |0_p, 1_{-p}\rangle \quad , \tag{3.70}$$

as expected. A simplifying circumstance is that, as is evident from the previous expression, the ket belonging to the $\pm p$ modes will not be evolved in time since the terms in the Hamiltonian (2.58) corresponding to these kets are zero; this is readily seen from (3.56). Therefore we can, using the already calculated expression for the other modes (3.62), write the expression for the time evolved ground state wave-

functions in the third phase:

$$|\pm p(t)\rangle = \left( \bigotimes_{0<q<\pi;q\in\Gamma^-\setminus\{p\}} \left[ \widetilde{\alpha}_q(t)\,|1_q,1_{-q}\rangle + \widetilde{\beta}_q(t)\,|0_q,0_{-q}\rangle \right] \right) \otimes |1_{\pm p},0_{\mp p}\rangle \otimes e^{\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|0_0\rangle \quad . \tag{3.71}$$

As for the even parity sector, in accordance with the discussion on the symmetry properties of the model, we will not need the time evolution of its ground states (albeit it is analogous to the given one) and express them by action with the parity operators on the even sector ones.

The main results from this section which we will use repeatedly in the following are (3.68) and (3.71), which determine the time evolution for all the modes in both parity sectors. The process of evaluating the correlation functions will follow the one of the static case in full.

### 3.3.2 1O and 2M phases—dynamic Majorana correlation functions

In the first two phases, we start with the even parity sector and discuss the odd parity sector using the symmetry properties of the model discussed in the introduction. The form of the ground states enables us to immediately find the actions of $b_q$ operators:

$$\begin{aligned} b_q\,|g^+(t)\rangle \propto\, & b_q \left[ \widetilde{\alpha}_q(t)\,|1_q,1_{-q}\rangle + \widetilde{\beta}_q(t)\,|0_q,0_{-q}\rangle \right] \otimes e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|0_\pi\rangle\,[1-\delta_{q,\pi}] + \\ & + b_\pi\,|\psi_q(t)\rangle \otimes e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|0_\pi\rangle\,\delta_{q,\pi} \\ =& \widetilde{\alpha}_q(t)\,|0_q,1_{-q}\rangle \otimes e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|0_\pi\rangle\,[1-\delta_{q,\pi}] \quad , \end{aligned} \tag{3.72}$$

where the Kronecker-delta symbols have come in handy for writing the total wave function as a sum of two terms, depending on whether the annihilation operator is that of the $\pi$ mode or not. Contributions that have vanished have done so because of their respective annihilation operators. We have also exploited (3.62) to write the unaltered time-evolved wave functions for modes other than $\pi$. A similar calculation for the creation operators yields:

$$\begin{aligned} b_q^\dagger\,|g^+(t)\rangle =& \widetilde{\beta}_q(t)\,|1_q,1_{-q}\rangle\,|1_q,0_{-q}\rangle \otimes e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|0_\pi\rangle\,[1-\delta_{q,\pi}] + \\ & + |\psi_q(t)\rangle \otimes e^{-\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t}\,|1_\pi\rangle\,\delta_{q,\pi} \quad . \end{aligned} \tag{3.73}$$

It is important to notice, as in the previous section, that the time evolution factor for the $\pi$ mode is the same in both cases so it can be omitted as the global phase factor which will vanish once the expectation values of interest are calculated. This goes for the $0$ mode in the odd parity sector as well. We can now proceed with obtaining the correlation functions (expectation values):

$$\begin{aligned}\langle g^+(t)|\, b_q b_k^\dagger \,|g^+(t)\rangle =&|\widetilde{\beta}_q(t)|^2\delta_{q,k}\left[1-\delta_{q,\pi}\right]+\delta_{q,k}\delta_{q,\pi}\\ =&|\widetilde{\beta}_q(t)|^2\delta_{q,k}+|\widetilde{\alpha}_\pi(t)|^2\delta_{q,k}\delta_{q,\pi}\ ,\end{aligned} \tag{3.74}$$

where we have exploited the orthonormality of the fermionic states for all the modes in the even parity sector and also the fact that each of the wave functions in (3.68) is normalised. However, another important remark is in order. Since we have written the correct form of the time evolution of the wave function corresponding to the $\pi$ mode, the emergence of the Bogoliubov angle for the $\pi$ mode may be unexpected, but it is of mathematical nature since we have chosen to write the result in a more convenient form; the expressions for the faulty Bogoliubov angles ought to be considered as they were when the static correlation functions were calculated. Continuing in a similar manner, we obtain the rest of the $b_q$ operator expectation values:

$$\langle g^+(t)|\, b_q^\dagger b_k \,|g^+(t)\rangle =|\widetilde{\alpha}_q(t)|^2\delta_{q,k}\left[1-\delta_{q,\pi}\right]\ , \tag{3.75a}$$

$$\langle g^+(t)|\, b_q b_k \,|g^+(t)\rangle =-\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\delta_{q,-k}\left[1-\delta_{q,\pi}\right]\left[1-\delta_{k,\pi}\right]\ , \tag{3.75b}$$

$$\langle g^+(t)|\, b_q^\dagger b_k^\dagger \,|g^+(t)\rangle =\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)\delta_{q,-k}\left[1-\delta_{q,\pi}\right]\left[1-\delta_{k,\pi}\right]\ , \tag{3.75c}$$

where the last terms in the last two equations are redundant, but written for clarity. As before, it is useful to check the internal consistency of these results.

We continue with the $c_j$ operators correlation functions[46] and exploit (3.74):

$$\begin{aligned}\langle g^+(t)|\, c_j c_l^\dagger \,|g^+(t)\rangle =&\frac{1}{N}\sum_{q,k\in\Gamma^+} e^{\imath(qj-kl)}\,\langle g^+(t)|\, b_q b_k^\dagger \,|g^+(t)\rangle\\ =&\frac{1}{N}\sum_{q,k\in\Gamma^+}\left[|\widetilde{\beta}_q(t)|^2\delta_{q,k}+|\widetilde{\alpha}_\pi(t)|^2\delta_{q,k}\delta_{q,\pi}\right]\\ =&\frac{1}{N}\sum_{q\in\Gamma^+\setminus\{\pi\}} e^{\imath q(j-l)}|\widetilde{\beta}_q(t)|^2+\frac{1}{N}(-1)^{j-l}\end{aligned} \tag{3.76}$$

[46] It is useful to notice that the following sums are over all the modes since they stem from the Fourier transform, not the ground state wave functions.

and similarly for the rest of the expectation values:

$$\langle g^+(t)|\, c_j^\dagger c_l \,|g^+(t)\rangle = \frac{1}{N} \sum_{q\in\Gamma^+\setminus\{\pi\}} e^{-\imath q(j-l)} |\widetilde{\alpha}_q(t)|^2 \ , \tag{3.77a}$$

$$\langle g^+(t)|\, c_j c_l \,|g^+(t)\rangle = \frac{1}{N} \sum_{q\in\Gamma^+\setminus\{\pi\}} e^{\imath q(j-l)} \left[-\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\right] \ , \tag{3.77b}$$

$$\langle g^+(t)|\, c_j^\dagger c_l^\dagger \,|g^+(t)\rangle = \frac{1}{N} \sum_{q\in\Gamma^+\setminus\{\pi\}} e^{-\imath q(j-l)} \left[\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)\right] \ . \tag{3.77c}$$

After the obligatory internal consistency checks, we proceed with the Majorana correlation functions and exploit (3.76) and (3.77) along with the properties (3.63) to obtain:

$$\begin{aligned}\langle A_j B_l\rangle_{g^+(t)} &= \imath\langle (c_j^\dagger + c_j)(c_l^\dagger - c_l)\rangle_{g^+(t)} \\ &= \frac{\imath}{N} \sum_{q\in\Gamma^+\setminus\{\pi\}} \Big[\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t) e^{-\imath q(j-l)} + \widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t) e^{\imath q(j-l)} \\ &\quad -|\widetilde{\alpha}_q(t)|^2 e^{-\imath q(j-l)} + |\widetilde{\beta}_q(t)|^2 e^{\imath q(j-l)}\Big] + \frac{\imath}{N}(-1)^{j-l} \ .\end{aligned} \tag{3.78}$$

The previous equation is now amended, just as in the case of the static correlation functions, by adding and subtracting the faulty Bogoliubov angles to the sums so as to render turning to integrals in the thermodynamic limit $N \to \infty$ possible. It is also observed that a completely analogous calculation yields the result for the ground state of the odd sector $|g^-(t)\rangle$ as well. In this way, a joint expression for the time-dependent Majorana correlation functions is obtained for the first two phases and also both parity sectors:

$$\boxed{\begin{aligned}\langle A_j B_l\rangle_{g^\pm(t)} =& \frac{\imath}{N} \sum_{q\in\Gamma^\pm} \Big[\Big(|\widetilde{\beta}_q(t)|^2 - |\widetilde{\alpha}_q(t)|^2\Big)\cos\left[q\,(j-l)\right] + \\ &+ \imath\Big(\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t) - \widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)\Big)\sin\left[q\,(j-l)\right]\Big] + \frac{2\imath}{N} f_{\phi_0}^{\pm}\,(j-l)\end{aligned}} \ , \tag{3.79}$$

with the function appearing in the last term defined in (3.25). Firstly, it is important to notice that this relation reduces to (3.26) for $t = 0$, as it should. Furthermore, the only[47] potentially faulty Bogoliubov angles will be those in the beginning, i.e. for the initial parameter value $\phi_0$.

In a similar manner, the remaining correlation functions are obtained for the first

[47] This can also be seen from the time-evolved coefficients in (3.62) since the Bogoliubov angles appear only for the initial parameter value $\phi_0$.

two phases as well:

$$\boxed{\langle A_j A_l \rangle_{g^{\pm}(t)} = \delta_{j,l} - \frac{\imath}{N} \sum_{q \in \Gamma^{\pm}} \left( \widetilde{\alpha}_q^*(t) \widetilde{\beta}_q(t) + \widetilde{\alpha}_q(t) \widetilde{\beta}_q^*(t) \right) \sin\left[q\,(j-l)\right]} \tag{3.80}$$

and

$$\boxed{\langle B_j B_l \rangle_{g^{\pm}(t)} = \delta_{j,l} + \frac{\imath}{N} \sum_{q \in \Gamma^{\pm}} \left( \widetilde{\alpha}_q^*(t) \widetilde{\beta}_q(t) + \widetilde{\alpha}_q(t) \widetilde{\beta}_q^*(t) \right) \sin\left[q\,(j-l)\right]} \,, \tag{3.81}$$

which both correctly reduce to (3.28) for $t = 0$.

### 3.3.3 $1$**O and** $2$**M phases—dynamic spin correlation functions**

Calculation of the dynamic Majorana correlation functions will be more complicated than that of their static counterparts since, *as per* (3.80) and (3.81), the $\langle A_j A_l \rangle$ and $\langle B_j B_l \rangle$ terms are generally different from Kronecker deltas. This implies that (again, in general) there will be significantly more nonvanishing contractions of these operators and to find the appropriate representations in terms of matrix determinants we need the concept of Pfaffian, which is defined and motivated with its properties explained in Appendix E and the reader should give it a read before continuing.

For the corresponding determinants we will define three types of abbreviations, having in mind the fact that all three dynamic Majorana correlation functions are translationally invariant in the sense that they only depend on the difference between the two sites of interest $r = l - j$. The first one is the time-dependent version of (3.40):

$$\widetilde{F}_2(j-l) \coloneqq \langle g^{\pm}(t)|\, A_j B_l \,|g^{\pm}(t)\rangle = -\,\langle g^{\pm}(t)|\, B_l A_j \,|g^{\pm}(t)\rangle \quad , \tag{3.82}$$

where the time dependence of $\widetilde{F}_2$ is implied, but omitted in writing lest it clutter the succeeding equations. Also note that the imaginary factor is omitted[48] in front of the correlation function. This is due to the fact that it will make writing the final expressions simpler, i.e. without lurking factors attached to each term. Secondly, since the $\langle A_j A_l \rangle$ and $\langle B_j B_l \rangle$ expectation values are now different, we define the

[48] Remember that these factors were used previously to render the abbreviations real.

appropriate function for each one:

$$\widetilde{F}_1(j-l) \coloneqq \langle g^{\pm}(t)|\, A_j A_l\, |g^{\pm}(t)\rangle \tag{3.83}$$

and

$$\widetilde{F}_3(j-l) \coloneqq \langle g^{\pm}(t)|\, B_j B_l\, |g^{\pm}(t)\rangle \quad , \tag{3.84}$$

with the numbers $1$, $2$ and $3$ chosen by the lexicographic order of expectation values. Then for the expectation values of operators such as (3.30) and (3.33) we will have the matrix of each dimension twice as large as that of the static case. Note also that these operators are the same for all phases and both static and dynamic regimes. More precise argumentation and additional literature required for obtaining these expressions is, as was already mentioned, relegated to Appendix E. The first matrix of interest is for the $x$ direction:

$$\left[(-\imath)^r\, \widetilde{C}^{xx}_{jl}(t)\right]^2 \coloneqq \left[(-\imath)^r\, \widetilde{C}^{xx}_{j-l}(t)\right]^2$$

$$= \left|\begin{array}{cccc|cccc} 0 & \widetilde{F}_1(-1) & \dots & \widetilde{F}_1(1-r) & \widetilde{F}_2(1) & \widetilde{F}_2(0) & \dots & \widetilde{F}_2(2-r) \\ \widetilde{F}_1(1) & 0 & \dots & \widetilde{F}_1(2-r) & \widetilde{F}_2(2) & \widetilde{F}_2(1) & \dots & \widetilde{F}_2(3-r) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_1(r-1) & \widetilde{F}_1(r-2) & \dots & 0 & \widetilde{F}_2(r) & \widetilde{F}_2(r-1) & \dots & \widetilde{F}_2(1) \\ \hline -\widetilde{F}_2(1) & -\widetilde{F}_2(2) & \dots & -\widetilde{F}_2(r) & 0 & \widetilde{F}_3(-1) & \dots & \widetilde{F}_3(1-r) \\ -\widetilde{F}_2(0) & -\widetilde{F}_2(1) & \dots & -\widetilde{F}_2(r-1) & \widetilde{F}_3(1) & 0 & \dots & \widetilde{F}_3(2-r) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\widetilde{F}_2(2-r) & -\widetilde{F}_2(r-1) & \dots & -\widetilde{F}_2(1) & \widetilde{F}_3(r-1) & \dots & \widetilde{F}_3(r-2) & 0 \end{array}\right| . \tag{3.85}$$

Similarly, for the $yy$ correlation function we obtain:

$$\left[(-\imath)^r\,\widetilde{C}^{yy}_{jl}(t)\right]^2 \coloneqq \left[(-\imath)^r\,\widetilde{C}^{yy}_{j-l}(t)\right]^2$$

$$= \frac{\begin{vmatrix} 0 & \widetilde{F}_1(-1) & \dots & \widetilde{F}_1(1-r) \\ \widetilde{F}_1(1) & 0 & \dots & \widetilde{F}_1(2-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_1(r-2) & \widetilde{F}_1(r-3) & \dots & 0 \end{vmatrix} \begin{vmatrix} \widetilde{F}_2(-1) & \widetilde{F}_2(-2) & \dots & \widetilde{F}_2(-r) \\ \widetilde{F}_2(0) & \widetilde{F}_2(-1) & \dots & \widetilde{F}_2(1-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_2(r-2) & \widetilde{F}_2(r-3) & \dots & \widetilde{F}_2(-1) \end{vmatrix}}{\begin{vmatrix} -\widetilde{F}_2(-1) & -\widetilde{F}_2(0) & \dots & -\widetilde{F}_2(r-2) \\ -\widetilde{F}_2(-2) & -\widetilde{F}_2(-1) & \dots & -\widetilde{F}_2(r-3) \\ \vdots & \vdots & \ddots & \vdots \\ -\widetilde{F}_2(-r) & -\widetilde{F}_2(r-1) & \dots & -\widetilde{F}_2(1) \end{vmatrix} \begin{vmatrix} 0 & \widetilde{F}_3(-1) & \dots & \widetilde{F}_3(1-r) \\ \widetilde{F}_3(1) & 0 & \dots & \widetilde{F}_3(2-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_3(1-r) & \dots & \widetilde{F}_3(r-2) & 0 \end{vmatrix}}, \tag{3.86}$$

with the distance between two sites of interest $r = l-j$, as before. These two matrices are both of dimension $2r \times 2r$.

Finally, for the $z$ direction correlation function we obtain in a similar way:

$$\left[-\widetilde{C}^{zz}_{jl}(t)\right]^2 \coloneqq \left[-\widetilde{C}^{zz}_{j-l}(t)\right]^2$$

$$= \frac{\begin{vmatrix} 0 & \widetilde{F}_1(-r) \\ \widetilde{F}_1(r) & 0 \end{vmatrix} \begin{vmatrix} \widetilde{F}_2(0) & \widetilde{F}_2(-r) \\ \widetilde{F}_2(r) & \widetilde{F}_2(0) \end{vmatrix}}{\begin{vmatrix} -\widetilde{F}_2(0) & -\widetilde{F}_2(r) \\ -\widetilde{F}_2(-r) & -\widetilde{F}_2(0) \end{vmatrix} \begin{vmatrix} 0 & \widetilde{F}_3(-r) \\ \widetilde{F}_3(r) & 0 \end{vmatrix}}. \tag{3.87}$$

### 3.3.4 3I phase—dynamic Majorana correlation functions

The time evolved ground states of the odd sector ground states in the third phase are given by (3.71). Following the preceding sections, the calculations of the dynamic Majorana correlation functions are analogous to the ones in previous two phases and thus we only cite the final expression here and list the results for each step in the

calculations in Appendix D:

$$\begin{aligned}
&\langle A_j B_l\rangle_{u_1,u_2}(t)\\
&=\frac{\imath}{N}\sum_{q\in\Gamma^-}\left[\left(|\widetilde{\beta}_q(t)|^2-|\widetilde{\alpha}_q(t)|^2\right)\cos\left[q\left(j-l\right)\right]-\imath\left(\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)-\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\right)\sin\left[q\left(j-l\right)\right]\right]-\\
&-\frac{2\imath}{N}\left[\left(|\widetilde{\beta}_p(t)|^2-|\widetilde{\alpha}_p(t)|^2\right)\cos\left[p\left(j-l\right)\right]-\imath\left(\widetilde{\alpha}_p^*(t)\widetilde{\beta}_p(t)-\widetilde{\alpha}_p(t)\widetilde{\beta}_p^*(t)\right)\sin\left[p\left(j-l\right)\right]\right]-\\
&-\frac{2\imath}{N}\left(u_1^*u_2e^{-\imath p(j+l)}+\text{c.c.}\right)
\end{aligned}\tag{3.88}$$

and we note that for $t=0$ the first row reduces to the first term in (3.46), the second row to the second term and the third row to the third term in the same equation. The other two Majorana correlation functions of interest are:

$$\begin{aligned}
&\langle A_j A_l\rangle_{u_1,u_2}(t)\\
&=\delta_{j,l}-\frac{\imath}{N}\sum_{q\in\Gamma^-}\left(\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)+\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\right)\sin\left[q\left(j-l\right)\right]+\\
&+\frac{2\imath}{N}\left(\widetilde{\alpha}_p^*(t)\widetilde{\beta}_p(t)+\widetilde{\alpha}_p(t)\widetilde{\beta}_p^*(t)\right)\sin\left[p\left(j-l\right)\right]-\frac{2\imath}{N}\left(|u_1|^2-|u_2|^2\right)\sin\left[p\left(j-l\right)\right]
\end{aligned}\tag{3.89}$$

and

$$\begin{aligned}
&\langle B_j B_l\rangle_{u_1,u_2}(t)\\
&=\delta_{j,l}+\frac{\imath}{N}\sum_{q\in\Gamma^-}\left(\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)+\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\right)\sin\left[q\left(j-l\right)\right]-\\
&-\frac{2\imath}{N}\left(\widetilde{\alpha}_p^*(t)\widetilde{\beta}_p(t)+\widetilde{\alpha}_p(t)\widetilde{\beta}_p^*(t)\right)\sin\left[p\left(j-l\right)\right]-\frac{2\imath}{N}\left(|u_1|^2-|u_2|^2\right)\sin\left[p\left(j-l\right)\right]
\end{aligned},\tag{3.90}$$

both of which reduce to (7.35) for $t=0$, as they should.

### 3.3.5 3I phase—dynamic spin correlation functions

Comparing the forms of the dynamic Majorana correlation functions for the first two phases and the third one we see that, since the two point spin operators we seek to evaluate are the same, the correlation functions will have the same form, although it is evident that the translational invariance in this case will be violated for the $\langle A_j B_l\rangle$ terms, as seen from (7.44). As for the static spin correlation functions in the AFM phase, this will indeed be the case. Also, consulting the form of (7.42) and (7.43) we see that, regardless of choice of the coefficients in ground states (2.81), the $\langle A_j A_l\rangle$

and $\langle B_j B_l \rangle$ correlation functions will in general be different from Kronecker deltas. Thus, we ought to combine the lack of translational invariance as well as the fact that the matrices will have both dimensions twice as large. As before, we begin by defining the appropriate abbreviations for all the Majorana correlation functions

$$\widetilde{H}_2^{u_1,u_2}(j,l) \coloneqq \langle A_j B_l \rangle_{u_1,u_2}(t) = -\langle B_l A_j \rangle_{u_1,u_2}(t) \ , \tag{3.91}$$

$$\widetilde{H}_1^{u_1,u_2}(j-l) \coloneqq \langle A_j A_l \rangle_{u_1,u_2}(t) \tag{3.92}$$

and

$$\widetilde{H}_3^{u_1,u_2}(j-l) \coloneqq \langle B_j B_l \rangle_{u_1,u_2}(t) \tag{3.93}$$

since the translational invariance still holds for $\langle A_j A_l \rangle$ and $\langle B_j B_l \rangle$ terms. It is instructive to note that we have once again omitted the imaginary unit perfactor in the first abbreviation since it would unnecessarily complicate the form of matrices we will soon write.

Operators for the two-point correlation functions are still of the same form given by (3.30) and (3.33) and their corresponding matrices[49] are (on the following page):

[49] We mention once again that the discussion of this and similar previous and forthcoming results are given in Appendix E.

$$\left[(-\imath)^r\,\widetilde{C}^{xx}_{jl}(t)\right]^2 \coloneqq$$

$$\left[(-\imath)^r\,\widetilde{C}^{xx}_{j-l}(t)\right]^2 = \frac{\begin{vmatrix} 0 & \widetilde{H}_1^{u_1,u_2}(-1) & \dots & \widetilde{H}_1^{u_1,u_2}(1-r) \\ \widetilde{H}_1^{u_1,u_2}(1) & 0 & \dots & \widetilde{H}_1^{u_1,u_2}(2-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{H}_1^{u_1,u_2}(r-1) & \widetilde{H}_1^{u_1,u_2}(r-2) & \dots & 0 \end{vmatrix} \begin{vmatrix} \widetilde{H}_2^{u_1,u_2}(j+1,j) & \widetilde{H}_2^{u_1,u_2}(j+1,j+1) & \dots & \widetilde{H}_2^{u_1,u_2}(j+1,l-1) \\ \widetilde{H}_2^{u_1,u_2}(j+2,j) & \widetilde{H}_2^{u_1,u_2}(j+2,j+1) & \dots & \widetilde{H}_2^{u_1,u_2}(j+2,l-1) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{H}_2^{u_1,u_2}(l,j) & \widetilde{H}_2^{u_1,u_2}(l,j+1) & \dots & \widetilde{H}_2^{u_1,u_2}(l,l-1) \end{vmatrix}}{\begin{vmatrix} -\widetilde{H}_2^{u_1,u_2}(j+1,j) & -\widetilde{H}_2^{u_1,u_2}(j+2,j) & \dots & -\widetilde{H}_2^{u_1,u_2}(l,j) \\ -\widetilde{H}_2^{u_1,u_2}(j+1,j+1) & -\widetilde{H}_2^{u_1,u_2}(j+2,j+1) & \dots & -\widetilde{H}_2^{u_1,u_2}(l,j+1) \\ \vdots & \vdots & \ddots & \vdots \\ -\widetilde{H}_2^{u_1,u_2}(j+1,l-1) & -\widetilde{H}_2^{u_1,u_2}(j+2,l-1) & \dots & -\widetilde{H}_2^{u_1,u_2}(l,l-1) \end{vmatrix} \begin{vmatrix} 0 & \widetilde{H}_3^{u_1,u_2}(-1) & \dots & \widetilde{H}_3^{u_1,u_2}(1-r) \\ \widetilde{H}_3^{u_1,u_2}(1) & 0 & \dots & \widetilde{H}_3^{u_1,u_2}(2-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{H}_3^{u_1,u_2}(r-1) & \widetilde{H}_3^{u_1,u_2}(r-2) & \dots & 0 \end{vmatrix}}\,, \tag{3.94}$$

$$\left[(-\imath)^r\,\widetilde{C}^{yy}_{jl}(t)\right]^2 \coloneqq$$

$$\left[(-\imath)^r\,\widetilde{C}^{yy}_{j-l}(t)\right]^2 = \frac{\begin{vmatrix} 0 & \widetilde{H}_1^{u_1,u_2}(-1) & \dots & \widetilde{H}_1^{u_1,u_2}(1-r) \\ \widetilde{H}_1^{u_1,u_2}(1) & 0 & \dots & \widetilde{H}_1^{u_1,u_2}(2-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{H}_1^{u_1,u_2}(r-1) & \widetilde{H}_1^{u_1,u_2}(r-2) & \dots & 0 \end{vmatrix} \begin{vmatrix} \widetilde{H}_2^{u_1,u_2}(j,j+1) & \widetilde{H}_2^{u_1,u_2}(j,j+2) & \dots & \widetilde{H}_2^{u_1,u_2}(j,l) \\ \widetilde{H}_2^{u_1,u_2}(j+1,j+1) & \widetilde{H}_2^{u_1,u_2}(j+1,j+2) & \dots & \widetilde{H}_2^{u_1,u_2}(j+1,l) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{H}_2^{u_1,u_2}(l-1,j+1) & \widetilde{H}_2^{u_1,u_2}(l-1,j+2) & \dots & \widetilde{H}_2^{u_1,u_2}(l-1,l) \end{vmatrix}}{\begin{vmatrix} -\widetilde{H}_2^{u_1,u_2}(j,j+1) & -\widetilde{H}_2^{u_1,u_2}(j+1,j+1) & \dots & -\widetilde{H}_2^{u_1,u_2}(l-1,j+1) \\ -\widetilde{H}_2^{u_1,u_2}(j,j+2) & -\widetilde{H}_2^{u_1,u_2}(j+1,j+2) & \dots & -\widetilde{H}_2^{u_1,u_2}(l-1,j+2) \\ \vdots & \vdots & \ddots & \vdots \\ -\widetilde{H}_2^{u_1,u_2}(j,l) & -\widetilde{H}_2^{u_1,u_2}(j+1,l) & \dots & -\widetilde{H}_2^{u_1,u_2}(l-1,l) \end{vmatrix} \begin{vmatrix} 0 & \widetilde{H}_3^{u_1,u_2}(-1) & \dots & \widetilde{H}_3^{u_1,u_2}(1-r) \\ \widetilde{H}_3^{u_1,u_2}(1) & 0 & \dots & \widetilde{H}_3^{u_1,u_2}(2-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{H}_3^{u_1,u_2}(r-1) & \widetilde{H}_3^{u_1,u_2}(r-2) & \dots & 0 \end{vmatrix}} . \tag{3.95}$$

Finally, for the $z$ direction correlation function we obtain in a similar way:

$$\left[-\widetilde{C}^{zz}_{j-l}(t)\right]^2 \coloneqq \left[-\widetilde{C}^{zz}_{jl}(t)\right]^2$$
$$= \frac{\begin{vmatrix} 0 & \widetilde{F}_1(j,l) & \widetilde{F}_2(j,j) & \widetilde{F}_2(j,l) \\ \widetilde{F}_1(l,j) & 0 & \widetilde{F}_2(l,j) & \widetilde{F}_2(l,l) \end{vmatrix}}{\begin{vmatrix} -\widetilde{F}_2(j,j) & -\widetilde{F}_2(l,j) & 0 & \widetilde{F}_3(j,l) \\ -\widetilde{F}_2(j,l) & -\widetilde{F}_2(l,l) & \widetilde{F}_3(l,j) & 0 \end{vmatrix}} . \tag{3.96}$$

# 4 Dynamic magnetisations

Having obtained all of the relevant combinations of the time-dependent correlation functions, we now take up calculating the magnetisations in different directions for the different phases. However, what interest us the most is the dynamic case in presence of frustration. The dynamic case with no frustration was already studied [37], as well as the frustrated static case [10]. We have successfully reproduced all of the correlation functions from both of these papers and will henceforth focus on the dynamic two-point correlation functions (static ones are there also for consistency checks and getting acquainted with the calculation process) and corresponding magnetisations. The reason we will employ these functions in the unfrustrated first phase[50] as well is that we intend to evolve the system between three different phases to observe potential peculiarities in its behaviour.

The way in which we will proceed was announced in the body of this work, but we reiterate and expand the discussion on the importance of parity once more in this introductory segment. Setting the two-point correlation function to be between antipodal points in the system and the taking its square root as a way of obtaining the one-point correlation function (which is essentially magnetization) relies on the *cluster decomposition hypothesis*, i.e. a supposition that the relation (1.3) [51] holds:

$$\lim_{r\to\infty}\left[\left\langle\sigma_j^\mu\sigma_{j+r}^\mu\right\rangle-\left\langle\sigma_j^\mu\right\rangle\left\langle\sigma_{j+r}^\mu\right\rangle\right]=0\ . \tag{4.1}$$

However, it was shown in previous works [10] that it can fail or be ambiguous in the presence of frustration in the static case and thus we seek to explore this possibility here as well, only for the time-evolving systems.

Obviously, for this test, a way of obtaining the one-point expectation values such as the ones appearing in the previous expression would be needed and it is difficult, as was previously explained based on parities of different states. However, for the Hamiltonian which we are working with (2.58), such a procedure was introduced in [10] and we will exploit it here as well. The main point relies on the fact that the ground states such as (2.63), (2.75), (2.81) and (2.80) have well defined parity

[50] Recall that, regardless of the boundary conditions, there is no frustration in this phase since the minimal energy mode is in the odd sector and can thus be excited alone.

[51] Formally, the limit of infinity corresponds to some fraction of number of spin sites $N$ in the thermodynamic limit.

along the $z$ axis, but not along the other two. This was not a problem for two-point correlation functions since their consecutive action on any of these ground states did not change the $z$ parity, but the one-point ones evidently do. Thus, it is necessary to construct states that have well-defined $x$ or $y$ parities so that the expectation values do not vanish immediately. Of course, when constructing these states, we are restricted to linear combinations of the eigenvectors of the system.

## *4.1* $1$*O and* $2$*M phases—dynamic magnetisations*

Bearing in mind the preceding discussion, we observe that in the first two phases, the state $|g^+(t)\rangle$ is in the even $z$ parity sector and thus the state $\Pi^x |g^+(t)\rangle$ will be in the odd one. Because of this and the fact that the parity operators commute with the Hamiltonian, its energy will be the same and it will thus, up to a phase factor, be equal to the ground state in the odd sector $|g^-(t)\rangle$. However, we wish to construct this type of state at the initial moment $t = 0$ and then evolve it in time—this is easily carried out since the parity operators commute with the Hamiltonian and the time-evolution operator is an exponentiated Hamiltonian[52] and thus the parity operators will commute with the time evolution operator. To put this into writing, we construct the time-dependent ground state with definite $x$ parity[53,54] as follows:

$$\begin{aligned} |g_x(t)\rangle =& U(t) \left( \left[ \cos\theta + \sin\theta e^{i\psi} \Pi^x \right] |g^+(t=0)\rangle \right) \\ =& \left[ \cos\theta + \sin\theta e^{i\psi} \Pi^x \right] U(t) |g^+(t=0)\rangle \\ =& \left[ \cos\theta + \sin\theta e^{i\psi} \Pi^x \right] |g^+(t)\rangle \quad , \end{aligned} \tag{4.2}$$

where we see that the proper choice based on the well-defined $x$ parity requirement is $\theta = \pi/4$ and $\psi = 0$ since then it is obvious that, when acting with the $\Pi^x$ on this state, we will obtain the same state as per $(\Pi^x)^1 = \mathbb{1}$. However, we will keep $\theta$ and $\psi$ general for now to demonstrate that this choice leads to the maximum value of magnetisation as well. We also note that we have used the commutativity of the parity and time-evolution operators to get to the second row.

We now choose a generic site $j$ of the spin chain and on it we evaluate the magnetisation in the $x$ direction. This magnetisation is defined in the usual way as the

[52] Because the Hamiltonian does not depend on time.
[53] This is one of the two announced states that break the $\mathbb{Z}_2$ symmetry.
[54] Note that the magnetisation along the other two axes vanishes in this state.

expectation value of the corresponding spin operator:

$$\begin{aligned} m_j^x(t) &= \langle g_x(t)|\, \sigma_j^x\, |g_x(t)\rangle \\ &= \cos^2\theta\, \langle g^+(t)|\, \sigma_j^x\, |g^+(t)\rangle + \sin^2\theta\, \langle g^+(t)|\, \Pi^x \sigma_j^x \Pi^x\, |g^+(t)\rangle + \\ &\quad + \sin\theta\cos\theta\, \left[e^{\imath\psi}\, \langle g^+(t)|\, \sigma_j^x \Pi^x\, |g^+(t)\rangle + e^{-\imath\psi}\, \langle g^+(t)|\, \Pi^x \sigma_j^x\, |g^+(t)\rangle\right] \\ &= \sin(2\theta)\cos\psi\, \left[e^{\imath\psi}\, \langle g^+(t)|\, \sigma_j^x \Pi^x\, |g^+(t)\rangle + e^{-\imath\psi}\, \langle g^+(t)|\, \sigma_j^x \Pi^x\, |g^+(t)\rangle\right] \\ &= \sin(2\theta)\cos\psi\, \langle g^+(t)|\, \Pi_j^x\, |g^+(t)\rangle \quad , \end{aligned} \tag{4.3}$$

where, since both $|g^+(t)\rangle$ and $\Pi^x\,|g^+(t)\rangle$ are eigenstates of $\Pi^z$, the states in the inner products in $\langle g^+(t)|\, \sigma_j^x\, |g^+(t)\rangle$ and $\langle g^+(t)|\, \Pi^x \sigma_j^x \Pi^x\, |g^+(t)\rangle$ will belong to different $z$ parity sectors and these products will necessarily vanish. The final row is obtained upon noticing that $\Pi^x \sigma_j^x = \sigma_j^x \Pi^x$ and introducing the operators:

$$\Pi_j^\alpha := \bigotimes_{l\neq j} \sigma_l^\alpha \tag{4.4}$$

that commute with the parity operator along the $z$ axis since the number of spins $N$ is odd and thus their expectation values can be different than zero.

To continue, we first notice that, as announced, the maximum absolute value of the magnetisation in the $x$ direction (4.3) will be obtained for $\psi = 0$ and $\theta = \pi/4$ and this is the state we choose in the following. The magnetisation then turns into an expectation value of the operator $\Pi_j^x$ that commutes with $\Pi^z$:

$$m_j^x(t) = \langle g^+(t)|\, \Pi_j^x\, |g^+(t)\rangle \quad , \tag{4.5}$$

meaning that it can be expressed in terms of Majorana correlation functions $A$ and $B$. To find this expansion, we choose, e.g. the $N$th site to calculate the magnetisation (the choice of the site is arbitrary, but the expansions are different so we ought to

make it) and recall the formulae (3.2) to obtain:

$$\begin{aligned}\Pi_N^x =&\sigma_1^x\sigma_2^x\ldots\sigma_{N-2}^x\sigma_{N-1}^x\\ =&\left[A_1\right]\left[\sigma_1^z A_2\right]\ldots\left[A_{N-2}\sigma_1^x\ldots\sigma_{N-3}^x\right]\left[\sigma_1^x\ldots\sigma_{N-2}^x A_{N-1}\right]\\ =&\left[A_1\sigma_1^z\right]A_2\ldots\left[A_{N-2}\sigma_{N-2}^z\right]A_{N-1}\\ =&(-\imath)^{\frac{N-1}{2}}\,B_1A_2B_3A_4\ldots B_{N-2}A_{N-1}\\ =&(-\imath)^{\frac{N-1}{2}}\bigotimes_{j=1}^{\frac{N-1}{2}}B_{2j-1}A_{2j}\ ,\end{aligned}\tag{4.6}$$

since the squares of all the spin operators are equal to identity.

Returning this expression into (4.5) we argue as before for its matrix form (notice that the step between the arguments of adjacent matrix elements is two in this case, as opposed to one in two-point functions) and we repeat the process[55] in full for the $y$ direction as well, using

$$\Pi_N^y = (\imath)^{\frac{N-1}{2}}\bigotimes_{j=1}^{\frac{N-1}{2}}A_{2j-1}B_{2j}\ .\tag{4.7}$$

If we now recall the appropriate abbreviations (3.82), (3.83) and (3.84), we can finally write both of the relevant matrices[56] (on the following page):

[55]Note that the state with well defined parity along the $y$ axis that also maximises the magnetisation in the same direction is $|g_y(t)\rangle = \frac{1}{\sqrt{2}}\left[1+\Pi^y\right]|g^+(t)\rangle$ .

[56]Reader should consult Appendix E for a short and incomplete introduction to this procedure.

$$\left[(-\imath)^{\frac{N-1}{2}}\, m_N^x(t)\right]^2 = \begin{vmatrix} 0 & \widetilde{F}_1(-2) & \dots & \widetilde{F}_1(3-N) & \widetilde{F}_2(1) & \widetilde{F}_2(-1) & \dots & \widetilde{F}_2(4-N) \\ \widetilde{F}_1(2) & 0 & \dots & \widetilde{F}_1(5-N) & \widetilde{F}_2(3) & \widetilde{F}_2(1) & \dots & \widetilde{F}_2(6-N) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_1(N-3) & \widetilde{F}_1(N-5) & \dots & 0 & \widetilde{F}_2(N-2) & \widetilde{F}_2(N-4) & \dots & \widetilde{F}_2(1) \\ \hline -\widetilde{F}_2(1) & -\widetilde{F}_2(3) & \dots & -\widetilde{F}_2(N-2) & 0 & \widetilde{F}_3(-2) & \dots & \widetilde{F}_3(3-N) \\ -\widetilde{F}_2(-1) & -\widetilde{F}_2(1) & \dots & -\widetilde{F}_2(N-4) & \widetilde{F}_3(2) & 0 & \dots & \widetilde{F}_3(5-N) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\widetilde{F}_2(4-N) & -\widetilde{F}_2(6-N) & \dots & -\widetilde{F}_2(1) & \widetilde{F}_3(N-3) & \widetilde{F}_3(N-5) & \dots & 0 \end{vmatrix}, \tag{4.8}$$

$$\left[(-\imath)^{\frac{N-1}{2}}\, m_N^y(t)\right]^2 = \begin{vmatrix} 0 & \widetilde{F}_1(-2) & \dots & \widetilde{F}_1(3-N) & \widetilde{F}_2(-1) & \widetilde{F}_2(-3) & \dots & \widetilde{F}_2(2-N) \\ \widetilde{F}_1(2) & 0 & \dots & \widetilde{F}_1(5-N) & \widetilde{F}_2(1) & \widetilde{F}_2(-1) & \dots & \widetilde{F}_2(4-N) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_1(N-3) & \widetilde{F}_1(N-5) & \dots & 0 & \widetilde{F}_2(N-4) & \widetilde{F}_2(N-6) & \dots & \widetilde{F}_2(-1) \\ \hline -\widetilde{F}_2(-1) & -\widetilde{F}_2(1) & \dots & -\widetilde{F}_2(N-4) & 0 & \widetilde{F}_3(-2) & \dots & \widetilde{F}_3(3-N) \\ -\widetilde{F}_2(-3) & -\widetilde{F}_2(-1) & \dots & -\widetilde{F}_2(N-6) & \widetilde{F}_3(2) & 0 & \dots & \widetilde{F}_3(5-N) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\widetilde{F}_2(2-N) & -\widetilde{F}_2(4-N) & \dots & -\widetilde{F}_2(-1) & \widetilde{F}_3(N-3) & \widetilde{F}_3(N-5) & \dots & 0 \end{vmatrix}. \tag{4.9}$$

Expression for the $z$ direction magnetisation is the most elementary one since the states $|g^{\pm}(t)\rangle$ already have a well defined parity along the $z$ axis and the expectation values of operators $\sigma_j^z$ is equal for both of them and thus for all their linear combinations:

$$m_j^z(t) = \langle g^{\pm}(t)| \sigma_j^z |g^{\pm}(t)\rangle = -\imath \langle g^{\pm}(t)| A_j B_j |g^{\pm}(t)\rangle = -\imath \langle A_j B_j \rangle_{g^{\pm}(t)} \tag{4.10}$$

upon using the following line of calculation:

$$\begin{aligned} \sigma_j^z =& 1 - 2c_j^\dagger c_j = c_j c_j^\dagger - c_j^\dagger c_j = c_j^2 - \left(c_j^\dagger\right)^2 + c_j c_j^\dagger - c_j^\dagger c_j \\ =& \left(c_j - c_j^\dagger\right)\left(c_j + c_j^\dagger\right) = -\imath A_j B_j \ . \end{aligned} \tag{4.11}$$

Equation (4.10) is already in the form known from (7.44).

## *4.2* $3$*I phase—dynamic magnetisations*

To obtain the magnetisations in the third phase we exploit an idea similar in nature to the one for the first two phases regarding the parity properties of ground states. However, here we will use a linear combination of two of the four ground state vectors and specifically those that have the opposite eigenvalues of the translation operator, soon to be motivated. From (2.87), the action of parity operator along the $x$ direction (2.10) (which induces a minus sign because the number of spins $N$ is odd) and the definitions of ground states in the AFM phase (2.81) and (2.80), it is observed that the eigenvalues of $|\pm p\rangle = a_{\pm p}^\dagger |0^-\rangle$, i.e. $e^{\imath(\pm)p}$ are the exponentiated negatives of the eigenvalues of $|\pm p'\rangle = a_{\pm p'}^\dagger a_\pi^\dagger |0^+\rangle$, i.e. $e^{(\imath\pi \pm p')} = e^{\imath(\mp p)}$ by virtue of (2.79) and (2.78). Thus, we can identify, up to a global phase:

$$\Pi^x |\mp p\rangle \propto |\pm p'\rangle \ . \tag{4.12}$$

It is now evident that the linear combinations of vectors having the opposite eigenvalues of the translation operator are, in pairs, $|p'\rangle$ and $\Pi^x |p\rangle$; $|-p'\rangle$ and $\Pi^x |-p\rangle$. As has been observed in [10] and [11], choosing a linear combination of two of these four vectors with the same eigenvalue with respect to the translation operator, we observe the behaviour termed *Mesoscopic ferromagnetic order* and for vectors with opposite eigenvalues, one termed *Incommensurate antiferromagnetic order* (IAO). Choosing

the most general ground state, i.e. a linear combination of all four vectors, mix of these effects emerges with one term corresponding to each. As will be explained in the following, we wish to focus on the incommensurate antiferromagnetic order and thus choose the state to be a linear combination of two of these with opposite eigenvalues (both pairs of opposites yield the same result and we choose the absolute values[57] of the coefficients to be equal since, as for the previous two phases, since this will maximise the absolute value of the magnetisation):

$$\begin{aligned} |g_{\text{IAO}}(t)\rangle =& U(t)\left(\frac{1}{\sqrt{2}}\left[|p(t=0)\rangle + e^{\imath\theta}\Pi^x\,|-p(t=0)\rangle\right]\right) \\ =& \frac{1}{\sqrt{2}}\left[|p(t)\rangle + e^{\imath\theta}\Pi^x\,|-p(t)\rangle\right] \quad , \end{aligned} \tag{4.13}$$

with $\theta$ once again denoting a phase factor between two vectors. We have exploited the fact that the time-evolution operator, dependent on the Hamiltonian only, commutes with the parity operators, specifically $\Pi^x$ in this case.

We define the magnetisation on a certain site as for the other two phases to be the expectation value of the spin operator corresponding to that site. For the $x$ direction, this yields:

$$\begin{aligned} m_j^x(t) =& \langle g_{\text{IAO}}(t)|\,\sigma_j^x\,|g_{\text{IAO}}(t)\rangle \\ =& \frac{1}{2}\left[\langle p(t)| + e^{-\imath\theta}\Pi^x\,\langle -p(t)|\right]\sigma_j^x\left[|p(t)\rangle + e^{\imath\theta}\Pi^x\,|-p(t)\rangle\right] \\ =& \frac{1}{2}\left[\langle p(t)|\,\sigma_j^x\,|p(t)\rangle + \langle -p(t)|\,\Pi^x\sigma_j^x\Pi^x\,|-p(t)\rangle + \left(e^{\imath\theta}\,\langle p(t)|\,\sigma_j^x\Pi^x\,|-p(t)\rangle + \text{c.c.}\right)\right] \\ =& \frac{1}{2}\left(e^{\imath\theta}\,\langle p(t)|\,\sigma_j^x\Pi^x\,|-p(t)\rangle + \text{c.c.}\right) \\ =& \mathfrak{Re}\left[e^{\imath\theta}\,\langle p(t)|\,\Pi_j^x\,|-p(t)\rangle\right] \quad , \end{aligned} \tag{4.14}$$

where we have, as before, used the fact that the parity operator $\Pi^x$ and $\sigma_j^x$ commute, as well as the fact that both $|p(t)\rangle$ and $\Pi^x\,|-p(t)\rangle$ are eigenstates of $\Pi^z$ and thus the states in the inner products in $\langle p(t)|\,\sigma_j^x\,|p(t)\rangle$ and $\langle -p(t)|\,\Pi^x\sigma_j^x\Pi^x\,|-p(t)\rangle$ will belong to different $z$ parity sectors so these products necessarily vanish.

We now exploit the mirroring and translation operators, introduced in the section on symmetry properties of the system. As we will soon see, the expectation value

[57] Note that the relative phase $\theta$ has not been set to zero; we will see that this factor will induce modulation of the magnetisation.

inside the expression for the magnetisation in the preceding equation will be purely real when we evaluate it on the $N$th site, i.e. choose $j = N$. For the $y$ direction, it will be purely imaginary and thus can in both cases be written in a particularly concise manner. We are able to exploit this fact to write operators of this kind for general $j$ in terms of that for $j = N$ since, because of relation (2.8), each spin operator can be connected to the one on the $N$th site via

$$\sigma_j^\alpha = \left(T^\dagger\right)^j \sigma_N^\alpha \left(T\right)^j \tag{4.15}$$

and we thus obtain for the general expression in (4.14) (note that the translation operator commutes with the time-evolution operator because of (2.9)):

$$\begin{aligned} \langle p(t)| \sigma_j^x \Pi^x |-p(t)\rangle &= \langle p(t)| \left(T^\dagger\right)^j \sigma_j^x \left(T\right)^j \Pi^x |-p(t)\rangle \\ &= \langle p(t)| \left(T^\dagger\right)^j \sigma_j^x \Pi^x \left(T\right)^j |-p(t)\rangle \\ &= e^{-\imath 2pj} \langle p(t)| \Pi_N^x |-p(t)\rangle \quad , \end{aligned} \tag{4.16}$$

upon using the commutation of the parity and the translation operators (2.11) as well for the second row and the eigenvalue equation of the former (2.87) for the final row.

The $N$th site is special in the respect of demonstrating purely real/imaginary expectation values because the JW transformation breaks the translational invariance of the system by identifying the first (and consequently the last) site of the spin chain. We now show that, as announced, this expectation value is purely real. To do so, use the action of the mirror operator on general state with odd number of excitations (2.88) and switch $p$ and $-p$ states in the expectation value (we use its Hermitian nature as well, specifically (2.24)):

$$\begin{aligned} \langle p(t)| \Pi_N^x |-p(t)\rangle &= \langle -p(t)| M_N \Pi_N^x M_N |p(t)\rangle = \langle -p(t)| M_N \sigma_N^x \Pi^x M_N |p(t)\rangle \\ &= \langle -p(t)| M_N \sigma_N^x M_N \Pi^x |p(t)\rangle \quad , \end{aligned} \tag{4.17}$$

upon remembering the commutation of the mirror operators with the parity operators (2.26). We further note that mirror operator with respect to the $N$th site will

obviously leave the spin operator on the same site invariant:

$$M_N \sigma_N^x M_N = \sigma_N^x \quad , \tag{4.18}$$

finally yielding for the desired expectation value:

$$\langle p(t)| \Pi_N^x |-p(t)\rangle = \langle -p(t)| \Pi_N^x |p(t)\rangle = \left(\langle p(t)| \Pi_N^x |-p(t)\rangle\right)^* \quad , \tag{4.19}$$

implying that this quantity is real. Consequently, upon returning to (4.14), we obtain the following expression:

$$m_j^x(t) = \mathfrak{Re}\left[e^{\imath(\theta-2pj)}\right] \langle p(t)| \Pi_N^x |-p(t)\rangle = \cos\left(2pj-\theta\right) \langle p(t)| \Pi_N^x |-p(t)\rangle \quad . \tag{4.20}$$

Analogous calculation for the $y$ direction demonstrates that the expectation value $\langle p(t)| \sigma_N^y \Pi^x |-p(t)\rangle$ is purely imaginary. All the other steps being the same, we use (2.20) to obtain $\Pi^x = (-\imath)^N \Pi^y \Pi^z$ and also the fact that $\Pi^z |\pm p\rangle = \pm |\pm p\rangle$ and then insert both of these into (4.14):

$$\langle p(t)| \sigma_N^y \Pi^x |-p(t)\rangle = (-\imath)^N \langle p(t)| \sigma_N^y \Pi^y \Pi^z |-p(t)\rangle = -(-\imath)^N \langle p(t)| \sigma_N^y \Pi^y |-p(t)\rangle \tag{4.21}$$

and thus the purely imaginary character of this quantity is evident since $\langle p(t)| \sigma_N^y \Pi^y |-p(t)\rangle$ is purely real[58] and $N$ is odd. From this we can infer the expression for the magnetisation in the $y$ direction for a general site:

$$\begin{aligned} m_j^y(t) =& \mathfrak{Re}\left[-e^{\imath(\theta-2pj)} (-\imath)^N \langle p(t)| \sigma_N^y \Pi^y |-p(t)\rangle\right] \\ =& \mathfrak{Re}\left[-e^{\imath\left(\theta-2pj-\frac{N\pi}{2}\right)}\right] \langle p(t)| \sigma_N^y \Pi^y |-p(t)\rangle \\ =& -\cos\left(2pj-\theta+\frac{N\pi}{2}\right) \langle p(t)| \sigma_N^y \Pi^y |-p(t)\rangle \\ =& \cos\left(2pj-\theta+\frac{N\pi}{2}+\pi\right) \langle p(t)| \Pi_N^y |-p(t)\rangle \quad . \end{aligned} \tag{4.22}$$

We can write both $x$ and $y$ direction magnetisations in a more convenient form if we note that (2.79) implies that $p = \frac{\pi}{2} + \frac{\pi}{2N}(-1)^{(N+1)/2}$ and also define the func-

[58] This is shown in the same manner as for the $\sigma_N^x \Pi^x$ since all of the deductions remain valid in both cases.

tion dependent on the the phase of the wavefunction (4.13), direction and the total number of spins in the system $N$:

$$f(\alpha,\theta,N) \coloneqq \begin{cases} (-1)^{\frac{N-1}{2}}\,\theta\ ; & \alpha = x\ , \\ (-1)^{\frac{N-1}{2}}\,\theta + \frac{\pi}{2}\ ; & \alpha = y \end{cases} \quad . \tag{4.23}$$

Then the expression for both $x$ and $y$ direction magnetisations on a general spin site and wave function phase finally becomes:

$$m_j^{\alpha}(t) = (-1)^j \cos\left[\frac{j\pi}{N} + f(\alpha,\theta,N)\right] \langle p(t)|\, \Pi_N^{\alpha}\, |-p(t)\rangle \quad , \quad \alpha = x, y\ . \tag{4.24}$$

As before, we will seek to write the previous expectation value as a product of Majorana operators $A$ and $B$. Remembering that we have obtained the expectation values of their two-operator products in a general state of the odd parity sector $|u_1, u_2\rangle$, given by (3.45), we can see somewhat easily that the announced combination of ground states in the odd sector with $u_1 = 1/\sqrt{2}$ and $u_1 = \pm 1/\sqrt{2}$ yields the following result (the $\langle p|\cdots|p\rangle$ and $\langle -p|\cdots|-p\rangle$ terms cancel out):

$$\langle \Pi_j^x \rangle_{u_1=\frac{1}{\sqrt{2}},u_2=\frac{1}{\sqrt{2}}} - \langle \Pi_j^x \rangle_{u_1=\frac{1}{\sqrt{2}},u_2=\frac{-1}{\sqrt{2}}} = \langle p(t)|\, \Pi_j^x\, |-p(t)\rangle + \langle -p(t)|\, \Pi_j^x\, |p(t)\rangle \tag{4.25}$$

and, since we have demonstrated that the expectation values on the RHS of the previous equation are purely real (and upon inserting $j = N$):

$$\langle p(t)|\, \Pi_N^x\, |-p(t)\rangle = \frac{1}{2}\left(\langle \Pi_N^x \rangle_{u_1=\frac{1}{\sqrt{2}},u_2=\frac{1}{\sqrt{2}}} - \langle \Pi_N^x \rangle_{u_1=\frac{1}{\sqrt{2}},u_2=\frac{-1}{\sqrt{2}}}\right)\ , \tag{4.26}$$

which is appropriate since the operator $\Pi_N^x$ can be expressed in terms of Majorana ones, as was done in (4.6). An analogous relation holds for the $y$ direction as well.

However, we now have to take into account the fact that $\langle AB\rangle$ Majorana correlation functions are not translationally invariant, as is evident from (7.44). With this in mind, we use the appropriate abbreviations (3.91), (3.92) and (3.93) to write the matrix representation (on the following page):

$$\left[(-\imath)^{\frac{N-1}{2}}\,\langle\Pi_N^x\rangle_{u_1,u_2}(t)\right]^2=\frac{\begin{vmatrix} 0 & \widetilde{H}_1^{u_1,u_2}(-2) & \dots & \widetilde{H}_1^{u_1,u_2}(3-N) & \widetilde{H}_2^{u_1,u_2}(2,1) & \widetilde{H}_2^{u_1,u_2}(2,3) & \dots & \widetilde{H}_2^{u_1,u_2}(2,N-2) \\ \widetilde{H}_1^{u_1,u_2}(2) & 0 & \dots & \widetilde{H}_1^{u_1,u_2}(5-N) & \widetilde{H}_2^{u_1,u_2}(4,1) & \widetilde{H}_2^{u_1,u_2}(4,3) & \dots & \widetilde{H}_2^{u_1,u_2}(4,N-2) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \widetilde{H}_1^{u_1,u_2}(N-3) & \widetilde{H}_1^{u_1,u_2}(N-5) & \dots & 0 & \widetilde{H}_2^{u_1,u_2}(N-1,1) & \widetilde{H}_2^{u_1,u_2}(N-1,3) & \dots & \widetilde{H}_2^{u_1,u_2}(N-1,N-2) \\ \hline -\widetilde{H}_2^{u_1,u_2}(2,1) & -\widetilde{H}_2^{u_1,u_2}(4,1) & \dots & -\widetilde{H}_2^{u_1,u_2}(N-1,1) & 0 & \widetilde{H}_3^{u_1,u_2}(-2) & \dots & \widetilde{H}_3^{u_1,u_2}(3-N) \\ -\widetilde{H}_2^{u_1,u_2}(2,3) & -\widetilde{H}_2^{u_1,u_2}(4,3) & \dots & -\widetilde{H}_2^{u_1,u_2}(N-1,3) & \widetilde{H}_3^{u_1,u_2}(2) & 0 & \dots & \widetilde{H}_3^{u_1,u_2}(5-N) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\widetilde{H}_2^{u_1,u_2}(2,N-2) & -\widetilde{H}_2^{u_1,u_2}(4,N-2) & \dots & -\widetilde{H}_2^{u_1,u_2}(N-1,N-2) & \widetilde{H}_3^{u_1,u_2}(N-3) & \widetilde{H}_3^{u_1,u_2}(N-5) & \dots & 0 \end{vmatrix}}{}, \tag{4.27}$$

$$\left[(-\imath)^{\frac{N-1}{2}}\,\Pi_N^y\rangle_{u_1,u_2}(t)\right]^2=\frac{\begin{vmatrix} 0 & \widetilde{H}_1^{u_1,u_2}(-2) & \dots & \widetilde{H}_1^{u_1,u_2}(3-N) & \widetilde{H}_2^{u_1,u_2}(1,2) & \widetilde{H}_2^{u_1,u_2}(1,4) & \dots & \widetilde{H}_2^{u_1,u_2}(1,N-1) \\ \widetilde{H}_1^{u_1,u_2}(2) & 0 & \dots & \widetilde{H}_1^{u_1,u_2}(5-N) & \widetilde{H}_2^{u_1,u_2}(3,2) & \widetilde{H}_2^{u_1,u_2}(3,4) & \dots & \widetilde{H}_2^{u_1,u_2}(3,N-1) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \widetilde{H}_1^{u_1,u_2}(N-3) & \widetilde{H}_1^{u_1,u_2}(N-5) & \dots & 0 & \widetilde{H}_2^{u_1,u_2}(N-2,2) & \widetilde{H}_2^{u_1,u_2}(N-2,4) & \dots & \widetilde{H}_2^{u_1,u_2}(N-2,N-1) \\ \hline -\widetilde{H}_2^{u_1,u_2}(1,2) & -\widetilde{H}_2^{u_1,u_2}(3,2) & \dots & -\widetilde{H}_2^{u_1,u_2}(N-2,2) & 0 & \widetilde{H}_3^{u_1,u_2}(-2) & \dots & \widetilde{H}_3^{u_1,u_2}(3-N) \\ -\widetilde{H}_2^{u_1,u_2}(1,4) & -\widetilde{H}_2^{u_1,u_2}(3,4) & \dots & -\widetilde{H}_2^{u_1,u_2}(N-2,4) & \widetilde{H}_3^{u_1,u_2}(2) & 0 & \dots & \widetilde{H}_3^{u_1,u_2}(5-N) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\widetilde{H}_2^{u_1,u_2}(1,N-1) & -\widetilde{H}_2^{u_1,u_2}(3,N-1) & \dots & -\widetilde{H}_2^{u_1,u_2}(N-2,N-1) & \widetilde{H}_3^{u_1,u_2}(N-3) & \widetilde{H}_3^{u_1,u_2}(N-5) & \dots & 0 \end{vmatrix}}{}. \tag{4.28}$$

Finally, we seek the $z$ direction magnetisations, which are obtained in the same way as for the previous two phases since the calculation to obtain (4.10) are the same in the AFM phase, only with different ground states, yielding:

$$m_j^z(t) = -\imath\langle A_j B_j\rangle_{u_1,u_2}(t) \tag{4.29}$$

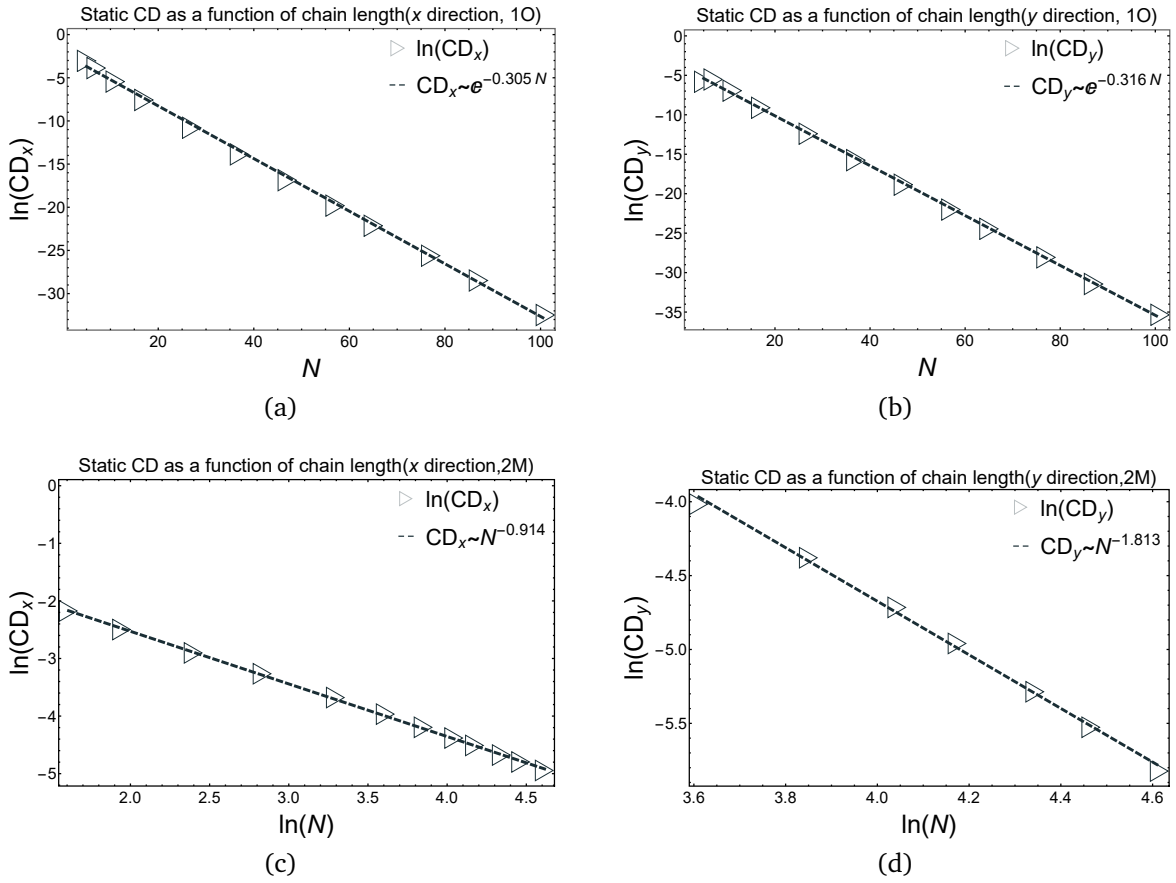



Figure 5.1: Static cluster decomposition ($t = 0$) for (a) $x$ direction, 1O ($\phi = -\pi/3.5$); (b) $y$ direction, 1O ($\phi = -\pi/3.5$); (c) $x$ direction, 2M ($\phi = -\pi/5.2$); (d) $y$ direction, 2M ($\phi = -\pi/5.2$).

# 5 Results

## *5.1 Static cluster decomposition ($t = 0$)*

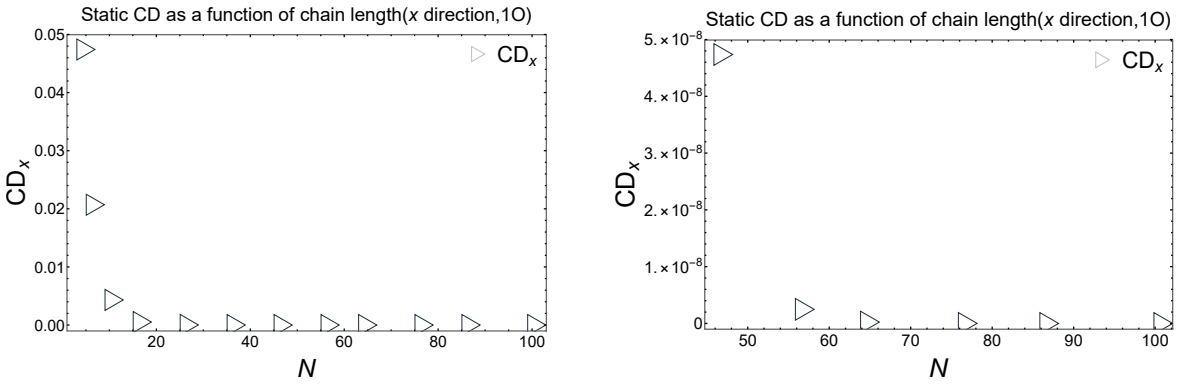
We have obtained the static CD results by taking only the first points in its time evolution. In this case we observe the expected behaviour, i.e. all of the CD terms decay as the size of the system increases.

In the first phase, one observes an exponential decay for both the $x$ and $y$ direction, while in the second phase, on the contrary, one observes algebraic decay, i.e. one with negative power law.

These four results are depicted in Figure 5.1.

We can see that the first three include all of the spin sites, corresponding to monotonous decay such as, e.g. the one depicted in Figure 5.2, i.e. that of $x$ direction in the first phase.

On the other hand, for the $y$ direction in the second phase, we see a peak at




(a) (b)

Figure 5.2: Static cluster decomposition ($t = 0$) for (a) $x$ direction, phase $1$O, all spin lengths; (b) $x$ direction, phase $1$O, half of spin lengths. Notice that we have discarded the lower spin numbers in the (b) part of the figure to demonstrate that, regardless of the current length, CD of the longer chain will be significantly lower in value; this behaviour echoes the exponential decay of CD as the chain length increases.

lower chain length and then again a decay, albeit an algebraic one. This behaviour is depicted in Figure $5.3$ and is indicative of the fact that one should consider only those numbers of spins that are a part of the decaying behaviour to avoid potential finite size effects.

Since the first phase corresponds to the unfrustrated case and the second to the frustrated one, we immediately see that our results are consistent with the known ones, both numeric and analytic [38–41]. Mathematically, the reason for the algebraic decay in the frustrated case is the extra term emerging in correlation function (3.26), i.e. the $f$ term that vanishes in the first phase. Physically, this term corresponds to a single delocalised excitation present in the ground state of the system. Thinking classically, one would naively expect this constant term to be insignificant, however it is important to notice that this excitation is delocalised and thus can have significant effect on the system, even in the thermodynamic limit, as has been shown repeatedly [10, 11].

## *5.2 Long times*

In Table 5.1, behaviour of the CD averaged out over long times is given for six possible transitions starting from the first two phases. Since all of them fall either into algebraic or exponential decay, we have only denoted the type in the table and left the precise numbers for the plots. However, one should note that the exponents usu-

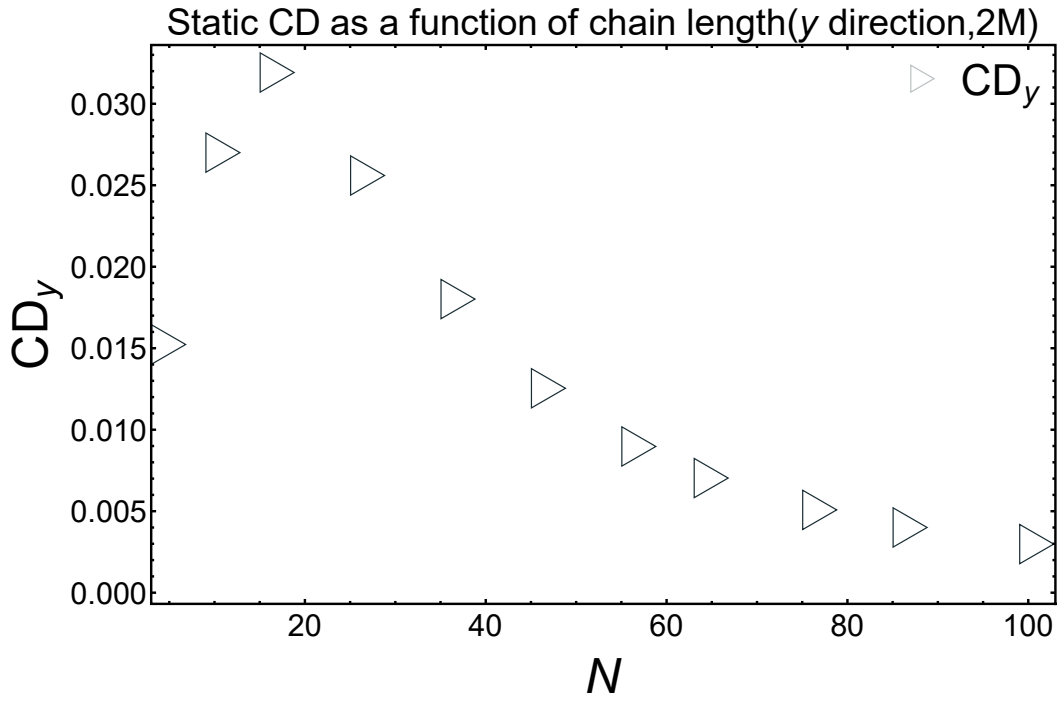



Figure 5.3: Nonscaled static cluster decomposition for $y$ direction and phase $2\mathrm{M}$ ($\phi = -\pi/5.2$). One can see that, due to finite size effects, there is a peak in the CD at low spin numbers, but as one enlarges the spin chain, it starts following an algebraic decay law.

ally depend on the initial and final parameter values and are thus not to be taken as a particularly relevant information.

We further emphasize that the averaging is done by means of a root-mean-square average since the CD expressions are in general oscillatory and thus cancellation can yield some unseemly results. However, in the dominant majority of the cases, averaging over the values directly would be sufficient, but our choice makes more sense intuitively as well since we are interested in how close the two terms in CDH are, not particularly which one is larger.

For the transitions, several different parameter values are shown in the forthcoming figures, noting that the behaviour persists over the range of values inside each phase, as long as we are not too close to its boundary so as not to approach a phase transition.

Let us start with six transitions from the first phase, as depicted in Figure 5.4.

We see that all decays except one are exponential (CD is exponentially decreasing with the system size). In general, there is a significantly faster decay of the CD when one evolves from $1\mathrm{O}$ to $3\mathrm{I}$ than from $1\mathrm{O}$ to $2\mathrm{M}$. This is intuitively understood due to the fact that the spectra of the system for the first two phases both demonstrate

Table 5.1: Table of averaged long time values of CD for evolutions starting in first two phases.

| final \ initial | 1 | | 2 | |
|---|---|---|---|---|
| 1 | $CD_x$ alg | $CD_y$ exp | $CD_x$ exp | $CD_y$ exp |
| 2 | $CD_x$ exp | $CD_y$ exp | $CD_x$ alg | $CD_y$ alg |
| 3 | $CD_x$ exp | $CD_y$ exp | $CD_x$ exp | $CD_y$ exp |

the lowest energy excitations as those of zero and $\pi$ modes and also have the same form of the ground states in both parity sectors. However, this picture is altered in the third phase since the four modes $\pm p$ and $\pm p'$ become of lower energy than the $0$ mode. Thus, the ground states are significantly different and as a consequence all the expectation values (hence their products and difference as well) decay rapidly as there is no overlap between the excited modes[59].

Furthermore, we have observed over several choices of initial and final parameters that the decay is also faster when evolving from the first phase to the second one than when remaining inside the first phase. Again, this is understood to be a consequence of the difference in spectra of the system in first two phases, i.e. existence of the energy gap in the first and lack thereof in the second.

Finally, one can also notice in Figure 5.4 that some of the spin number ranges start at higher numbers, again due to peaks that are consequences of finite size effects. One such behaviour is depicted in Figure **??**. It was also observed over several different parameter choices that decay for $1O \rightsquigarrow 1O$ evolutions is delayed, i.e. shifted towards higher spin chain lengths, such as the one in Figure 5.5.

Further still, one can see that in Figure 5.4, plot (d) is over larger chain lengths $N$ than the rest. This is due to the fact that the system exhibits finite size effects at smaller $N$ and these follow a significantly different law, as can be seen in Figure 5.6. The CD value exhibits a peak at very low chain lengths and then proceeds to decay with a reasonably precise power law.

Finally, one should observe a different behaviour of the $y$ direction CD when the evolution remains in the first phase. It is of algebraic decay with power of approximately two for several parameter ranges and thus corresponds to mesoscopic behaviour in the sense that it vanishes in the thermodynamic limit, but is present for

[59]Note that, since the Hamiltonian after the quench commutes with the translation operator (all of the symmetries remain because quench is global), total momentum is conserved.

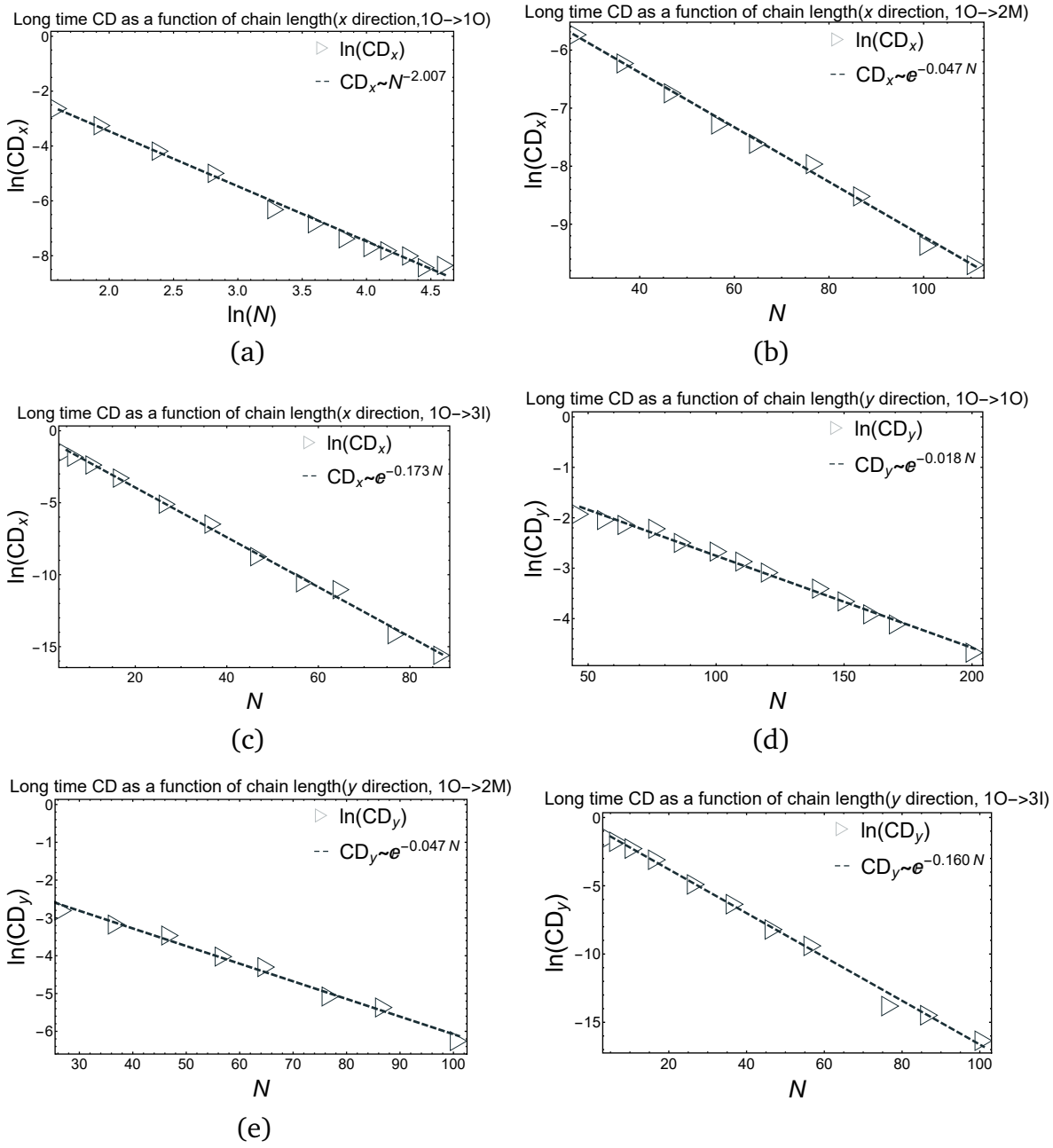



Figure 5.4: Long time average of CD for transitions starting in the first phase (a) $x$ direction, 1O$\rightsquigarrow$1O $(-\pi/3.0 \rightsquigarrow -\pi/3.5)$ (b) $x$ direction, 1O$\rightsquigarrow$2M $(-\pi/3.3 \rightsquigarrow -\pi/5.2)$ (c) $x$ direction, 1O$\rightsquigarrow$3I $(-\pi/3.0 \rightsquigarrow +\pi/4.5)$ (d) $y$ direction, 1O$\rightsquigarrow$1O $(-\pi/2.5 \rightsquigarrow -\pi/3.5)$ (e) $y$ direction, 1O$\rightsquigarrow$2M $(-\pi/3.0 \rightsquigarrow -\pi/4.9)$ (f) $y$ direction, 1O$\rightsquigarrow$3I $(-\pi/3.0 \rightsquigarrow +\pi/4.5)$ .

finite systems. This is in agreement with the fact that the decay is shifted towards higher spin numbers for this type of evolution.

It is also noticeable that there are some deviations of points from the lines of precise decay laws, but these are due to our relatively imprecise method of averaging over $100$ points in an interval that is the same for most of the evolutions. In those that did not display precise agreement with the fits, averaging was carried out over

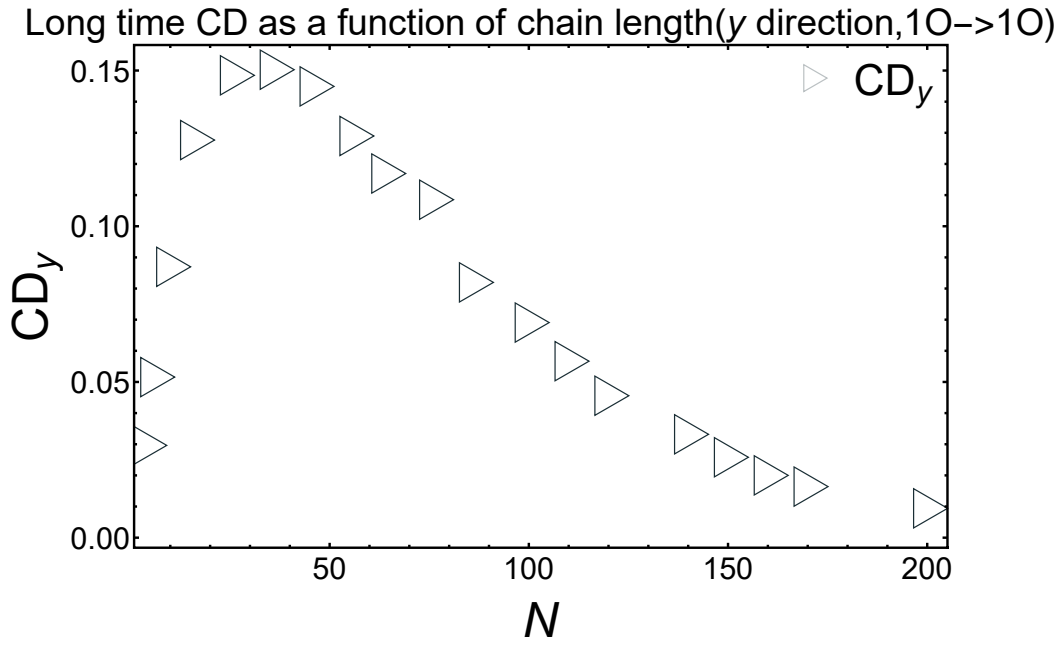



Figure 5.5: Long time average of cluster decomposition for $y$ direction and evolution $1O \rightsquigarrow 1O$ $(-\pi/2.5 \rightsquigarrow -\pi/3.5)$. One can see that, due to finite size effects, there is a peak in the CD at low spin numbers, but as one enlarges the spin chain, it starts following an exponential decay law. Furthermore, in a range of cases of $1O \rightsquigarrow 1O$ evolution, it was observed that the decay is shifted towards higher chain lengths.

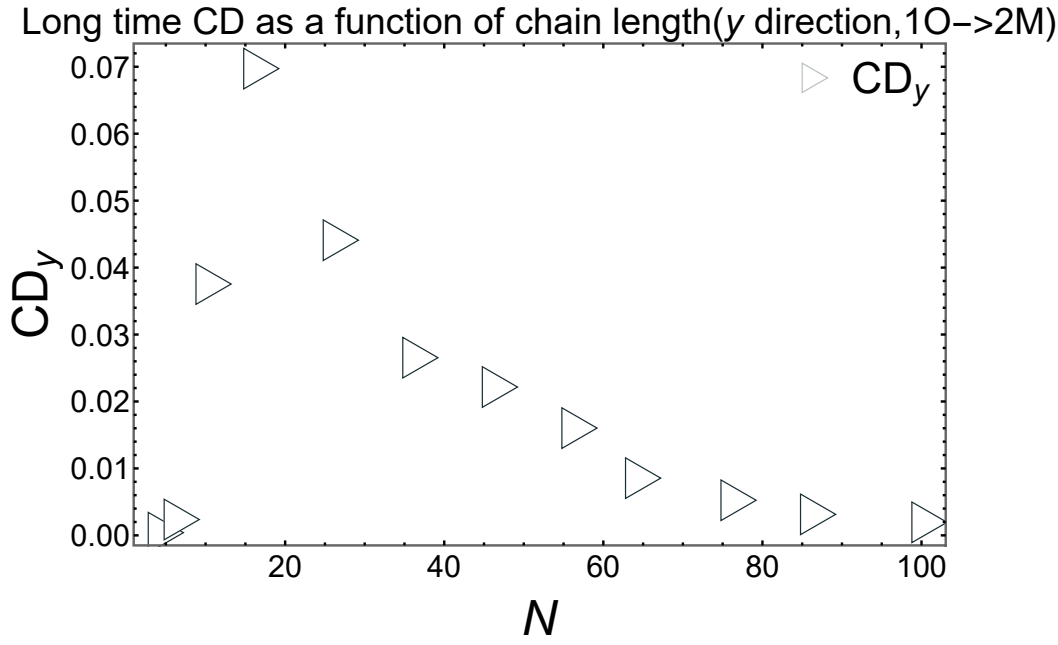



Figure 5.6: Long time average of CD for $1O \rightsquigarrow 2M$ $(-\pi/2.5 \rightsquigarrow -\pi/3.5)$ evolution and $y$ direction without any scaling of the axes. We see that, due to finite size effects, there is a peak in CD at low chain length and that the first part of the plot does not follow the decay behaviour observed for larger chain lengths.

longer time intervals. In practice, to obtain even more precise results, one ought to do averages of this kind over several intervals of different length and number of points

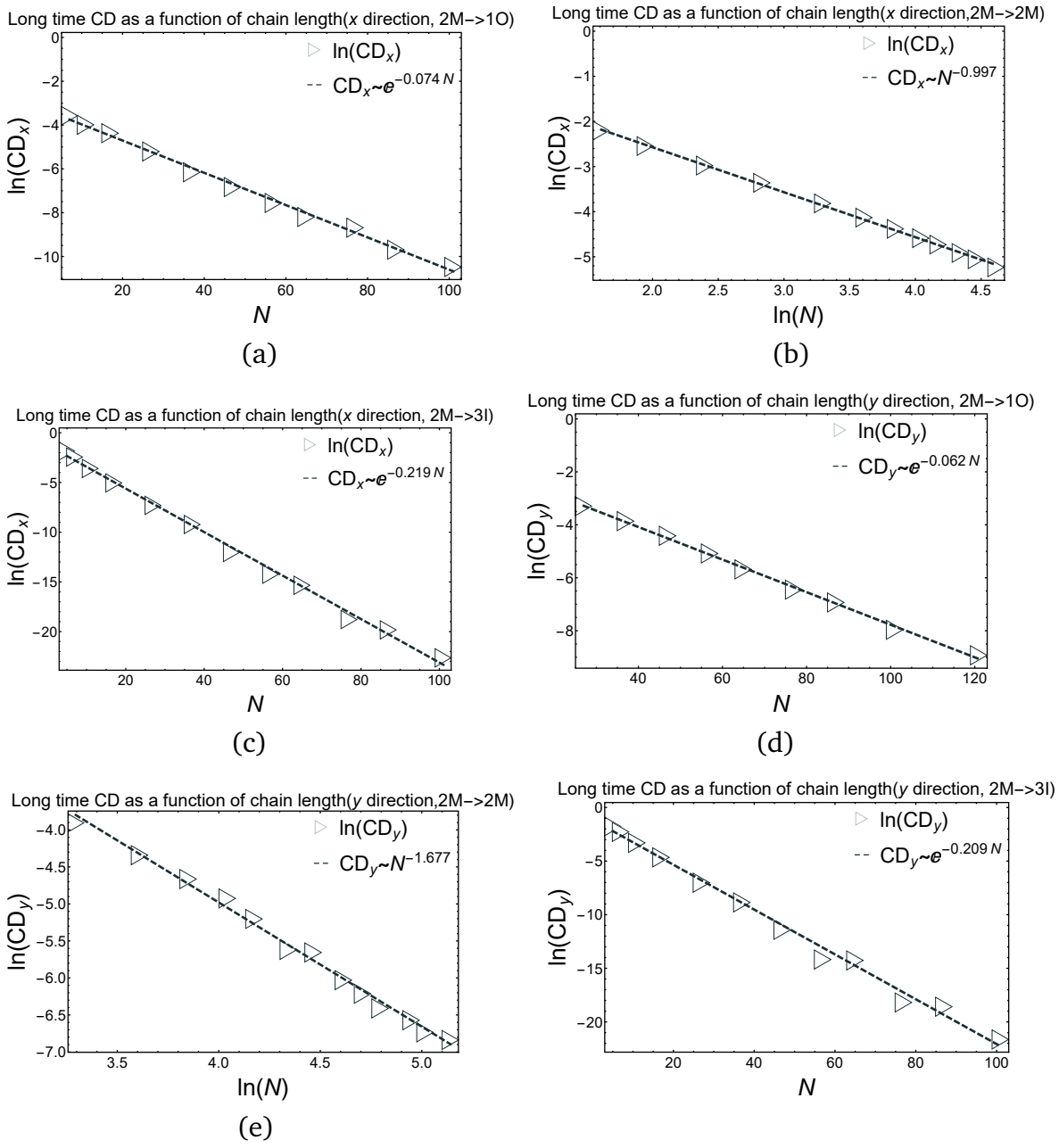



Figure 5.7: Long time average of CD for transitions starting in the second phase (a) $x$ direction, $2\text{M}\rightsquigarrow 1\text{O}$ $(-\pi/4.8 \rightsquigarrow -\pi/3.0)$ (b) $x$ direction, $2\text{M}\rightsquigarrow 2\text{M}$ $(-\pi/4.5 \rightsquigarrow -\pi/5.0)$ (c) $x$ direction, $2\text{M}\rightsquigarrow 3\text{I}$ $(-\pi/4.5 \rightsquigarrow +\pi/4.5)$ (d) $y$ direction, $2\text{M}\rightsquigarrow 1\text{O}$ $(-\pi/4.8 \rightsquigarrow -\pi/3.0)$ (e) $y$ direction, $2\text{M}\rightsquigarrow 2\text{M}$ $(-\pi/4.5 \rightsquigarrow -\pi/5.0)$ (f) $y$ direction, $2\text{M}\rightsquigarrow 3\text{I}$ $(-\pi/4.5 \rightsquigarrow +\pi/4.5)$ .

to check at what range does the average become stable and proceed accordingly.

The evolutions starting from the second phase in the long time regime yield similar results as the ones starting from the first phase and are shown in Figure 5.7.

First, the exponential decays when crossing the $\phi = 0$ are, over a range of parameter values, larger than the ones when crossing between $1\text{O}$ and $2\text{M}$ and vice versa. Once again, this is due to the significant difference in lowest energy modes and thus

the form of ground state as well. Similarly, there are mostly exponential decays for the rest, but expectedly with the decay rates higher when crossing between phases than remaining in the same one, as is reasonable based on the presence of the energy gap in the first phase and lack thereof in the second.

As for the evolutions starting in the first phase, one observes an algebraic decay of the magnetisation along both $x$ and $y$ directions when the system remains in the second phase during evolution, again implying a mesoscopic regime in which the CD persists for finite systems.

To conclude, we reiterate the important observation of the emergence of mesoscopic magnetisation in three of the long-time regimes in which we remain inside the first two phases. This term was coined and demonstrated in previous work [10] and has now been shown to hold for several dynamic regimes as well. Besides this, we have observed a delayed decay, i.e. the one shifted towards higher spin numbers of the $y$ direction long time CD when the system remains in the same phase during the evolution, albeit with different parameter value, i.e. $1$O$\rightsquigarrow$1O and $2$M$\rightsquigarrow$2M. At the moment, we intend to explain this behaviour after obtaining the data for the remaining $3$ time evolutions starting in the third ($3$I) phase since in this phase the system is frustrated as well and could thus shed some light on the observed phenomena.

Finally, we briefly mention that the CDH was not discussed for the $z$ direction since its expressions tend to be trivial in the sense of exponential decay regardless of the phase, as was shown in the static case [10]. This is due to the fact that the matrices corresponding to their correlation functions are of fixed size, i.e. they do not scale with the system size as, e.g. the ones for $x$ and $y$ directions do.

# 6 Conclusion

The aim of this thesis was to explore the validity of the cluster decomposition hypothesis and its behaviour for the long time ranges in different phases of the $1$D XY model, both for $x$ and $y$ directions.

Process was carried out in several steps, starting with solution to the model in absence of external magnetic field by means of the Jordan-Wigner transformation and Bogoliubov rotation, along with introduction of the three distinct phases based on the value of the anisotropy parameter $\phi$. In this way, we have obtained the ground states and spectra of the model and shown that it is doubly degenerate in the first two phases and quadruply degenerate in the third one. Based on these results, we have derived the analytic expressions for the two-point correlation functions in both static and dynamic case for all three phases. Afterwards, dynamic one-point correlation functions were obtained as well by evaluating them in the ground states of well-defined parities along the $x$ and $y$ directions. This was possible since the ground state was degenerate in all three phases and we were consequently able to construct the appropriate states as linear combinations of degenerate ones.

We continued by discussing the static correlation functions as a $t \to 0$ limit of the dynamic ones. It was shown that their behaviour is in agreement with known results and that the cluster decomposition decays with system size in different phases. In the first phase, i.e. unfrustrated one it was shown that the decay was exponential. On the contrary, in the second, i.e. frustrated phase it follows an algebraic law in the system size.

For the evolutions crossing the $\phi = 0$ threshold, we have demonstrated that all of the CD expressions decay exponentially, as was expected due to the significant difference of the minimal energy states above and below $\phi = 0$. Furthermore, we have also analysed the cluster decomposition behaviour in long-time regime for the evolutions between the first two phases and shown that, when there is crossing between $1$O and $2$M, the CD once again demonstrates an exponential decay, although at consistently slower rate compared to the $\phi = 0$ crossing. This type of decay is understandable due to presence of energy gap in the first phase but not in the second.

The conclusion is similar for the $1$O$\rightsquigarrow$$1$O long-time evolutions and CD in the $y$ direction, but not the $x$. This regime, along with both directions in $2$M$\rightsquigarrow$$2$M demon-

strate an algebraic decay with system size. This implies a mesoscopic behaviour and CDH that does not hold for finite sized systems. Furthermore, at least one of these evolutions, the long-time CD in the $y$ direction and the first phase displays decay shifted towards higher spin numbers, implying again that the two-point correlation functions cannot be decomposed until the system is very large.

At the moment, we intend to explain this last couple of behaviours after analysing the data for the remaining time-evolutions starting in the third ($3$I) phase since in this phase the system is frustrated as well and could thus shed light on this phenomenon. Such evolutions will be explored in an upcoming paper since, when starting in the third phase, translational invariance is broken and there are thus additional subtleties in both the definition and evaluation of the cluster decomposition hypothesis, compared to the first two.

In the end, we emphasise that the importance of our result lies in the fact that it implies constraints on the validity of the often used cluster decomposition principle and in certain phases prevents one from exploiting it without ensuring that the system is sufficiently large, which requires an additional layer of rigour and care compared to how this principle is usually used.

# Appendices

## Appendix A Miscellaneous

The purpose of this appendix is to list the results which are obtained and consistent with previous papers and elucidate some of the calculations done while solving the XY model as well.

### *A.1 Consistency with previous papers*

Dispersion given in (2.58) is equal to the one given by (15) in [10], as we show working backwards, i.e. by starting with the equation from the paper:

$$\begin{aligned}\epsilon(q) = 2|e^{\imath 2q}\cos\phi + \sin\phi| =& 2\sqrt{\left(\cos\phi\cos(2q) + \sin\phi\right)^2 + \left(\cos\phi\sin(2q)\right)^2} \\ =& 2\sqrt{1 + \sin(2\phi)\cos(2q)} \quad \checkmark\end{aligned} \tag{A.1}$$

Furthermore, we mention the correlation functions given by (3.28) and (3.26) which correspond, respectively, to (18) in [10], while (7.35) and (3.46) correspond to (55) and (56) in [11], respectively.

### *A.2 Fermionic nature of the $b_q$ operators*

As was mentioned after introducing the Fourier transform (7.15), the fermionic nature of the $b_q$ operators is seen from the symmetry of the Fourier transform (7.15), but we demonstrate it here nevertheless:

$$\left\{b_q, b_k^\dagger\right\} = \frac{1}{N}\sum_{q,k\in\Gamma^\pm} e^{-\imath(qj-kl)} \left\{c_j, c_l^\dagger\right\} = \frac{1}{N}\sum_{q\in\Gamma^\pm} e^{-\imath q(j-l)} = \delta_{q,k} \tag{A.2}$$

using (7.15), (2.35) and the delta function identity $\sum_{q\in\Gamma^\pm} e^{-\imath q(j-l)} = N\delta_{j,l}$. Similarly, for the other anticommutators:

$$\{b_q, b_k\} = \frac{1}{N}\sum_{q,k\in\Gamma^\pm} e^{-\imath(qj+kl)} \{c_j, c_l\} = 0 \tag{A.3}$$

upon using the relation (2.36) and the final relation is obtained by taking the Hermitian conjugate of the preceding one:

$$\left\{b_q^\dagger, b_k^\dagger\right\} = 0 \ . \tag{A.4}$$

Hence, we have demonstrated that the $b_q$ operators are consistently[60] fermionic.

## *A.3 Fermionic and collective nature of the $a_q$ operators*

To demonstrate the fermionic nature of the $a_q$ operators, we use the results for the $b_q$ operators obtained in the preceding section and the transformation (2.57):

$$\begin{aligned}\left\{a_q, a_k^\dagger\right\} =& \left\{\cos\theta_q b_q + \imath \sin\theta_q b_{-q}^\dagger, \cos\theta_k b_k^\dagger - \imath \sin\theta_k b_{-k}\right\} \\ =& \cos\theta_q \cos\theta_k \left\{b_q, b_k^\dagger\right\} + \sin\theta_q \sin\theta_k \left\{b_{-q}^\dagger, b_{-k}\right\} \\ =& \cos^2\theta_q \delta_{q,k} + \sin^2\theta_q \delta_{q,k} \\ =& \delta_{q,k} \ ,\end{aligned} \tag{A.5}$$

specifically upon using (A.2), (A.3) and (A.4).

Continuing, we obtain the other anticommutation relations of interest in a similar manner:

$$\begin{aligned}\{a_q, a_k\} =& \left\{\cos\theta_q b_q + \imath \sin\theta_q b_{-q}^\dagger, \cos\theta_k b_k + \imath \sin\theta_k b_{-k}^\dagger\right\} \\ =& \imath \cos\theta_q \sin\theta_k \left\{b_q, b_{-k}^\dagger\right\} + \imath \sin\theta_q \cos\theta_k \left\{b_{-q}^\dagger, b_k\right\} \\ =& -\imath \cos\theta_q \sin\theta_q \delta_{q,-k} + \imath \sin\theta_q \cos\theta_q \delta_{q,-k} \\ =& 0 \ ,\end{aligned} \tag{A.6}$$

upon using the same formulae again. Taking the Hermitian conjugate of the preceding equation also yields:

$$\left\{a_q^\dagger, a_k^\dagger\right\} = 0 \ . \tag{A.7}$$

Zeros of the squares of these operators are, as usual, seen from the anticommutation relations of the same operators, i.e. (A.6) and (A.7).

Having proven their fermionic nature, it is illustrative to ponder their collective nature, which is evident from the transformation (2.57) since they represent linear

[60] That their squares are zero is seen easily from (A.3) and (A.4).

combinations of Fourier transforms of the physical spin operators. Much has been written on the topic of quasiparticles and collective phenomena in general and we thus refer the reader to the standard literature [42, 43]. However, for intuitive convenience, we will emphasise here that the excitations we mention in the body of the thesis ought to be interpreted as collective excitations of the physical system as a whole, rather than imagining them as single particles. Furthermore, the high non-locality of the JW transformation implies that the distinct parts of the system will be parts of excitations simultaneously; dramatic consequences of this fact in terms of boundary conditions being enough to destroy the local order or induce a phase transition even in the thermodynamic limit of macroscopic number of spin sites have already been demonstrated [10, 11].

# Appendix B Diagonalisation and the Bogoliubov angle definition

We will solve the eigenvalue problem for the matrix in (2.53), i.e.:

$$\begin{bmatrix} C_{q,\phi} & \imath S_{q,\phi} \\ -\imath S_{q,\phi} & -C_{q,\phi} \end{bmatrix} \tag{B.1}$$

by diagonalising it directly to illustrate some of the peculiarities that arise in the frustrated case. We remark that this corresponds not to analysing the system all at once, but rather inspecting the subspaces spanned by the two opposite momenta $q$ and $-q$ and seeking to solve their eigenvalue problem. From this it is also evident that the basis[61,62] in which the previous matrix is given is that of the vectors:

$$|0_q, 0_{-q}\rangle \coloneqq |0_q\rangle\,|0_{-q}\rangle \quad \text{and} \quad |1_q, 1_{-q}\rangle \coloneqq a_q^\dagger a_{-q}^\dagger\,|0_q, 0_{-q}\rangle \ , \tag{B.2}$$

where the first vector corresponds to $\binom{0}{1}$ and the second one to $\binom{1}{0}$.

It is easily seen that the energy of the quasiparticle vacuum state $\lambda_{q,\phi}$ of a given

[61] It is evident from (B.1) that there are no mixed basis elements, such as $|0_q, 1_{-q}\rangle$.

[62] Furthermore, to prove that the matrix (B.1) is indeed correct in a given basis, it is easy to calculate the matrix elements in, e.g. (2.46).

subsystem is obtained by solving the equation:

$$\lambda_{q,\phi}^2 - 4\left(C_{q,\phi}^2 + S_{q,\phi}^2\right) = 0 \ , \tag{B.3}$$

and the appropriate choice of the minus sign gives the energy as:

$$\begin{aligned}\lambda_{q,\phi} = -2\sqrt{C_{q,\phi}^2 + S_{q,\phi}^2} &= -2\sqrt{(1+\sin(2\phi))\cos^2 q + (1-\sin(2\phi))\sin^2 q} \\ &= -2\sqrt{1+\sin(2\phi)\cos(2q)} = -2|e^{\imath 2q}\cos\phi + \sin\phi| \ ,\end{aligned} \tag{B.4}$$

where we have exploited (A.1) to write $\lambda_{q,\phi}$ in two convenient equivalent forms. Note that the factor of two has emerged in the Hamiltonian terms since for all the modes $q$ except[63] $0$ and $\pi$ the Hamiltonian term for the $-q$ is the same as the one for $q$ and thus we have indicated this directly. Furthermore, observe that this implies that the total energy of the vacuum state of the system is given by the sum of $\lambda_{q,\phi}$ over all of the positive momenta $q$ and reduces to (2.67), as it should.

With eigenenergies known, we solve for the vacuum state wavefunction $|\psi_{q,\phi}\rangle = \left[\beta_q + \alpha_q a_q^\dagger a_{-q}\dagger\right]|0_q, 0_{-q}\rangle$ for each $q$ and $-q$ momenta pair:

$$\begin{bmatrix} C_{q,\phi} & \imath S_{q,\phi} \\ -\imath S_{q,\phi} & -C_{q,\phi} \end{bmatrix} \begin{pmatrix} \alpha_q \\ \beta_q \end{pmatrix} = \lambda_{q,\phi} \begin{pmatrix} \alpha_q \\ \beta_q \end{pmatrix} \ , \tag{B.5}$$

yielding[64]:

$$\begin{aligned}|\psi_{q,\phi}\rangle &\propto \left[1 - \imath\left(\frac{|e^{\imath 2q}\cos\phi + \sin\phi| - C_{q,\phi}}{S_{q,\phi}}\right) b_q^\dagger b_{-q}^\dagger\right]|0_q, 0_{-q}\rangle \\ &= \left[1 - \imath\tan\theta_q \, b_q^\dagger b_{-q}^\dagger\right]|0_q, 0_{-q}\rangle \ ,\end{aligned} \tag{B.6}$$

where the *Bogoliubov angle* $\theta_q$ is defined uniquely by the arctangent function as:

$$\theta_q \coloneqq \arctan\frac{|e^{\imath 2q}\cos\phi + \sin\phi| - C_{q,\phi}}{S_{q,\phi}} = \arctan\frac{|e^{\imath 2q}\cos\phi + \sin\phi| - [\cos\phi + \sin\phi]\cos q}{[\cos\phi - \sin\phi]\sin q} \ . \tag{B.7}$$

To justify the rigmarole the previous couple of equations are, note that $\theta_q$ defined in

[63] The Hamiltonian for these two modes has no factor of two.

[64] It is instructive to act upon this wave function with appropriate annihilation operator $a_q$ and demonstrate that it yields zero, as it should by (2.64). The ground state in the latter is a product state of those of form (B.6).

this way is endowed with the property:

$$\theta_{-q} = -\theta_q \tag{B.8}$$

and thus it holds for the coefficients in the wavefunction that:

$$\cos\theta_{-q} = \cos\theta_q \quad \text{and} \quad \sin\theta_{-q} = -\sin\theta_q \ . \tag{B.9}$$

It is now more transparent that we have made this choice since it is somewhat natural in terms of the expected behaviour of sine and cosine functions. Notice that if we had written the coefficients in (B.6) straight away as sine and cosine, they would have properties opposite to those in (2.56) so this process was indeed necessary for our convenience. We furthermore note that there would be no physical difference when calculating the ground states and correlation functions since this exchange would alter the wave functions up to a factor of minus, however in other calculations differences arise [11] and it is important to be consistent with the unique choice we make throughout the calculations.

We can now finally write the normalised wavefunction (B.6) of the quasiparticle vacuum as:

$$|\psi_q\rangle = \left[\cos\theta_q - \imath \sin\theta_q \ b_q^\dagger b_{-q}^\dagger\right] |0_q, 0_{-q}\rangle \ \ , \tag{B.10}$$

where it is evident that we have identified:

$$\alpha_q = -\imath \sin\theta_q \quad \text{and} \quad \beta_q = \cos\theta_q \ , \tag{B.11}$$

from which it immediately holds that:

$$\alpha_{-q} = -\alpha_q \quad \text{and} \quad \beta_{-q} = \beta_q \ . \tag{B.12}$$

Notice also that (B.10) is invariant under the transformation $q \rightsquigarrow -q$ since $|1_q, 1_{-q}\rangle = a_q^\dagger a_{-q}^\dagger |0_q, 0_{-q}\rangle = -a_{-q}^\dagger a_q^\dagger |0_q, 0_{-q}\rangle = |1_{-q}, 1_q\rangle$ for the fermionic qusiparticles determined by the $a$ operators and this was to be expected because the exchange of these modes does not induce any changes in the system. With opposite properties (2.56), the wave function would gain a minus sign upon said transformation, which again adds only an arbitrary phase to the wavefunction and thus leaves the physics of the

system invariant.

In the end, we reiterate that the total vacuum wave function is a state product of terms of the form (B.10):

$$|0^{\pm}\rangle = \bigotimes_{0<q<\pi;\ q\in\Gamma^{\pm}} \left[\cos\theta_q - \imath \sin\theta_q\ b_q^{\dagger} b_{-q}^{\dagger}\right] |0\rangle \tag{B.13}$$

and again notice that the product goes over only the positive modes $q$, as is congruent with the fact that the Hamiltonian (2.58) can be written in such a way, albeit with the diagonal matrices corresponding to $0$ and $\pi$ modes written separately since they have no negative counterparts. This fact will be quite useful when considering the time evolution of the system, since it will be possible to analyse the subspaces of different modes separately similarly to the process of diagonalisation.

# Appendix C Static correlation functions for the $3$I phase

In this appendix we provide an overview of all the results necessary for deriving the relevant correlation functions (3.46) and (7.35) in the third phase. Note, however, that the state of interest is (3.45) and thus the expectation values of different kind will be needed. To explicitly see exactly which terms are of importance, let us express the expectation value of a generic operator $O$ in the $|u_1, u_2\rangle$ state:

$$\begin{aligned}\langle O\rangle_{u_1,u_2} =& \left[u_1^* \langle p| + u_2^* \langle -p|\right] O \left[u_1 |p\rangle + u_2 |-p\rangle\right] \\ =& |u_1|^2 \langle p| O |p\rangle + |u_2|^2 \langle -p| O |-p\rangle + (u_1^* u_2 \langle p| O |-p\rangle + \text{c.c.})\end{aligned} \tag{C.1}$$

and we thus conclude that four types of expectation values will be needed in general. As we will soon see, many of them are equal or related in a trivial manner.

## *C.1 Majorana correlation functions for the $3$I phase*

Begin with the correlation function terms in terms of the operators $a_q$ and use the definition of the ground state wave function (2.81). The relevant combinations of

the operators are:

$$\langle \pm p| \, a_q a_k^\dagger \, |\pm p\rangle = \delta_{q,k} \left[1 - \delta_{q,\pm p}\right] \ , \tag{C.2a}$$

$$\langle \pm p| \, a_q a_k^\dagger \, |\mp p\rangle = -\, \delta_{q,\mp p}\delta_{k,\pm p} \ , \tag{C.2b}$$

$$\langle \pm p| \, a_q^\dagger a_k \, |\pm p\rangle = \delta_{q,\pm p}\delta_{k,\pm p} \ , \tag{C.2c}$$

$$\langle \pm p| \, a_q^\dagger a_k \, |\mp p\rangle = \delta_{q,\pm p}\delta_{k,\mp p} \ , \tag{C.2d}$$

$$\langle \pm p| \, a_q a_k \, |\pm p\rangle = \langle \pm p| \, a_q a_k \, |\mp p\rangle = \langle \pm p| \, a_q^\dagger a_k^\dagger \, |\pm p\rangle = \langle \pm p| \, a_q^\dagger a_k^\dagger \, |\mp p\rangle = 0 \ . \tag{C.2e}$$

As before, it is instructive to notice the internal consistency of these equations, regarding the anticommutation relations for the $a_q$ operators (A.5), (A.6) and (A.7).

We continue with turning to the $b_q$ operators, exploiting (3.9) to obtain:

$$\langle \pm p| \, b_q b_k^\dagger \, |\pm p\rangle = -\cos^2\theta_p \delta_{q,\pm p}\delta_{k,\pm p} + \sin^2\theta_p \delta_{q,\mp p}\delta_{k,\mp p} + \frac{1+\cos(2\theta_q)}{2}\delta_{q,k} \ , \tag{C.3a}$$

$$\langle \pm p| \, b_q b_k^\dagger \, |\mp p\rangle = -\, \delta_{q,\mp p}\delta_{k,\pm p} \ , \tag{C.3b}$$

$$\langle \pm p| \, b_q^\dagger b_k \, |\pm p\rangle = \cos^2\theta_p \delta_{q,\pm p}\delta_{k,\pm p} - \sin^2\theta_p \delta_{q,\mp p}\delta_{k,\mp p} + \frac{1-\cos(2\theta_q)}{2}\delta_{q,k} \ , \tag{C.3c}$$

$$\langle \pm p| \, b_q^\dagger b_k \, |\mp p\rangle = \delta_{q,\pm p}\delta_{k,\mp p} \ , \tag{C.3d}$$

$$\langle \pm p| \, b_q b_k \, |\pm p\rangle = -\imath\frac{\sin(2\theta_{\pm p})}{2}\left[\delta_{q,\pm p}\delta_{k,\mp p} - \delta_{q,\mp p}\delta_{k,\pm p}\right] + \imath\frac{\sin(2\theta_q)}{2}\delta_{q,-k} \ , \tag{C.3e}$$

$$\langle \pm p| \, b_q b_k \, |\mp p\rangle = 0 \ , \tag{C.3f}$$

$$\langle \pm p| \, b_q^\dagger b_k^\dagger \, |\pm p\rangle = -\imath\frac{\sin(2\theta_{\pm p})}{2}\left[\delta_{q,\pm p}\delta_{k,\mp p} - \delta_{q,\mp p}\delta_{k,\pm p}\right] + \imath\frac{\sin(2\theta_q)}{2}\delta_{q,-k} \ , \tag{C.3g}$$

$$\langle \pm p| \, b_q^\dagger b_k^\dagger \, |\mp p\rangle = 0 \ . \tag{C.3h}$$

Internal consistency checks should not even be mentioned at this point, but it is also useful to notice the similarities between the functions for the first two phases and the importance of certain modes ($0$ mode for those two phases and the $\pm p$ modes for the third phase), both for $a_q$ and $b_q$ operators.

Finally, we return to the coordinate space via the inverse Fourier transform (7.15)

to obtain the correlation functions in terms of the $c_j$ operators:

$$\langle \pm p| \, c_j c_l^\dagger \, |\pm p\rangle = \frac{1}{N} \sum_{q \in \Gamma^-} e^{\imath q(j-l)} \frac{1+\cos(2\theta_q)}{2} + \frac{1}{N} \left[ \sin^2 \theta_p e^{-\imath(\pm p)(j-l)} - \cos^2 \theta_p e^{\imath(\pm p)(j-l)} \right] \ , \tag{C.4a}$$

$$\langle \pm p| \, c_j c_l^\dagger \, |\mp p\rangle = -\frac{1}{N} e^{-\imath(\pm p)(j+l)} \ , \tag{C.4b}$$

$$\langle \pm p| \, c_j^\dagger c_l \, |\pm p\rangle = \frac{1}{N} \sum_{q \in \Gamma^-} e^{\imath q(j-l)} \frac{1-\cos(2\theta_q)}{2} + \frac{1}{N} \left[ -\sin^2 \theta_p e^{\imath(\pm p)(j-l)} + \cos^2 \theta_p e^{-\imath(\pm p)(j-l)} \right] \ , \tag{C.4c}$$

$$\langle \pm p| \, c_j^\dagger c_l \, |\mp p\rangle = \frac{1}{N} e^{-\imath(\pm p)(j+l)} \ , \tag{C.4d}$$

$$\langle \pm p| \, c_j c_l \, |\pm p\rangle = \frac{\imath}{N} \sum_{q \in \Gamma^-} e^{\imath q(j-l)} \frac{\sin(2\theta_q)}{2} + \frac{1}{N} \sin(2\theta_{\pm p}) \sin\left[\pm p\,(j-l)\right] \ , \tag{C.4e}$$

$$\langle \pm p| \, c_j c_l \, |\mp p\rangle = 0 \ , \tag{C.4f}$$

$$\langle \pm p| \, c_j^\dagger c_l^\dagger \, |\pm p\rangle = -\frac{\imath}{N} \sum_{q \in \Gamma^-} e^{\imath q(j-l)} \frac{\sin(2\theta_q)}{2} - \frac{1}{N} \sin(2\theta_{\pm p}) \sin\left[\pm p\,(j-l)\right] \ , \tag{C.4g}$$

$$\langle \pm p| \, c_j^\dagger c_l^\dagger \, |\mp p\rangle = 0 \ . \tag{C.4h}$$

It is from this last set of equations that the relations (3.46) and (7.35) are obtained. We also remark that, since the problematic mode in the odd sector which our ground state $|u_1, u_2\rangle$ is a part of is the $0$ mode and upon exploiting (2.60) it is seen that there is no need for the correction of the Bogoliubov angle in the third phase we are considering at the moment.

# Appendix D Dynamic correlation functions for the $3$I phase

In this appendix, we list the relevant results necessary to calculate the dynamic correlation functions in the third phase. We exploit the expression for the time-evolved ground states in the odd sector of this phase (3.71) and first find the actions of the

$b_q$ operators on them to be:

$$
\begin{aligned}
& b_q \left|\pm p(t)\right\rangle \\
& \left( \bigotimes_{0<q<\pi; q\in\Gamma^- \setminus \{1,p\}} \widetilde{\alpha}_q(t) \left|0_q, 1_{-q}\right\rangle \right) \otimes \left|1_{\pm p}, 0_{\mp p}\right\rangle \otimes e^{\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t} \left|0_0\right\rangle \left[1-\delta_{q,p}\right]\left[1-\delta_{q,-p}\right]\left[1-\delta_{q,0}\right] + \\
& + \left( \bigotimes_{0<q<\pi; q\in\Gamma^- \setminus \{p\}} \left[ \widetilde{\alpha}_q(t) \left|1_q, 1_{-q}\right\rangle + \widetilde{\beta}_q(t) \left|0_q, 0_{-q}\right\rangle \right] \right) \otimes \left|0_p, 0_{-p}\right\rangle \otimes e^{\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t} \left|0_0\right\rangle \delta_{q,\pm p}
\end{aligned}
\tag{D.1}
$$

and

$$
\begin{aligned}
& b_q^\dagger \left|\pm p(t)\right\rangle \\
& \left( \bigotimes_{0<q<\pi; q\in\Gamma^- \setminus \{1,p\}} \widetilde{\beta}_q(t) \left|1_q, 0_{-q}\right\rangle \right) \otimes \left|1_{\pm p}, 0_{\mp p}\right\rangle \otimes e^{\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t} \left|0_0\right\rangle \left[1-\delta_{q,p}\right]\left[1-\delta_{q,-p}\right]\left[1-\delta_{q,0}\right] - \\
& - \left( \bigotimes_{0<q<\pi; q\in\Gamma^- \setminus \{p\}} \left[ \widetilde{\alpha}_q(t) \left|1_q, 1_{-q}\right\rangle + \widetilde{\beta}_q(t) \left|0_q, 0_{-q}\right\rangle \right] \right) \otimes \left|1_{\pm p}, 1_{\mp p}\right\rangle \otimes e^{\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t} \left|0_0\right\rangle \delta_{q,\mp p} + \\
& + \left( \bigotimes_{0<q<\pi; q\in\Gamma^- \setminus \{p\}} \left[ \widetilde{\alpha}_q(t) \left|1_q, 1_{-q}\right\rangle + \widetilde{\beta}_q(t) \left|0_q, 0_{-q}\right\rangle \right] \right) \otimes \left|1_{\pm p}, 0_{\mp p}\right\rangle \otimes e^{\imath\sqrt{2}\cos\left(\phi-\frac{\pi}{4}\right)t} \left|1_0\right\rangle \delta_{q,0}
\end{aligned}
\tag{D.2}
$$

with the expressions written out in a somewhat cumbersome fashion to again illustrate a slightly different way of calculating the correlation functions and as a consistency check.

We proceed with calculating all of the expectation values (correlation functions) for the $b_q$ operators and write the delta terms in a shorter way (one should convince

oneself of its validity):

$$\langle \pm p(t)|\, b_q b_k^\dagger \,|\pm p(t)\rangle = |\widetilde{\beta}_q(t)|^2 \delta_{q,k}\left[1-\delta_{q,p}-\delta_{q,-p}-\delta_{q,0}\right]+\delta_{q,k}\delta_{q,\mp p}+\delta_{q,k}\delta_{q,0}\ , \tag{D.3a}$$

$$\langle \pm p(t)|\, b_q b_k^\dagger \,|\mp p(t)\rangle = -\,\delta_{q,\mp p}\delta_{k,\pm p}\ , \tag{D.3b}$$

$$\langle \pm p(t)|\, b_q^\dagger b_k \,|\pm p(t)\rangle = |\widetilde{\alpha}_q(t)|^2 \delta_{q,k}\left[1-\delta_{q,p}-\delta_{q,-p}-\delta_{q,0}\right]+\delta_{q,k}\delta_{q,\pm p}\ , \tag{D.3c}$$

$$\langle \pm p(t)|\, b_q^\dagger b_k \,|\mp p(t)\rangle = \delta_{q,\pm p}\delta_{k,\mp p}\ , \tag{D.3d}$$

$$\langle \pm p(t)|\, b_q b_k \,|\pm p(t)\rangle = -\,\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\delta_{q,-k}\left[1-\delta_{q,p}-\delta_{q,-p}-\delta_{q,0}\right]\ , \tag{D.3e}$$

$$\langle \pm p(t)|\, b_q b_k \,|\mp p(t)\rangle = 0\ , \tag{D.3f}$$

$$\langle \pm p(t)|\, b_q^\dagger b_k^\dagger \,|\pm p(t)\rangle = \widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)\delta_{q,-k}\left[1-\delta_{q,p}-\delta_{q,-p}-\delta_{q,0}\right]\ , \tag{D.3g}$$

$$\langle \pm p(t)|\, b_q^\dagger b_k^\dagger \,|\mp p(t)\rangle = 0 \tag{D.3h}$$

and check the internal consistency as before while also noting that they correctly reduce to (C.3) for $t=0$.

We continue with the corresponding relations for the $c_j$ operators, exploiting the Fourier transform (7.15) to obtain:

$$\langle \pm p(t)|\, c_j c_l^\dagger \,|\pm p(t)\rangle = \frac{1}{N}\sum_{q\in\Gamma^-\setminus\{p,-p,0\}} e^{\imath q(j-l)}|\widetilde{\beta}(t)|^2+\frac{1}{N}\left[e^{\imath(\mp p)(j-l)}+1\right]\ , \tag{D.4a}$$

$$\langle \pm p(t)|\, c_j c_l^\dagger \,|\mp p(t)\rangle = -\,\frac{1}{N}e^{-\imath(\pm p)(j+l)}\ , \tag{D.4b}$$

$$\langle \pm p(t)|\, c_j^\dagger c_l \,|\pm p(t)\rangle = \frac{1}{N}\sum_{q\in\Gamma^-\setminus\{p,-p,0\}} e^{\imath q(j-l)}|\widetilde{\alpha}(t)|^2+\frac{1}{N}e^{-\imath(\pm p)(j-l)}\ , \tag{D.4c}$$

$$\langle \pm p(t)|\, c_j^\dagger c_l \,|\mp p(t)\rangle = \frac{1}{N}e^{-\imath(\pm p)(j+l)}\ , \tag{D.4d}$$

$$\langle \pm p(t)|\, c_j c_l \,|\pm p(t)\rangle = -\,\frac{1}{N}\sum_{q\in\Gamma^-\setminus\{p,-p,0\}} e^{\imath q(j-l)}\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\ , \tag{D.4e}$$

$$\langle \pm p(t)|\, c_j c_l \,|\mp p(t)\rangle = 0\ , \tag{D.4f}$$

$$\langle \pm p(t)|\, c_j^\dagger c_l^\dagger \,|\pm p(t)\rangle = -\,\frac{1}{N}\sum_{q\in\Gamma^-\setminus\{p,-p,0\}} e^{\imath q(j-l)}\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)\ , \tag{D.4g}$$

$$\langle \pm p(t)|\, c_j^\dagger c_l^\dagger \,|\mp p(t)\rangle = 0\ , \tag{D.4h}$$

which are internally consistent and also reduce to (C.4), as they ought to.

It is from this last set of equation that the expressions (7.44), (7.42) and (7.43) are obtained. Notice that, as for the static correlation functions in this phase, there is no need of eliminating any faulty Bogoliubov angles.

# Appendix E Expectation values, determinants and Toeplitz matrices

As can be observed throughout the thesis body, most of the important physical are reduced to problems of evaluating matrix determinants. Furthermore, these matrices are always of one of two forms: Toeplitz matrices or Pfaffians.

To begin, let us consider the matrix in (3.41). We first observe that it has a particular form, i.e. that its left-to-right diagonals all have the same value—these matrices are known as Toeplitz matrices and study of their determinants, especially their asymptotic behaviour is a branch in and of itself. Coincidentally, their development is intimately related to research on the properties of Ising and XY models [35]. Being able to write the physical quantities in this way is extremely useful since it is then possible to obtain analytic expressions for their expansions. This was done formally for the systems we are interested in and it has been shown that the unfrustrated ($1$O) and frustrated ($2$M) phases exhibit exponential and algebraic decay of the two-point correlation functions, respectively [41]. This fact is based on the extra constant term emerging in the matrix entries in the frustrated case due to the single delocalised excitation in the ground state.

To obtain their Toeplitz form based on different contractions of operators, we consult the determinant formulation of Wick's theorem for certain systems [9, 44]. From a practical viewpoint, we can just write all of the operators in particular order both as the rows and columns and then fill the matrix with their contractions (one should convince oneself of this process intuitively by focusing on one row in the determinant and consider the possible contractions inside the Wick's theorem). To this end, we also note that $\langle A_j A_l \rangle$ and $\langle B_j B_l \rangle$ contractions vanish except for $j = l$, but these terms will be the reason for the matrix reducing to Toeplitz form. Particularly, let us consider formula (3.41) with the sites being $j = 1$ and $l = 3$. Then, as per expression (3.30) there will be four Majorana operators: $A_2, A_3, B_1, B_2$[65] Ordering these operators as suggested and contracting them (beearing in mind that $\langle A_j A_l \rangle$ and $\langle B_j B_l \rangle$ are Kronecker-deltas, but also that the determinant is antisymmetric)

[65]Note that there will be some additional factors based on interchanging these operators since they are fermionic, but we are only interested in matrix form at the moment.

yields:

| | $A_2$ | $A_3$ | $B_1$ | $B_2$ |
|---|---|---|---|---|
| $A_2$ | $0$ | $0$ | $\langle A_2 B_1 \rangle$ | $\langle A_2 B_2 \rangle$ |
| $A_3$ | $0$ | $0$ | $\langle A_3 B_1 \rangle$ | $\langle A_3 B_2 \rangle$ |
| $B_1$ | $\langle B_1 A_2 \rangle$ | $\langle B_1 A_3 \rangle$ | $0$ | $0$ |
| $B_2$ | $\langle B_2 A_2 \rangle$ | $\langle B_2 A_3 \rangle$ | $0$ | $0$ |

. (E.1)

Furthermore, to simplify this expression, we first recall that switching operators $A_j$ and $B_l$ induces only a minus sign and also that the upper left and lower right blocks in it are zero matrices. Thus, the matrix is of the form:

$$\begin{bmatrix} 0 & D \\ -D^{\mathrm{T}} & 0 \end{bmatrix} \tag{E.2}$$

and using the result

$$\begin{bmatrix} 0 & D \\ -D^{\mathrm{T}} & 0 \end{bmatrix} = \begin{bmatrix} D & 0 \\ 0 & D^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{bmatrix} , \tag{E.3}$$

one gets that this expectation value can be written in terms of the upper right corner of (E.4), i.e. it is reducible to Toeplitz form[66].

To generalise this result to the case of more complicated $\langle A_j A_l \rangle$ and $\langle B_j B_l \rangle$ terms, i.e. not Kronecker-deltas, we proceed as before and take a look at the same example (again note that the diagonal terms are zero because of total antisymmetry):

| | $A_2$ | $A_3$ | $B_1$ | $B_2$ |
|---|---|---|---|---|
| $A_2$ | $0$ | $\langle A_2 A_3 \rangle$ | $\langle A_2 B_1 \rangle$ | $\langle A_2 B_2 \rangle$ |
| $A_3$ | $\langle A_3 A_2 \rangle$ | $0$ | $\langle A_3 B_1 \rangle$ | $\langle A_3 B_2 \rangle$ |
| $B_1$ | $\langle B_1 A_2 \rangle$ | $\langle B_1 A_3 \rangle$ | $0$ | $\langle B_1 B_2 \rangle$ |
| $B_2$ | $\langle B_2 A_2 \rangle$ | $\langle B_2 A_3 \rangle$ | $\langle B_2 B_1 \rangle$ | $0$ |

(E.4)

and upon using the fact that $A_j$ and $B_l$ are fermionic, we see that this matrix is indeed totally antisymmetric and that it has a form of a Pfaffian. As for Toeplitz matrices, exploration of Pfaffians is a huge body of research [45–47] and will be not be pursued

[66] E.g. one can write the easy determinant expansion in full for this case and then proceed inductively for general dimension.

in the current work since we have made use of numerical evaluation because of the analytic expression being extremely tedious and cumbersome to evaluate. However, we will mention that one can see that for vanishing upper left and lower right blocks in the matrix (i.e. the determinant reducible to Toeplitz form), one can use the Pfaffian property for matrix $A$ of dimension $N$:

$$\mathrm{pf}\begin{bmatrix} 0 & A \\ -A^{\mathrm{T}} & 0 \end{bmatrix} = (-1)^{\frac{1}{2}N(N-1)} \det A \tag{E.5}$$

and we see that reduces it to Toeplitz form directly.

In the end, we emphasize that essentially all of the expectation values for both one- and two-point correlation functions are of this form and that this is a consequence of the fact that they emerge from the Wick's theorem for the operators that are fermionic, i.e. their products are antisymmetric upon changing their order.

# 7 Prošireni sažetak

## *7.1 Uvod*

Jednodimenzionalni XY lanac egzaktno je rješiv model koji predstavlja generalizaciju jednodimenzionalnog Isingovog modela uz dodatnu interakciju u smjeru ortogonalnom na inicijalnu. Odnos među ove dvije interakcije opisan je *parametrom anizotropije* $\phi$ u kojem su sadržani njihova relativna magnituda i predznak pa je stoga njegov Hamiltonijan jednak:

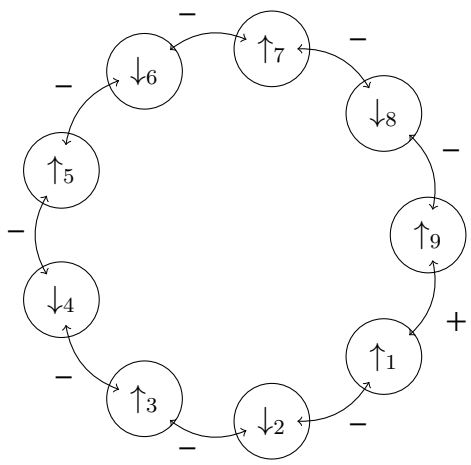
$$H = \sum_{j=1}^{N} \left[ \cos\phi \; \sigma_j^x \sigma_{j+1}^x + \sin\phi \; \sigma_j^y \sigma_{j+1}^y \right] \;\; , \tag{7.1}$$

gdje $\sigma^{x,y}$ uobičajeno označavaju spinske Paulijeve matrice. Vidimo da ovaj model posjeduje razne simetrije poput one translacijske, ali i činjenice da transformacija $\phi \rightsquigarrow \phi + \pi/2$ zamjenjuje interakcije u $x$ i $y$ smjeru. Na temelju potonje, zaključujemo da bez smanjenja općenitosti možemo restringirati vrijednosti $\phi$ na jednu polovinu jedinične kružnice, odnosno intervala od $0$ do $2\pi$.

Da bismo motivirali interes za proučavanjem ovog modela, zadržimo se kratko na konceptu *frustracije*. Neformalno, frustracija odgovara nemogućnosti istovremene minimizacije globalnog Hamiltonijana i svih njegovih lokalnih podsustava, što je obično posljedica više sukobljenih interakcija. Konkretno, možemo promotriti spinski sustav s antiferomagnetskom interakcijom na Slici 7.1. Želeći da sve interakcije među spinovima budu minimalne, krenemo od prvog spina i svaki idući orijentiramo suprotno. Vidimo da kada dođemo do posljednjeg, on će nužno biti paralelan sa početnim; ovakva nemogućnost se javlja u svim zatvorenim lancima sa neparnim brojem spinova $N$.

Nastavno na spomen frustracije i činjenicu da je dovoljno promatrati polovinu jedinične kružnice, uvedimo oznake za tri različite faze u kojima se naš sustav može naći ovisno o vrijednosti parametra $\phi$:

- 1. faza (*uređena*): $\phi \in \langle -3\pi/4, -\pi/4 \rangle$—ime joj potječe od neiščezavajućeg parametra uređenja (magnetizacije) $\langle \sigma_j^y \rangle$ u slučaju zatvorenog spinskog lanca (periodičkih rubnih uvjeta) i neparnog broja spinova u njemu $N$
- 2. faza (*mezoskopska*): $\phi \in \langle -\pi/4, 0 \rangle$—ime joj potječe od pojave feromagnetske




Slika 7.1: Frustrirani sustav od devet spinova u $2$D konfiguraciji takvoj da spinove nije moguće orijentirati tako da su sve lokalne interakcije istovremeno minimalne.

magnetizacije u $x$ smjeru koja pada polinomno s veličinom spinskog lanca u slučaju periodičkih rubnih uvjeta i neparnog broja spinova $N$

- $3$. faza (*nesrazmjerna*): $\phi \in \langle 0, +\pi/4 \rangle$—ime joj potječe od nesrazmjerno moduliranog antiferomagnetskog uređenja, također uočenog za lanac s periodičkim rubnim uvjetima i neparnim brojem spinova $N$

Iz njihova kratkog opisa, da se zaključiti da su u sve tri faze periodički rubni uvjeti i neparan broj spinova ključni za pojavu navedenih fizikalnih obilježja. Ova dva zahtjeva označavamo terminom *frustrirani rubni uvjeti*. Ipak, treba biti pažljiv i napomenuti da sustav u prvoj fazi ne pokazuje frustraciju jer je dominantna interakcija feromagnetska. S druge strane, neparan broj spinova je nužan za pojavu neiščezavajućeg parametra uređenja jer je osnovno stanje sustava u tom slučaju degenerirano, a u suprotnom parametar uređenja iščezava. U drugoj i trećoj fazi sustav uistinu jest frustriran zato što mu je, osim frustriranih rubnih uvjeta, dominantna interakcija antiferomagnetska. U sve tri faze, izostanak frustriranih rubnih uvjeta uništava opaženo ponašanje.

Nakon što smo predstavili tri faze u kojima se sustav može naći, naglasimo da će nam od velike važnosti biti mogućnost računanja očekivanih vrijednosti jednog i dvaju spinskih operatora, odnosno redom magnetizacija $\langle \sigma_j^\mu \rangle$ i korelacijskih funkcija $\langle \sigma_j^\mu \sigma_l^\mu \rangle$. Magnetizacije je obično teško računati direktno, posebno zbog činjenice da naš postupak dijagonalizacije Hamiltonijan razdvaja u dva nepreklapajuća sektora pariteta duž osi $z$ i to s osnovnim stanjima koja imaju dobro definiran paritet duž te osi. Naravno, očekivane vrijednosti operatora $\sigma_j^x$ i $\sigma_j^y$ u tim stanjima iščezavaju jer

djelovanje tih operatora nužno mijenja paritet stanja. No, kako je Hamiltonijan degeneriran u sve tri faze, moguće je konstruirati stanja s dobro definiranim paritetima u $x$ i $y$ smjerovima.

Jedan način da se pokuša zaobići ova poteškoća je korištenje *principa dekompozicije nakupina* (PDN):

$$\lim_{r\to\infty}\left[\left\langle\sigma_j^\mu\sigma_{j+r}^\mu\right\rangle-\left\langle\sigma_j^\mu\right\rangle\left\langle\sigma_{j+r}^\mu\right\rangle\right]=0\ , \tag{7.2}$$

gdje $\mu$ označava smjer ($x$, $y$ ili $z$). U suštini, ovaj princip pretpostavlja da se korelacija među dva spinska položaja može izračunati kao umnožak pojedinih očekivanih vrijednosti u slučaju kada njihova udaljenost divergira. U ovom kontekstu, divergencija znači da su pozicije antipodalne u lancu čija duljina raste neograničeno. Uz ovo, postoji i dodatna suptilnost ovisno o tome koliko brzo se ova vrijednost približava nuli, polinomno ili eksponencijalno.

Prva poteškoća u primjeni PDN leži u činjenici da nije uvijek očito na koji način uzeti limese, kao što je diskutirano u prijašnjim radovima [10], odnosno trebamo li prvo uzeti limes divergirajućeg $N$ ili prvo postaviti $r$ iz jednadžbe (7.2) na udaljenost antipodalnih točaka $(N\pm1)/2$ pa tek onda uzeti limes za $N$. U navedenom radu je pokazano da ova dvosmislenost vodi na dva bitno različita ponašanja za očekivanu vrijednost spinskog operatora, odnosno magnetizaciju u smjeru $x$.

Cilj ovog diplomskog rada je proširiti ovu diskusiju na slučaj vremenski ovisnog PDN tako što ćemo promotriti evoluciju sustava nakon globalne promjene parametra $\phi$ u $t=0$.

## *7.2 Rješenje XY modela*

### 7.2.1 Simetrijska svojstva XY modela

Prva očita simetrija modela je njegova translacijska invarijantnost, koju matematički formuliramo kao komutaciju unitarnog operatora translacije po spinskim položajima i Hamiltonijana:

$$[T,H]=0\ , \tag{7.3}$$

gdje je operator translacije definiran pomoću:

$$T\left|\psi\right\rangle = \bigotimes_{j=1}^{N} \left(\sigma_j^-\right)^{n_{j+1}} \left|\uparrow_j\right\rangle \ . \tag{7.4}$$

Uz ovo, definiramo i operatore pariteta po svakoj od osiju kao operatore koji u suštini broje koliko je preokrenutih spinova u lancu u pojedinom smjeru:

$$\Pi^{\mu} \coloneqq \bigotimes_{j=1}^{N} \sigma_j^{\mu} \ , \tag{7.5}$$

gdje $\mu$ označava smjer $x$, $y$ ili $z$.

Operatori pariteta komutiraju s Hamiltonijanom (7.1), ali antikomutiraju međusobno u slučaju neparnog $N$, implicirajući barem dvostruku degeneraciju svakog osnovnog stanja, neovisno o fazi.

Konačno, uvodimo operator zrcaljenja u odnosu na $k$-tu poziciju u lancu:

$$M_j\left|\psi\right\rangle = \bigotimes_{l=1}^{N} \left(\sigma_l^-\right)^{n_{2j-l}} \left|\uparrow_l\right\rangle \tag{7.6}$$

koji očito komutira s operatorima pariteta, a koristan je za izračun očekivanih vrijednosti spinskih operatora u trećoj fazi.

### 7.2.2 Jordan-Wignerova transformacija

Da bismo pronašli svojstvena stanja i energije Hamiltonijana (7.1), krećemo od standardnog pokušaja kvantizacije, odnosno zapisa spinskih operatora pomoću operatora dizanja i spuštanja:

$$\sigma_j^{\pm} = \frac{1}{2}\left[\sigma_j^x \pm \imath\sigma_j^y\right] \ . \tag{7.7}$$

Nakon što Hamiltonijan zapišemo koristeći isključivo njih, primijetimo da je konzistentna kvantizacija onemogućena činjenicom da su operatori $\sigma^{\pm}$ fermionski na istom položaju u lancu, ali bozonski na različitima. Da bismo mogli nastaviti, uvodimo novi skup Jordan-Wignerovih (JW) operatora $c_j$ koji su povezani s operatorima dizanja i spuštanja na sljedeći način:

$$c_j^{\dagger} \coloneqq \left(\bigotimes_{l=1}^{j-1} \sigma_l^z\right) \otimes \sigma_j^- \quad \text{i} \quad c_j \coloneqq \left(\bigotimes_{l=1}^{j-1} \sigma_l^z\right) \otimes \sigma_j^+ \ . \tag{7.8}$$

Može se pokazati da su operatori $c_i$ konzistentno fermionski i stoga naš Hamiltonijan prelazi u pogodan oblik jednom kad ga napišemo koristeći samo njih:

$$\begin{aligned} H = -\sqrt{2}\Bigg[\sum_{j=1}^{N}\left[\sin\left(\phi-\frac{\pi}{4}\right)c_j^\dagger c_{j+1}^\dagger - \cos\left(\phi-\frac{\pi}{4}\right)c_j^\dagger c_{j+1}\right] + \\ +\Pi^z\sqrt{2}\left[\sin\left(\phi-\frac{\pi}{4}\right)c_N^\dagger c_1^\dagger - \cos\left(\phi-\frac{\pi}{4}\right)c_N^\dagger c_1\right]\Bigg] + \text{H.c.}\ . \end{aligned} \tag{7.9}$$

S obzirom da $H$ i operator pariteta u $z$ smjeru $\Pi^z$ komutiraju, imaju zajednička svojstvena stanja. Kako paritet u smjeru $z$ može poprimiti samo dvije vrijednosti $\pm 1$, s obzirom na odabir rubnih uvjeta u (7.9), $H$ možemo razdvojiti na dva nepreklapajuća sektora pariteta:

$$H = \left(\frac{1+\Pi^z}{2}\right)H^+\left(\frac{1+\Pi^z}{2}\right) + \left(\frac{1-\Pi^z}{2}\right)H^-\left(\frac{1-\Pi^z}{2}\right)\ , \tag{7.10}$$

gdje oba člana imaju sličan oblik, iako odgovaraju različitim Fockovim prostorima:

$$H^\pm = -\sqrt{2}\sum_{j=1}^{N}\left[\sin\left(\phi-\frac{\pi}{4}\right)c_j^{\pm\dagger}c_{j+1}^{\pm\dagger} - \cos\left(\phi-\frac{\pi}{4}\right)c_j^{\pm\dagger}c_{j+1}^{\pm}\right] + \text{H.c.} \tag{7.11}$$

Paritet pojedinog sektora označava parnost broja JW fermiona koji su u njemu pobuđeni.

### 7.2.3 Fourierov transformat

Da bismo različite položaje u spinskom lancu pretvorili u fazne faktore, definiramo diskretni Fourierov transformat JW operatora $c_j$:

$$c_j^\pm = \frac{1}{\sqrt{N}}\sum_q e^{\imath qj}b_q \quad \leftrightarrow \quad b_q = \frac{1}{\sqrt{N}}\sum_j e^{-\imath qj}c_j^\pm \tag{7.12}$$

i primjećujemo da iz njegove definicije slijedi da su modovi po kojima sumiramo u dva sektora pariteta:

$$q \in \Gamma^+ = \left\{-\frac{N-2}{N}\pi,\ ...,\ -\frac{1}{N}\pi,\ \frac{1}{N}\pi,\ ...,\ \frac{N-2}{N}\pi,\ \pi\right\} \tag{7.13}$$

te

$$q \in \Gamma^- = \left\{-\frac{N-1}{N}\pi,\ ...,\ -\frac{2}{N}\pi,\ 0,\ \frac{2}{N}\pi,\ ...,\ \frac{N-1}{N}\pi\right\}. \tag{7.14}$$

Na temelju ovih skupova vrijednosti, naš FT zapisujemo preciznije:

$$c_j^{\pm} = \frac{1}{\sqrt{N}} \sum_{q \in \Gamma^{\pm}} e^{\imath q j} b_q \quad \leftrightarrow \quad b_q = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-\imath q j} c_j^{\pm} \ . \tag{7.15}$$

Zamjenom JW operatora u (7.11) njihovim FT, dolazimo do oblika koji se može zapisati na elegantan način kao suma po svim modovima:

$$H^{\pm} = \sum_{q \in \Gamma^{\pm}} \begin{pmatrix} b_q^{\dagger} & b_{-q} \end{pmatrix} \begin{bmatrix} C_{q,\phi} & -\imath S_{q,\phi} \\ \imath S_{q,\phi} & -C_{q,\phi} \end{bmatrix} \begin{pmatrix} b_q \\ b_{-q}^{\dagger} \end{pmatrix} \tag{7.16}$$

uz pokrate

$$C_{q,\phi} = \sqrt{2} \cos\left(\phi - \frac{\pi}{4}\right) \cos q \quad \text{i} \quad S_{q,\phi} = \sqrt{2} \sin\left(\phi - \frac{\pi}{4}\right) \sin q \ . \tag{7.17}$$

### 7.2.4 Bogoljubovljeva rotacija

Da bismo dijagonalizirali svaki od sumanada u (7.16), rješavamo problem dijagonalizacije $2 \times 2$ matrice tako da zahtijevamo da bude dijagonalna u operatorima $a_q$ koji su linearne kombinacije operatora $b_q$:

$$\begin{pmatrix} a_q \\ a_{-q}^{\dagger} \end{pmatrix} = \begin{bmatrix} \cos\theta_q & \imath \sin\theta_q \\ \imath \sin\theta_q & \cos\theta_q \end{bmatrix} \begin{pmatrix} b_q \\ b_{-q}^{\dagger} \end{pmatrix} \quad \text{za} \quad q \neq 0, \pi \ , \tag{7.18}$$

gdje je Bogoljubovljev kut $\theta_q$ definiran pomoću:

$$\theta_q \coloneqq \arctan \frac{|e^{\imath 2q} \cos\phi + \sin\phi| - [\cos\phi + \sin\phi] \cos q}{[\cos\phi - \sin\phi] \sin q} \quad \text{za} \quad q \neq 0, \pi \ . \tag{7.19}$$

Primijetimo da je Hamiltonijan dijagonalan za modove $0$ i $\pi$ te da stoga nema potrebe za Bogoljubovljevom rotacijom.

Koristeći (7.18), Hamiltonijan (7.16) uistinu svodimo na dijagonalan oblik koji zapisujemo kao:

$$H^{\pm} = \sum_{q \in \Gamma^{\pm}} \epsilon(q) \left[ a_q^{\dagger} a_q - \frac{1}{2} \right] \quad \text{za} \quad q \neq 0, \pi \quad \text{i} \quad \epsilon(q) = 2\sqrt{1 + \sin(2\phi)\cos(2q)} \ . \tag{7.20}$$

Iz ovog konačnog izraza napokon možemo odrediti svojstvena stanja i energije sustava u sve tri faze.

### 7.2.5 Svojstvena stanja i spektri

**Prva (uređena) faza** U ovoj fazi je energija moda $0$ negativna, a moda $\pi$ i svih ostalih modova pozitivna. Na temelju zahtjeva parnog broja čestica u parnom sektoru, za njegovo osnovno stanje uzimamo kvazičestični vakuum; a u neparnom sektoru moramo pobuditi barem jedan mod pa biramo onaj najmanje energije, odnosno mod $0$. Tada su osnovna stanja u svakom od sektora:

$$\text{parni: } |g^+\rangle = |0^+\rangle \quad \text{i} \quad \text{neparni: } |g^-\rangle = a_0^\dagger\,|0^-\rangle \quad , \tag{7.21}$$

gdje kvazičestični vakuum $|0^\pm\rangle$ poništavaju operatori $a_q$.

Analogno standardnom rješenju BCS problema, može se pokazati da je osnovno stanje u svakom od sektora dano izrazom:

$$|0^\pm\rangle = \bigotimes_{0<q<\pi;\ q\in\Gamma^\pm} \left[\cos\theta_q - \imath \sin\theta_q\ b_q^\dagger b_{-q}^\dagger\right] |0\rangle \quad , \tag{7.22}$$

gdje $|0\rangle$ označava vakuum za operatore $b$.

Djelovanjem Hamiltonijana u obliku (7.20) na svako od ovih stanja, pokazuje se da su njihove energije jednake za neparan $N$ i da stoga sustav pokazuje dvostruku degeneraciju osnovnog stanja. Usto, kako je energija moda $0$ manja od svih ostalih, a ujedno i veća od energije moda $\pi$ (i to s razlikom koja se ne smanjuje u termodinamičkom limesu $N \to \infty$), zaključujemo da u prvoj fazi postoji procjep u energijskom spektru sustava.

**Druga (mezoskopska) faza** U ovoj fazi je energija moda $\pi$ negativna, a moda $0$ i svih ostalih modova pozitivna. Na temelju zahtjeva parnog broja čestica u parnom sektoru, za njegovo osnovno stanje uzimamo kvazičestični vakuum, jer iako mu mod $\pi$ pripada i mogao bi smanjiti energiju osnovnog stanja, zbog zahtjeva parnosti broja pobuđenja bismo morali dodati još barem jedno pobuđenje, a sva ostala imaju energiju po iznosu veću od one moda $\pi$. U neparnom sektoru moramo pobuditi barem jedan mod pa ponovno biramo onaj najmanje energije među onima koji pripadaju tom sektoru, odnosno mod $0$. Tada su osnovna stanja u svakom od sektora kao i u prvoj fazi:

$$\text{parni: } |g^+\rangle = |0^+\rangle \quad \text{i} \quad \text{neparni: } |g^-\rangle = a_0^\dagger\,|0^-\rangle \quad . \tag{7.23}$$

Kao i u prvoj fazi, djelovanjem Hamiltonijana u obliku (7.20) na svako od ovih stanja, pokazuje se da su njihove energije jednake za neparan $N$ i da stoga sustav pokazuje dvostruku degeneraciju osnovnog stanja. No, u ovom slučaju je spektar sustava kontinuiran u termodinamičkom limesu zato što se energije ostalih modova mogu proizvoljno približiti energiji moda $0$.

**Treća (nesrazmjerna) faza** U trećoj fazi do izražaja dolaze modovi $\pm p' \in \Gamma^+$:

$$p' = \begin{cases} \frac{\pi}{2}\left(1+\frac{1}{N}\right) \ ; & N \bmod 4 = 1 \ , \\ \frac{\pi}{2}\left(1-\frac{1}{N}\right) \ ; & N \bmod 4 = 3 \end{cases} \tag{7.24}$$

i $\pm p \in \Gamma^-$:

$$p = \begin{cases} \frac{\pi}{2}\left(1-\frac{1}{N}\right) \ ; & N \bmod 4 = 1 \ , \\ \frac{\pi}{2}\left(1+\frac{1}{N}\right) \ ; & N \bmod 4 = 3 \end{cases} \tag{7.25}$$

koji imaju niže energije od moda $0$ i stoga nova osnovna stanja postaju:

$$|\pm p'\rangle = a^\dagger_{\pm p'} a^\dagger_\pi |0^+\rangle \quad \text{i} \quad |\pm p\rangle = a^\dagger_{\pm p} |0^-\rangle \tag{7.26}$$

takva da im je energija jednaka, odnosno da je osnovno stanje četverostruko degenerirano.

## *7.3 Statičke korelacijske funkcije*

Kao što je najavljeno u motivacijskom dijelu, od interesa su nam korelacijske funkcije i magnetizacije, a krećemo od računanja korelacijskih funkcija jer je jednostavnije.

Naravno, nas zanimaju korelacijske funkcije za operatore $\sigma^\mu_j$, no osnovna stanja sustava nisu zadana pomoću njih. Stoga, ove operatore pretvorimo u operatore $c_j$ koristeći JW transformaciju, onda njih u operatore $b_q$ pomoću FT i konačno u $a_q$ koristeći Bogoljubovljevu rotaciju. Na ovaj način, dolazimo do operatora čije je djelovanje na stanja sustava jasno i stoga lako koračanjem unatrag dođemo do korelacijskih funkcija za spinske operatore.

Zbog kompleksnosti pripadnih izraza, definiramo *Majorana fermionske operatore*:

$$A_j \coloneqq \left(\bigotimes_{l=1}^{j-1} \sigma_l^z\right) \otimes \sigma_j^x = c_j^\dagger + c_j \quad \text{i} \quad B_j \coloneqq \left(\bigotimes_{l=1}^{j-1} \sigma_l^z\right) \otimes \sigma_j^y = \imath\left(c_j^\dagger - c_j\right) \tag{7.27}$$

pomoću kojih je korelacijske funkcije moguće izraziti kao npr.

$$C_{jl}^{xx} = \langle g^\pm | \, \sigma_j^x \sigma_l^x \, | g^\pm \rangle = (-\imath)^{l-j} \, \langle g^\pm | \bigotimes_{m=j}^{l-1} B_m A_{m+1} \, | g^\pm \rangle \tag{7.28}$$

u prve dvije faze i slično za smjerove $y$ i $z$.

Očekivane vrijednosti umožaka fermionskih operatora zapisujemo u pogodnom matričnom obliku koristeći *Wickov teorem za fermionske operatore* pa npr. očekivana vrijednost u izrazu (7.28) odgovara determinanti:

$$C_{jl}^{xx} = (-1)^r \begin{vmatrix} G(1) & G(0) & G(-1) & \dots & G(2-r) \\ G(2) & G(1) & G(0) & \dots & G(3-r) \\ G(3) & G(2) & G(1) & \dots & G(4-r) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G(r) & G(r-1) & G(r-2) & \dots & G(1) \end{vmatrix} \tag{7.29}$$

uz

$$G(j-l) \coloneqq -\imath \, \langle g^\pm | \, A_j B_l \, | g^\pm \rangle = \imath \, \langle g^\pm | \, B_l A_j \, | g^\pm \rangle \ . \tag{7.30}$$

Valja primijetiti da u ovoj fazi, od tri moguće vrste kontrakcija Majorana operatora $A_j$ i $B_j$: $\langle A_j A_l \rangle$, $\langle B_j B_l \rangle$ i $\langle A_j B_l \rangle$ susrećemo samo posljednju, što je odraz translacijske invarijantnosti korelacijske funkcije. Slično vrijedi i za drugu fazu, dok se u trećoj javljaju i $\langle A_j A_l \rangle$ i $\langle B_j B_l \rangle$ članovi.

Analitički izraz za svakog od njih izračunat je koristeći prethodno opisani proces[67] te se pokaže da za prve dvije faze vrijedi:

$$\boxed{\langle g^\pm | \, A_j A_l \, | g^\pm \rangle = \langle g^\pm | \, B_j B_l \, | g^\pm \rangle = \delta_{j,l}} \tag{7.31}$$

[67] Uz određene suptilnosti vezano za činjenicu da Bogoljubovljeva rotacija u pojedinim fazama vodi na rotaciju Hamiltonijana za modove $0$ i $\pi$ u kojima je već dijagonalan. Za ove modove treba napraviti korekcije u sumama.

i

$$\boxed{\langle g^{\pm}|\, A_j B_l \,|g^{\pm}\rangle = \frac{\imath}{N}\sum_{q\in\Gamma^{\pm}} e^{\imath 2\theta_q} e^{-\imath q(j-l)} + \frac{2\imath}{N} f_{\phi}^{\pm}\,(j-l)} \tag{7.32}$$

uz

$$f_{\phi}^{\pm}\,(j-l) \coloneqq \begin{cases} 0\ ; \quad \phi \in \langle -\frac{\pi}{2}, -\frac{\pi}{4}\rangle\ , \\ -\,(\mp 1)^{j-l+1}\ \ ; \quad \phi \in \langle -\frac{\pi}{4}, 0\rangle\ . \end{cases} \tag{7.33}$$

Primijetimo da funkcija $f_{\phi}^{\pm}$ iščezava u prvoj fazi, u skladu s činjenicom da sustav u njoj ne pokazuje frustraciju jer je dominantna interakcija feromagnetska.

Analogni račun za treću fazu daje

$$\boxed{\langle A_j B_l\rangle_{u_1,u_2} = \frac{\imath}{N}\sum_{q\in\Gamma^{-}} e^{\imath 2\theta_q} e^{-\imath q(j-l)} - \frac{2\imath}{N}\cos\left[p\,(j-l) - 2\theta_p\right] - \frac{2\imath}{N}\left(u_1^{*} u_2 e^{-\imath p(j+l)} + \text{c.c.}\right)} \tag{7.34}$$

i

$$\boxed{\langle A_j A_l\rangle_{u_1,u_2} = \langle B_j B_l\rangle_{u_1,u_2} = \delta_{j,l} - \frac{2\imath}{N}\left(|u_1|^2 - |u_2|^2\right)\sin\left[p\,(j-l)\right]}\ . \tag{7.35}$$

### 7.3.1 Problem vremenske evolucije

Da bismo mogli doći do dinamičkih korelacijskih funkcija i magnetizacija, trebamo riješiti problem vremenske evolucije za XY model.

U tu svrhu koristimo vremensku neovisnost njegova Hamiltonijana i separabilnost po potprostorima da riješimo diferencijalnu jednadžbu vremenske evolucije koja odgovara globalnoj promjeni parametra $\phi$ u $t = 0$:

$$\imath\frac{\mathrm{d}}{\mathrm{d}t} U_{q,\phi_1}(t) = U_{q,\phi_1}(t) H_{\phi_1,q}\ , \tag{7.36}$$

a za modove $0$ i $\pi$ daje trivijalne evolucije koje predstavljaju samo zajedničke globalne

faktore, dok za ostale daje:

$$\begin{aligned}\begin{pmatrix}\widetilde{\alpha}_q(t)\\ \widetilde{\beta}_q(t)\end{pmatrix} =: |\psi_q(t)\rangle = U_{q,\phi_1}(t)\,|\psi_q\rangle = \begin{bmatrix}U^{11}_{q,\phi_1}(t) & U^{12}_{q,\phi_1}(t)\\ U^{21}_{q,\phi_1}(t) & U^{22}_{q,\phi_1}(t)\end{bmatrix}\begin{pmatrix}\alpha_q\\ \beta_q\end{pmatrix}\\ = \begin{pmatrix}U^{11}_{q,\phi_1}(t)\alpha_{q,\phi_0} + U^{12}_{q,\phi_1}(t)\beta_{q,\phi_0}\\ U^{21}_{q,\phi_1}(t)\alpha_{q,\phi_0} + U^{22}_{q,\phi_1}(t)\beta_{q,\phi_0}\end{pmatrix}\\ = \begin{pmatrix}\alpha_{q,\phi_0}\cos\left[\lambda_{q,\phi_1}t\right] + \frac{2}{\lambda_{q,\phi_1}}\left[-\imath C_{q,\phi_1}\alpha_{q,\phi_0} + S_{q,\phi_1}\beta_{q,\phi_0}\right]\sin\left[\lambda_{q,\phi_1}t\right]\\ \beta_{q,\phi_0}\cos\left[\lambda_{q,\phi_1}t\right] + \frac{2}{\lambda_{q,\phi_1}}\left[-S_{q,\phi_1}\alpha_{q,\phi_0} + \imath C_{q,\phi_1}\beta_{q,\phi_0}\right]\sin\left[\lambda_{q,\phi_1}t\right]\end{pmatrix},\end{aligned} \tag{7.37}$$

uz pokrate

$$\alpha_q = -\imath\sin\theta_q \quad \text{i} \quad \beta_q = \cos\theta_q\ . \tag{7.38}$$

### 7.3.2 Dinamičke korelacijske funkcije

Jednom kada smo pronašli kako osnovna stanja sustava u sve tri faze izgledaju tijekom evolucije u vremenu, potpuno analognim postupkom kao i za statički slučaj dolazimo do rezultata za korelacijske funkcije Majorana operatora.

Tako u prve dvije faze vrijedi:

$$\boxed{\langle A_j A_l\rangle_{g^{\pm}(t)} = \delta_{j,l} - \frac{\imath}{N}\sum_{q\in\Gamma^{\pm}}\left(\widetilde{\alpha}^*_q(t)\widetilde{\beta}_q(t) + \widetilde{\alpha}_q(t)\widetilde{\beta}^*_q(t)\right)\sin\left[q\,(j-l)\right]} \tag{7.39}$$

i

$$\boxed{\langle B_j B_l\rangle_{g^{\pm}(t)} = \delta_{j,l} + \frac{\imath}{N}\sum_{q\in\Gamma^{\pm}}\left(\widetilde{\alpha}^*_q(t)\widetilde{\beta}_q(t) + \widetilde{\alpha}_q(t)\widetilde{\beta}^*_q(t)\right)\sin\left[q\,(j-l)\right]} \tag{7.40}$$

te

$$\boxed{\begin{aligned}\langle A_j B_l\rangle_{g^{\pm}(t)} =& \frac{\imath}{N}\sum_{q\in\Gamma^{\pm}}\Big[\left(|\widetilde{\beta}_q(t)|^2 - |\widetilde{\alpha}_q(t)|^2\right)\cos\left[q\,(j-l)\right] +\\ &+ \imath\left(\widetilde{\alpha}_q(t)\widetilde{\beta}^*_q(t) - \widetilde{\alpha}^*_q(t)\widetilde{\beta}_q(t)\right)\sin\left[q\,(j-l)\right]\Big] + \frac{2\imath}{N}f^{\pm}_{\phi_0}(j-l)\end{aligned}}\ . \tag{7.41}$$

S druge strane, za treću fazu vrijedi:

$$\begin{aligned}&\langle A_j A_l\rangle_{u_1,u_2}(t)\\ &=\delta_{j,l}-\frac{\imath}{N}\sum_{q\in\Gamma^-}\left(\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)+\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\right)\sin\left[q\left(j-l\right)\right]+\\ &\quad+\frac{2\imath}{N}\left(\widetilde{\alpha}_p^*(t)\widetilde{\beta}_p(t)+\widetilde{\alpha}_p(t)\widetilde{\beta}_p^*(t)\right)\sin\left[p\left(j-l\right)\right]-\frac{2\imath}{N}\left(|u_1|^2-|u_2|^2\right)\sin\left[p\left(j-l\right)\right]\end{aligned} \tag{7.42}$$

i

$$\begin{aligned}&\langle B_j B_l\rangle_{u_1,u_2}(t)\\ &=\delta_{j,l}+\frac{\imath}{N}\sum_{q\in\Gamma^-}\left(\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)+\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\right)\sin\left[q\left(j-l\right)\right]-\\ &\quad-\frac{2\imath}{N}\left(\widetilde{\alpha}_p^*(t)\widetilde{\beta}_p(t)+\widetilde{\alpha}_p(t)\widetilde{\beta}_p^*(t)\right)\sin\left[p\left(j-l\right)\right]-\frac{2\imath}{N}\left(|u_1|^2-|u_2|^2\right)\sin\left[p\left(j-l\right)\right]\end{aligned} \tag{7.43}$$

te

$$\begin{aligned}&\langle A_j B_l\rangle_{u_1,u_2}(t)\\ &=\frac{\imath}{N}\sum_{q\in\Gamma^-}\left[\left(|\widetilde{\beta}_q(t)|^2-|\widetilde{\alpha}_q(t)|^2\right)\cos\left[q\left(j-l\right)\right]-\imath\left(\widetilde{\alpha}_q^*(t)\widetilde{\beta}_q(t)-\widetilde{\alpha}_q(t)\widetilde{\beta}_q^*(t)\right)\sin\left[q\left(j-l\right)\right]\right]-\\ &\quad-\frac{2\imath}{N}\left[\left(|\widetilde{\beta}_p(t)|^2-|\widetilde{\alpha}_p(t)|^2\right)\cos\left[p\left(j-l\right)\right]-\imath\left(\widetilde{\alpha}_p^*(t)\widetilde{\beta}_p(t)-\widetilde{\alpha}_p(t)\widetilde{\beta}_p^*(t)\right)\sin\left[p\left(j-l\right)\right]\right]-\\ &\quad-\frac{2\imath}{N}\left(u_1^*u_2e^{-\imath p(j+l)}+\text{c.c.}\right)\end{aligned}, \tag{7.44}$$

gdje valja primijetiti da korelacijske funkcije više ne ovise samo o razlici $j$ i $l$, odnosno da je translacijska invarijantnost narušena.

Lako se pokazuje da se svi ovi izrazi svode na izračunate statičke očekivane vrijednosti u limesu $t=0$. Također, fizikalne korelacijske funkcije ponovno su dane determinantama matrica, ali složenijeg oblika nego u statičkom slučaju zato što članovi $\langle A_j A_l\rangle$ i $\langle B_j B_l\rangle$ više nisu Kronecker-delte. Jedan takav primjer je matrica korelacija

u $y$ smjeru za sustav čija evolucija kreće iz jedne od prve dvije faze:

$$\left[(-\imath)^r\,\widetilde{C}^{yy}_{jl}(t)\right]^2 \coloneqq \left[(-\imath)^r\,\widetilde{C}^{yy}_{j-l}(t)\right]^2$$

$$= \frac{\begin{vmatrix} 0 & \widetilde{F}_1(-1) & \dots & \widetilde{F}_1(1-r) \\ \widetilde{F}_1(1) & 0 & \dots & \widetilde{F}_1(2-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_1(r-2) & \widetilde{F}_1(r-3) & \dots & 0 \end{vmatrix} \begin{vmatrix} \widetilde{F}_2(-1) & \widetilde{F}_2(-2) & \dots & \widetilde{F}_2(-r) \\ \widetilde{F}_2(0) & \widetilde{F}_2(-1) & \dots & \widetilde{F}_2(1-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_2(r-2) & \widetilde{F}_2(r-3) & \dots & \widetilde{F}_2(-1) \end{vmatrix}}{\begin{vmatrix} -\widetilde{F}_2(-1) & -\widetilde{F}_2(0) & \dots & -\widetilde{F}_2(r-2) \\ -\widetilde{F}_2(-2) & -\widetilde{F}_2(-1) & \dots & -\widetilde{F}_2(r-3) \\ \vdots & \vdots & \ddots & \vdots \\ -\widetilde{F}_2(-r) & -\widetilde{F}_2(r-1) & \dots & -\widetilde{F}_2(1) \end{vmatrix} \begin{vmatrix} 0 & \widetilde{F}_3(-1) & \dots & \widetilde{F}_3(1-r) \\ \widetilde{F}_3(1) & 0 & \dots & \widetilde{F}_3(2-r) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{F}_3(1-r) & \dots & \widetilde{F}_3(r-2) & 0 \end{vmatrix}}, \tag{7.45}$$

gdje funckije $\widetilde{F}_1(r)$, $\widetilde{F}_3(r)$ i $\widetilde{F}_2(r)$ do na faktore redom odgovaraju korelacijskim funkcijama $\langle A_j A_l\rangle$, $\langle B_j B_l\rangle$ i $\langle A_j A_l\rangle$ i $\langle A_j B_l\rangle$ uz $r = l - j$.

### 7.3.3 Dinamičke magnetizacije

Nakon što su sve korelacijske funkcije izračunate, okrećemo se suptilnijem problemu računanja magnetizacija. Naime, svojstvena stanja Hamiltonijana su istovremeno i svojstvena stanja operatora pariteta u smjeru $z$ pa stoga operatori $\sigma^x_j$ i $\sigma^y_j$ mijenjaju njihov paritet te njihova očekivana vrijednost u njima nužno iščezava. No, s obzirom na degeneraciju stanja sustava u sve tri faze, moguće je konstruirati linearne kombinacije osnovnih stanja kojima ove očekivane vrijednosti ne iščezavaju.

Kao primjer takve konstrukcije, promotrimo vremenski ovisna osnovna stanja oba sektora u prve dvije faze $|g^{\pm}(t)\rangle$. S obzirom na to da operator pariteta u npr. $x$ smjeru $\Pi^x$ mijenja $z$ paritet ovog stanja, vidimo da će npr. stanje $\Pi^x\,|g^+(t)\rangle$ do na fazni pomak odgovarati stanju $|g^-(t)\rangle$. Stoga, možemo konstruirati općenito osnovno stanje kao kombinaciju $|g^+(t)\rangle$ i $\Pi^x\,|g^+(t)\rangle$ uz određene relativne koeficijente. Pokazuje se da postoji njihov odabir takav da dobiveno stanje bude svojstveno stanje operatora $\Pi^x$ te istovremeno da očekivana vrijednost istog operatora (magnetizacija) bude maksimalna. To stanje s neiščezavajućim paritetom u smjeru $x$ je

$$|g_x(t)\rangle = \frac{1}{\sqrt{2}}\left[1 + \Pi^x\right]|g^+(t)\rangle \tag{7.46}$$

te analogno za $y$ smjer.

Očekivane vrijednosti pojedinih operatora se sada, koristeći ovako konstruirana stanja, ponovno mogu prikazati pomoću determinanti vremenski ovisnih matrica.

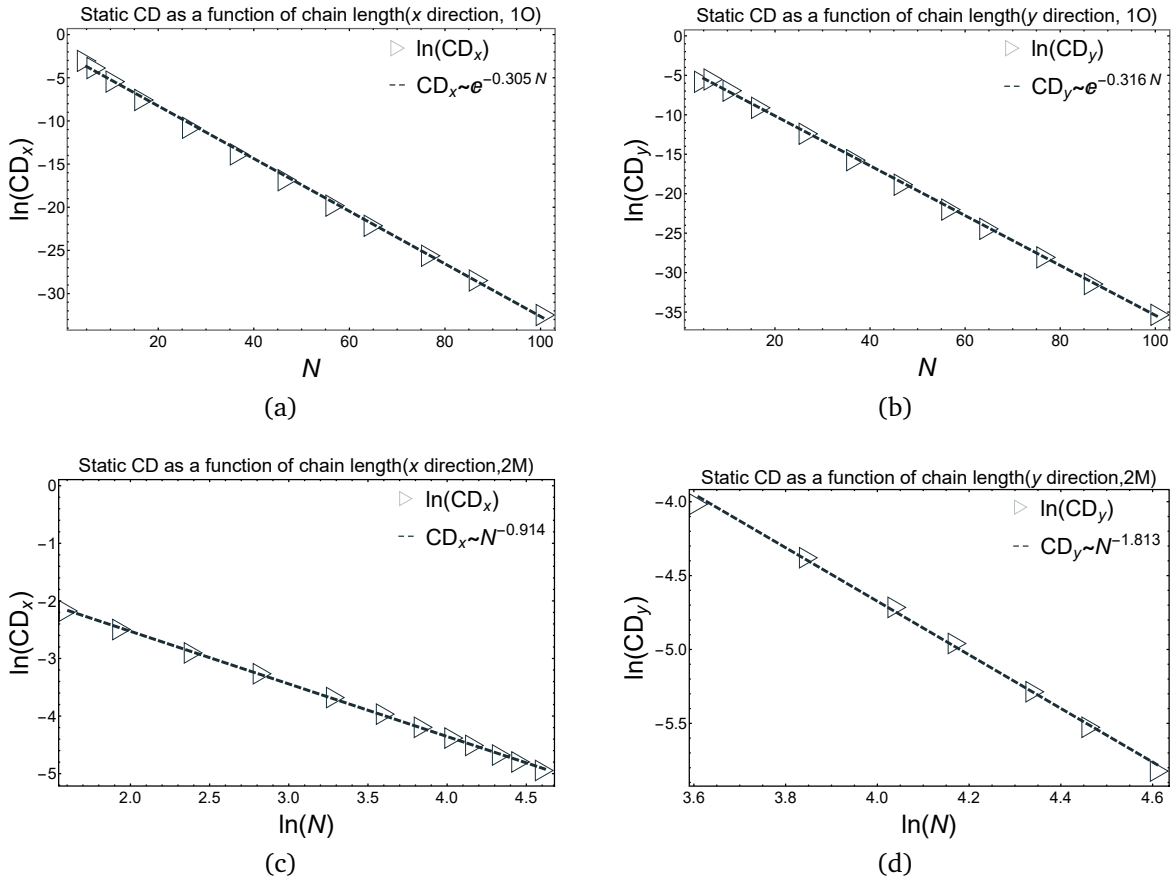
Za magnetizacije u prve dvije faze postupak je jednostavniji nego za treću. Naime, u trećoj fazi je potrebno koristiti rezultate koji opisuju djelovanje operatora zrcaljenja i translacije na stanja sustava te na taj način doći do prikladnog izraza za njihovu vrijednost. U ovom se slučaju dolazi do najavljene magnetizacije koja je nesrazmjerno modulirana duž spinskog lanca. Također, u ovoj fazi dijelovi matrica korelacijskih funkcija više ne ovise samo o udaljenosti dvaju položaja $r$ nego i o njihovim pojedinačnim vrijednostima, sukladno s činjenicom da korelacijske funkcije više nisu translacijski invarijantne.

## *7.4 Rezultati i zaključci*

Analiza statičkog principa dekompozicije nakupina u prve dvije faze prikazana je na Slici 7.2 i pokazuje slaganje sa poznatim rezultatima [10, 41]. Konkretno, u prvoj (nefrustriranoj) fazi sve korelacije pa tako i DN trnu eksponencijalno, dok u drugoj (frustriranoj) dominantni članovi postaju algebarski (polinomni)) u veličini sustava $N$.

Rezultati analize principa dekompozicije nakupina za duga vremena i $6$ evolucija koje počinju u jednoj od prve dvije faze prikazani su na Slikama 7.3 i 7.4 na kojima se da uočiti da većini evolucija odgovara eksponencijalno trnjenje DN, no u tri se javlja algebarsko, implicirajući da u sustavu postoji mezoskopsko ponašanje, odnosno korelacijske funkcije se ne mogu rastavljati za konačne sustave. Uz ovo, u barem jednoj od evolucija, uočljiva je odgoda trnućeg ponašanja prema većem broju spinova, u skladu s prethodnim zaključkom. Podaci u ovom režimu dobiveni su tako da se usrednji po $100$ točaka u nekom intervalu koji je udaljen od vremenskog ishodišta. S obzirom na oscilatornu prirodu članova u PDN, usrednjavanje je vršeno kvadratno, što ima i intuitivnog smisla jer nas u suštini zanima koliko su dva člana u (7.2) udaljena, a ne nužno koji od njih je veći.

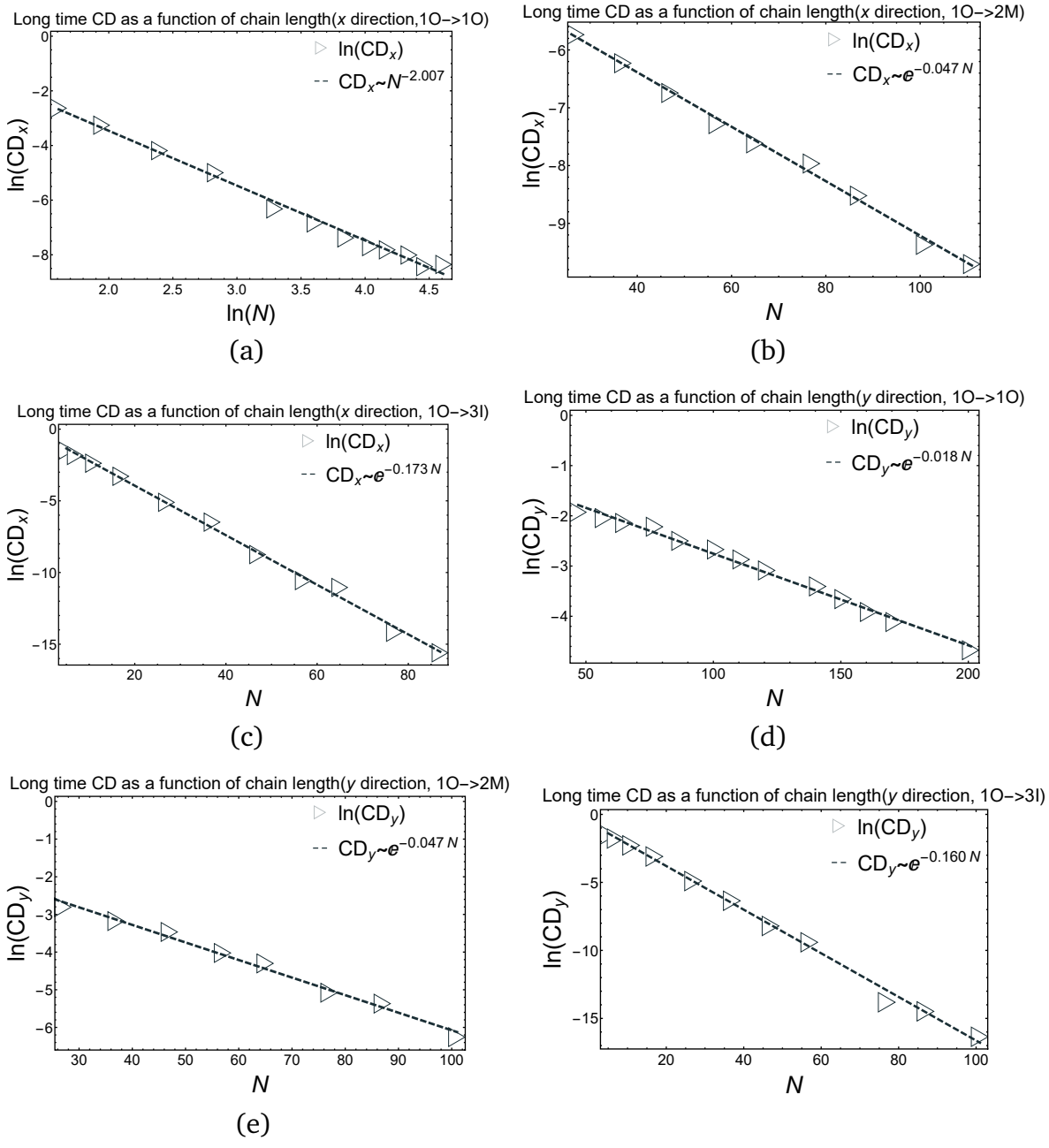
Da zaključimo, podsjetimo se bitne pojave mezoskopskog ponašanja u nekoliko režima dugih vremena u kojima prilikom evolucije ostajemo u jednoj od prve dvije faze. Ovakvo ponašanje detaljno je diskutirano u prethodnim radovima [10] te je



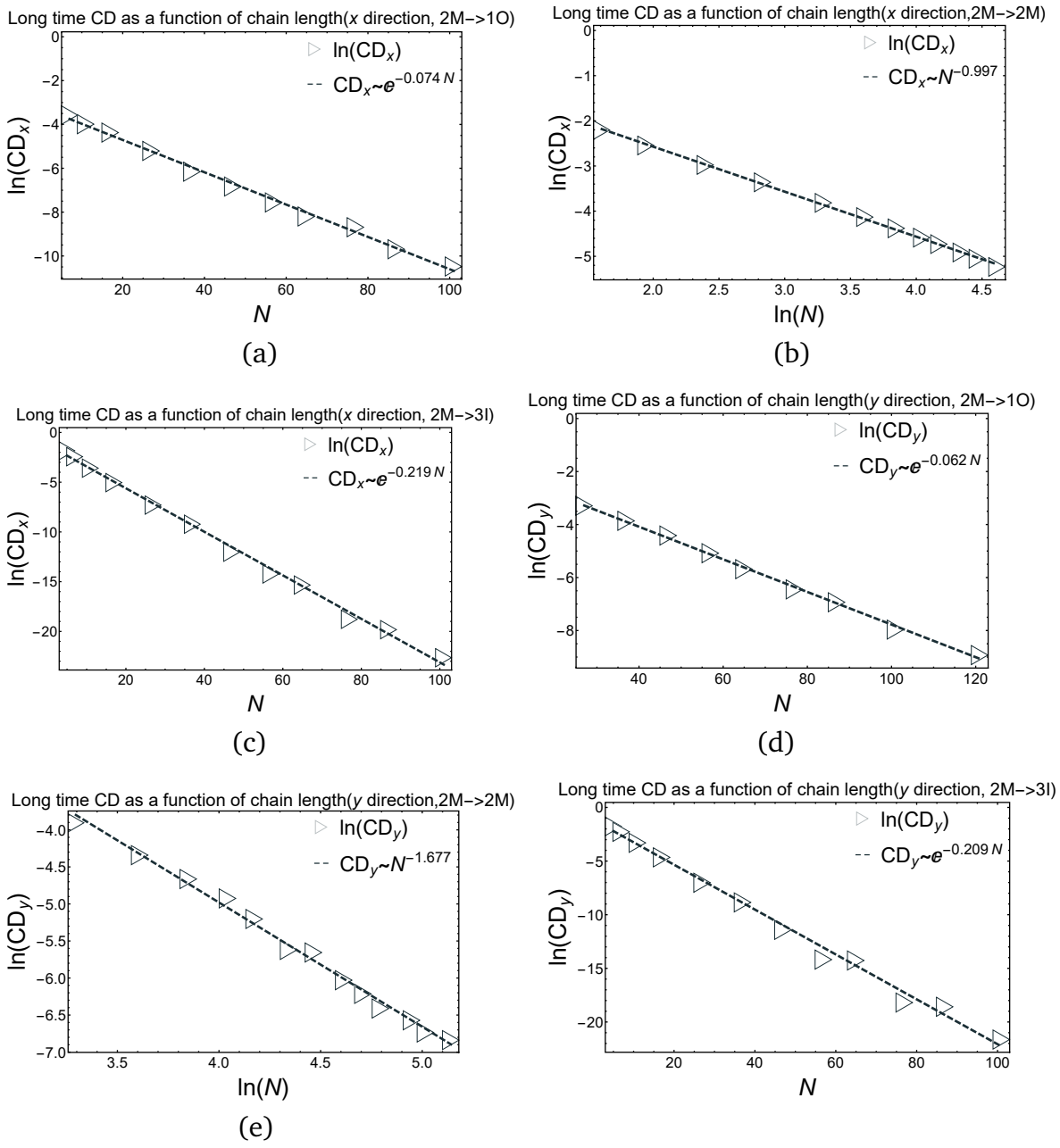

Slika 7.2: Statički princip dekompozicije nakupina za (a) $x$ smjer, 1O ($\phi = -\pi/3.5$); (b) $y$ smjer, 1O ($\phi = -\pi/3.5$); (c) $x$ smjer, 2M ($\phi = -\pi/5.2$); (d) $y$ smjer, 2M ($\phi = -\pi/5.2$).

ovim radom pokazano da se javlja i u vremenski ovisnim sustavima. Trenutni plan za objašnjenje ovog ponašanja je analogna analiza za evolucije koje kreću iz treće faze jer je u njoj sustav također frustriran pa se ima smisla nadati da će moći pružiti bolji uvid u opažene fenomene.

Na kraju, ističemo važnost dobivenih rezultata s obzirom da daju ograničenja na primjenjivost principa dekompozicije nakupina i u određenim sustavima sprečavaju njegovo korištenje za konačne veličine. U takvim situacijama, potreban je dodatan sloj rigora i pažnje u odnosu na to kako se ovaj princip uobičajeno primjenjuje.




Slika 7.3: Usrednjene vrijednosti DN za vremenske trenutke daleko od $t = 0$ i evolucije koje počinju u prvoj fazi (a) $x$ smjer, 1O$\rightsquigarrow$1O $(-\pi/3.0 \rightsquigarrow -\pi/3.5)$ (b) $x$ smjer, 1O$\rightsquigarrow$2M $(-\pi/3.3 \rightsquigarrow -\pi/5.2)$ (c) $x$ smjer, 1O$\rightsquigarrow$3I $(-\pi/3.0 \rightsquigarrow +\pi/4.5)$ (d) $y$ smjer, 1O$\rightsquigarrow$1O $(-\pi/2.5 \rightsquigarrow -\pi/3.5)$ (e) $y$ smjer, 1O$\rightsquigarrow$2M $(-\pi/3.0 \rightsquigarrow -\pi/4.9)$ (f) $y$ smjer, 1O$\rightsquigarrow$3I $(-\pi/3.0 \rightsquigarrow +\pi/4.5)$ .




Slika 7.4: Usrednjene vrijednosti DN za vremenske trenutke daleko od $t = 0$ i evolucije koje počinju u drugoj fazi (a) $x$ smjer, 2M$\rightsquigarrow$1O $(-\pi/4.8 \rightsquigarrow -\pi/3.0)$ (b) $x$ smjer, 2M$\rightsquigarrow$2M $(-\pi/4.5 \rightsquigarrow -\pi/5.0)$ (c) $x$ smjer, 2M$\rightsquigarrow$3I $(-\pi/4.5 \rightsquigarrow +\pi/4.5)$ (d) $y$ smjer, 2M$\rightsquigarrow$1O $(-\pi/4.8 \rightsquigarrow -\pi/3.0)$ (e) $y$ smjer, 2M$\rightsquigarrow$2M $(-\pi/4.5 \rightsquigarrow -\pi/5.0)$ (f) $y$ smjer, 2M$\rightsquigarrow$3I $(-\pi/4.5 \rightsquigarrow +\pi/4.5)$ .

## *7.5 Nazivi slika i tablica na hrvatskom jeziku*

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