Studying time-dependent symmetry breaking with the path integral approach

Author: Jorrit RIJNBEEK

Supervisors: Dr. Carmine ORTIX
Prof. dr. Jeroen VAN DEN BRINK

Co-Supervisor: Dr. Jasper VAN WEZEL

September 11, 2009
Abstract

Symmetry breaking is studied in many systems by introducing a static symmetry breaking field. By taking the right limits, one can prove that certain symmetries in a system will be broken spontaneously. One might wonder what the results are when the symmetry breaking field depends on time, and if it differs from a static case. It turns out that it does.

The study focuses on the Lieb-Mattis model for an antiferromagnet. It is an infinite range model in the sense that all the spins on one sublattice interact with all spins on the other sublattice. This model has a wide range of applications as it effectively contains the thin spectrum for the familiar class of Heisenberg models.

In order to study time-dependent symmetry breaking of the Lieb-Mattis model, one needs the path integral mechanism. It turns out that for solving a general quadratic Hamiltonian, only two solutions of the classical Euler-Lagrange equation of motion need to be known. Furthermore, the introduction of a boundary condition to the system is investigated, where the problem is limited to half-space. The effects of the boundary condition can be implemented at the very end when a set of wave functions and the propagator of the time-dependent system is known.

The Lieb-Mattis model of an antiferromagnet is studied with the developed path integral mechanism. A linear symmetry breaking field is introduced and its consequences are computed. An instantaneous state can be defined, which represents the results that a static treatment would have given us by simply implementing the time-dependence at the end. This is compared with the true dynamical state that is calculated by means of the path integral mechanism.

A density of defects is defined, which is a measure of the difference between the dynamical symmetry-broken ground state and the instantaneous one. The behaviour of the density of defects can be summarised in a phase diagram, which is controlled by two system parameters: the initial time that the field is switched on, and the final time.

The phase diagram consists of three regions. First of all, it contains a defect creation regime in which the defect density increases but does not saturate before the final time is reached. Secondly, there exists a defect saturation regime where the defects are present and are saturated at the final time. Finally, there exists a defect free region, in which no defects can be found.

The results of the linear field case can be generalised to other shapes of the time-dependent symmetry-breaking field. The same phases can be identified in the phase diagram and only the quantitative behaviour of the phase diagram changes. Therefore one concludes that in general the way in which a symmetry is broken matters for the resulting symmetry broken ground state.
Contents

I. Introduction 5

1. Introduction to spontaneous symmetry breaking and motivation 7
  1.1. The crystal and the thin spectrum ................................. 7
  1.2. Spontaneous symmetry breaking in the crystal ................. 9
  1.3. Motivation ....................................................... 10

2. The method: path integrals 11
  2.1. Path integral formalism ......................................... 12
  2.2. Quadratic Hamiltonians ........................................... 15
  2.3. Wave functions ................................................... 18
  2.4. Boundary conditions in the classical way ...................... 22
    2.4.1. Static field ................................................ 23
    2.4.2. Exponential field .......................................... 25
    2.4.3. Linear field ............................................... 28
    2.4.4. Conclusion and physical analog ............................ 31
  2.5. Boundary conditions in the quantum way: the Kleinert argument .... 32
  2.6. Conclusion ...................................................... 35

3. Theoretical study of time-dependent symmetry breaking of the Lieb-Mattis model 36
  3.1. Derivation of the Lieb-Mattis Hamiltonian .................... 36
  3.2. Breaking the symmetry dynamically ............................. 38
  3.3. Theoretical study of a linear symmetry-breaking field ........ 40
    3.3.1. Shape of the symmetry-breaking field and the equations of motion ... 41
    3.3.2. The dynamical basis ...................................... 43
    3.3.3. The overlaps and the dynamical state .................... 47
    3.3.4. Energy of the dynamical state ........................... 51
    3.3.5. Density of defects ....................................... 51
    3.3.6. Generalisation to other time-dependent symmetry-breaking fields ... 56
    3.3.7. Influence of the perturbing state $\gamma_2(S, \tau)$ on the dynamical state $\Psi(S, \tau)$, energy $E(\tau)$, and the density of defects $\rho(\tau)$ ......................... 58
  3.4. Conclusion ...................................................... 59

4. Summary 62

A. Factorisation 65
B. Pauli-van Vleck formula 66
C. Energy levels 68
D. Derivation of the equation of motion 70
E. Derivation of $\omega_r$ and the $\gamma_1(S, t)$ state 71

Bibliography 72
Introduction

The very first question you might like to answer before reading this thesis could be: what is symmetry and what is a broken symmetry? A symmetry in a physical system means that the system is invariant after some kind of transformation. This transformation can be anything, for example a translation through space or a rotation around a particular axis. Symmetries arise in all realms of physics and besides their beauty they appeal to physicists due to the fact that practically all laws in nature arise from a symmetry.

Symmetries can be broken. The easiest and most familiar example in daily life is 3-dimensional space here on earth. Two directions, north and west for instance, are in a sense the same. If one would be at a desert for instance, one could not recognise the difference (neglect any navigational clues like the sun or other stars) between north and west, but for sure one could recognise the difference between up and down, due to the gravitational force. So this symmetry of 3-dimensional space is broken: not all directions are equal. In this case, gravity breaks the symmetry.

Spontaneous symmetry breaking is exactly what it says: the symmetry gets broken spontaneously. One could picture the gravitational force breaking symmetry in a quite non-subtle, brute way. Spontaneous symmetry breaking is a bit more subtle. A funny way to picture it is imagining a ball lying on top of a symmetric hill. The tiniest displacement would push the ball downwards, picking some direction in which to roll down. The symmetry has been broken because the ball rolled down in only one, now special, direction.

Spontaneous symmetry breaking is related to the fact that the tiniest, or infinitesimal, external influence can break the perfect symmetry that existed without the externality. An essential feature of spontaneous symmetry breaking is the existence of non-commuting limits. In other words: the ordering of the limits matters. In the ball example one has to consider the shape of the hill as well. Suppose that the top of the hill is a bit flattened initially. If one removes the displacement of the ball before making the hill sharp, the ball remains on top of the hill. However, if one makes the hill sharp before removing the displacement of the ball from the centre, the ball falls down. In this example, the difference between these operations is precisely the non-commuting limit.

The concept of spontaneous symmetry breaking arises in many areas of physics, for example condensed matter physics and high energy physics. The superconductor is an interesting system in which this mechanism plays an essential role. Another one is the Lieb-Mattis model for an antiferromagnet, which is studied in this thesis. In high energy physics, the Higgs Mechanism is a well-known exponent of this phenomenon.

The goal of this project is to find an answer to the fundamental question: does the precise way in which a symmetry is broken matter? Does it matter if the symmetry-breaking externality has a certain shape, a certain time-dependence? We will try to find the answers to these question by use of the Lieb-Mattis model for an antiferromagnet.

This thesis is structured as follows. It starts with a short introductory chapter on spontaneous
symmetry breaking, mainly illustrated by the example of the harmonic crystal. After that, it will treat the formalism and methods necessary to solve this problem: Feynman’s path integral approach to quantum mechanics. We will apply this method in the third chapter to investigate the effects of dynamical symmetry breaking.
1. Introduction to spontaneous symmetry breaking and motivation

This master’s research project is a continuation of part of the work done in this group before in the context of Jasper van Wezel’s PhD [1]. In a particular paper that arose from that work [2], the concept of spontaneous symmetry breaking is introduced by means of the harmonic crystal. The way the symmetry gets broken instantaneously is illustrated nicely, and also the concept of the thin spectrum gets introduced. To gain understanding of (spontaneous) symmetry breaking, we will follow the same approach.

An important question to ask ourselves is: why do crystals, fixed at a certain position, exist? The informed reader may know that quantum mechanics tells us that if there is a certain symmetry in a system, each equivalent configuration due to the symmetry has equal weight.

For the crystal the principle that a symmetry causes equivalent states to have equivalent weight would mean that the crystal, being fully symmetric in space translations, should be completely delocalised! But in nature crystals appear to be fixed. They have lost all the quantum fluctuations: crystals are classical objects. One notices a table or chair at one fixed position, not floating around the room, or worse, the universe.

So how come? Are our laws of quantum mechanics incorrect? This conclusion would be a bit rash. A closer inspection in our quantum mechanical model will reveal that in fact spontaneous symmetry breaking governs this 'transition' from quantum physics to classical physics.Apparently, the translational symmetry gets broken in some way, making a certain position more favourable than others.

In this chapter, we will look at the harmonic crystal as an example of how this symmetry breaking precisely works. We will start our analysis with a Hamiltonian that describes the crystal, and diagonalise it. However, at a certain position in Fourier space the diagonalising transformation blows up. If we investigate this point a bit further, we will find that this is where the thin spectrum arises and the symmetry gets broken spontaneously. After that, we will motivate this project in section 1.3.

1.1. The crystal and the thin spectrum

The crystal can be described by a 1-dimensional chain of atoms $j$, which all have some kinetic energy due to their momentum (vibrations), and some potential energy due to the coupling with nearest neighbours. The easiest way to picture this potential energy is to imagine the atoms to be connected with their nearest neighbours by little springs, each exerting a tiny harmonic spring force. Casting these considerations into a Hamiltonian we can write down:
\[ H = \sum_j \frac{p_j^2}{2m} + \frac{\kappa}{2} \sum_j (x_j - x_{j+1})^2, \] (1.1)

with \( p_j \) the momentum of atom \( j \), \( m \) the mass, \( \kappa \) some spring coupling constant and \( x_j \) the position of atom \( j \). In any quantum textbook, for example [3], one would find that the system is transformed to new coordinates for the atoms: the position of the atom relative to the equilibrium position. Then one could Fourier transform the Hamiltonian and find phonons: collective wave-like modes of the atoms. Please note that we treat the 1-dimensional case, although extending the analysis to the 3-dimensional case is quite easy\(^1\).

However, we will take a different approach, based on [2], because the thin spectrum gets introduced in an insightful way.

We start our analysis by defining the bosonic operators:
\[
\begin{align*}
  b_j^\dagger &= \left( \frac{(2m\kappa)^{1/4}}{2m\kappa} - i \frac{p_j}{2m\kappa} \right) \frac{1}{\sqrt{2\hbar}} \\
  b_j &= \left( \frac{(2m\kappa)^{1/4}}{2m\kappa} + i \frac{p_j}{2m\kappa} \right) \frac{1}{\sqrt{2\hbar}}
\end{align*}
\] (1.2)

The term bosonic refers to the commutation relationship that the creation and annihilation operators obey. One can rewrite the operators \( x \) and \( p \) in terms of these bosons, and find the Hamiltonian to be:
\[
H = \hbar \sqrt{\frac{\kappa}{2m}} \sum_j 2(b_j^\dagger b_j + b_j b_j^\dagger) - (b_j^\dagger + b_j)(b_{j+1}^\dagger + b_{j+1}).
\] (1.3)

If we now perform a Fourier transformation our Hamiltonian reads:
\[
H = \hbar \sqrt{\frac{\kappa}{2m}} \sum_k \left( A_k b_k^\dagger b_k + \frac{B_k}{2} (b_k^\dagger b_{-k}^\dagger + b_k b_{-k}) + 1 \right),
\] (1.4)

where \( A_k = 2 - \cos(ka) \), \( B_k = -\cos(ka) \) and \( a \) is the lattice separation constant (distance between atoms). Remember that we are trying to diagonalise the problem, but there are still terms that involve a \( b_k \) and a \( b_{-k} \). Furthermore, there are terms that create two bosons, and terms that annihilate two. This is the moment to perform a Bogoliubov transformation. The aim of this is to transform to new, again bosonic, operators \( \beta_k = \cosh(u_k) b_{-k} + \sinh(u_k) b_k^\dagger \) to diagonalise the non-diagonal term in (1.4). Note that \( u_k \) is picked in such a way that the diagonalisation is fulfilled. In principle this is always possible, because it is a system of two equations with two variables. The transformed Hamiltonian reads, after throwing away the integral over a full period of a cosine, which is obviously zero:
\[
H = 2\hbar \sqrt{\frac{\kappa}{m}} \sum_k \sin \left( \frac{ka}{2} \right) (n_k + 1/2).
\] (1.5)

\(^1\)Actually, spontaneous symmetry breaking and long range ordering do not exist in 1 dimension, but because we can easily extend this analysis and results to 3 dimensions, we will perform the easier 1-dimensional calculation here.
At this point a note of caution is necessary: this transformation does not work out whenever
$k \to 0$ because then the hyperbolic functions $\cosh(u_k)$ and $\sinh(u_k)$ in the Bogoliubov trans-
formation blow up (a singular point). This is because $A_k^2 = B_k^2$, and because by definition
$\cosh(2u_k) = \frac{A_k}{A_k^2 - B_k^2}$ and $\sinh(2u_k) = \frac{B_k}{A_k^2 - B_k^2}$ both hyperbolic functions become infinite.

Therefore, we should treat the $k = 0$ point separately and with a bit more care. Be aware
that this point corresponds with the movement of the crystal as a whole: the wavelength of such
a movement is infinitely long and thus $k = 0$. We know that in Fourier space at $k = 0$ our
Hamiltonian reads:

$$H_{k=0} = \hbar \sqrt{\frac{\kappa}{2m}} \left( 1 - \frac{1}{2} \left( b_0^\dagger - b_0 \right) \right)^2,$$

where, if we due to the definitions of the bosons realise that $(b_0^\dagger - b_0)^2 = \frac{-2}{\hbar \sqrt{2m \kappa}} p_0^2$ and that
$N p_{k=0}^2 = p_{tot}^2$, we find

$$H_{k=0} = \frac{p_{tot}^2}{2Nm} + \hbar \sqrt{\frac{\kappa}{2m}},$$

with $p_{tot}$ the collective momentum of the system as a whole. The important part of this Hamilton-
ian is the first term. One can immediately see that if $N$ is large there are a lot of states, differing
in $p_{tot}$, that are very close in energy ($\sim 1/N$). This is the thin spectrum.

One might wonder what the effect of the existence of a thin spectrum is. In fact, it turns out
that in the thermodynamic limit ($N \to \infty$) the contribution to the free energy vanishes [4]. This
also means that, considering thermodynamics, the thin spectrum has no influences whatsoever,
at least not measurable. The implications of the thin spectrum are hidden beneath the surface.

1.2. Spontaneous symmetry breaking in the crystal

The absolute ground state of the $k = 0$ Hamiltonian (the movement of the crystal as a whole)
obviously has a fixed and definite momentum $p_{tot} = 0$. According to Heisenberg’s uncertainty
relationship, the position must have maximum uncertainty then. This means that the crystal
should be at any place in space at the same time in some kind of superposition. Still we observe
crystals at one specific position. How does this happen?

The argument is very subtle. Suppose there is a very small symmetry breaking potential,
which tends to localise the crystal: $B x_{tot}^2$. This is a harmonic oscillator potential for the col-
lective (centre-of-mass) coordinate, where $B$ represents the strength of the force associated with
this potential. Thus, the resulting wave function will be the ground-state of a harmonic oscillator:

$$\psi_0(x_0) = \left( \frac{m \omega N}{\pi \hbar} \right)^{1/4} \exp \left\{ - \frac{m \omega N}{2\hbar} x_{tot}^2 \right\},$$

where $\omega = \sqrt{\frac{B}{mN}}$. If one now takes the limit $B \to 0$, one recovers a completely delocalised
wave function, which confirms the quantum solution and conserves the translational symme-
try. So, without the externality we are still in the quantum regime. However, if one takes the thermodynamic limit $N \to \infty$ before sending $B \to 0$, one finds a totally different result: the wave function becomes a completely localised delta-function at the centre of the potential where $x_{tot} = 0$ [4].

Whenever the results depend on the order of taking a limit, this limit is called singular. As we mentioned in the introduction, this dependence defines spontaneous symmetry breaking. If you kill the symmetry breaking term before taking the thermodynamic limit, of course, one should recover the quantum, fully symmetric state. If one goes to the thermodynamic limit before killing the symmetry breaking term, the crystal will localise. This is why we observe crystals at one position instead of spread out through space.

\subsection*{1.3. Motivation}

This ends our brief introduction into (spontaneous) symmetry breaking. We looked at the case of the crystal and looked at how spontaneous symmetry breaking governs the transition from quantum mechanics to the real word.

In this project we would like to investigate what happens if the symmetry breaking field is time-dependent. For instance, in the case of the harmonic crystal, what would happen if $Bx_{tot}^2$ becomes a time-dependent term?

As we mentioned, we will use the Lieb-Mattis model to find the answer to this question. For now, we will take a step back from symmetry breaking and consider the method we will need to tackle our physical problem later on: the path integral approach to quantum mechanics.
2. The method: path integrals

In this chapter we will introduce the fundamental concepts of the path integral formalism. This formalism is a different, but equivalent, approach to quantum mechanics than the more familiar operator formalism. Feynman developed it during his thesis work [6] and since then many have studied and exploited this powerful mechanism.

In the end, the path-integral formulation is all about adding probabilities: the probabilities of particular paths the particle or system took. Suppose we are interested in the probability of moving a particle from position and time \((x_a, t_a)\) to \((x_b, t_b)\), which is called the amplitude or propagator. The task then is to add all the possible paths, where each path gets assigned a certain weight. This weight, as we will see later, is determined by the action of this path. With the propagator, one can easily calculate the time-evolution of a wave function and therefore, the quantum system is solved.

An important ingredient for the path-integral approach is the quantum-Hamiltonian, which, in general, can be time-dependent. In the past few decades there has been a surge of interest in the quantum theory (finding wave functions, energy levels, etc.) of precisely those time-dependent Hamiltonians [7–11]. Many phenomena in different areas of physics can be modelled by these. As an exotic example, it has recently been shown that the problem of relic (very old, big bang related) gravitons in a cosmological background can be mapped to that of a generalised time-dependent unforced harmonic oscillator [12]. In other words, the applications of time-dependent Hamiltonians extend to all different branches of physics.

The exact quantum theory of generalised time-dependent harmonic oscillators can be solved by all kinds of methods. These include canonical transformations [13], invariant methods [9,11] and, of course, the path integral mechanism, which is a very powerful tool to solve these time-dependent systems. In this thesis we will focus on the latter.

Khandekar and Lawande [7] evaluated the general propagator for a one-dimensional quadratic action. Although their procedure is valid for any kinetic term and perturbative force in the Hamiltonian, the derivation of a complete set of wave functions can be achieved in only a few cases. This is because an exact treatment relies on solving the non-linear differential Pinney’s equation [14]. Thus, only a few number of cases have been solved. More recently, Yeon and collaborators [15] evaluated the general propagator and the wave functions in the case of a bound generalised quadratic Hamiltonian.

For this work a different and easier approach due to Song [16–18] is used. It relies on finding the classical solution of the Hamiltonian, with which an exact solution for the propagator and a set of wave functions can be obtained. In section (2.1) we will start with a rather technical, but necessary derivation of the path integral formula. In section (2.2) we will treat the more specific theory that we need to tackle our physical problem. Section (2.3) deals with finding wave functions with the use of propagators. Section (2.4) will use a way of treating boundary conditions classically, while section (2.5) will use a way of treating boundary conditions quantum
mechanically. Finally, we will draw some conclusions.

2.1. Path integral formalism

For the following derivation of the propagator formula the line of Kleinert’s book on path integrals [19] will be followed. We will work with localised particle states in one dimension, but the path integral approach is equally valid in more dimension or with different states.

The fundamental quantity we would like to calculate with the path integral formalism is the propagator or time evolution amplitude: \( G(q_b, t_b | q_a, t_a) \). This corresponds to the probability that if we would start out at a state \((q_a, t_a)\) we would end up at a state \((q_b, t_b)\). This means we are interested in how states develop through time. The Schrödinger equation exactly fulfils that role in quantum mechanics,

\[
\frac{i}{\hbar} \frac{\partial \Psi(q, t)}{\partial t} = \hat{H}(q, t) \Psi, \tag{2.1}
\]

where \( \hat{H}(q, t) \) is a time-dependent quantum Hamiltonian. When the Hamiltonian does not depend on time one can find the wave functions the way one learns in a first quantum mechanics course [20]: solving the time-independent Schrödinger equation and add factors of \( e^{-iE_{t}/\hbar} \) to include the time development of states. When the Hamiltonian does depend on time, the treatment is different and of course more complicated. We integrate Schrödinger’s equation to find the time-evolution operator:

\[
\hat{U}(t_b, t_a) = \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} dt \hat{H}(t) \right\}, \tag{2.2}
\]

where \( \hat{T} \) is the time-ordering symbol, which makes sure we integrate over each infinitesimal time in the right order. In this expression one recognises the fact that \( \hat{H} \) is the generator of translations through time. The time-evolution operator acts on a state as

\[
\hat{U}(t_b, t_a) |\Psi(t_a)\rangle = |\Psi(t_b)\rangle. \tag{2.3}
\]

So this operator does precisely what we need, namely evolving a state from time \( t_a \) to time \( t_b \). A property of the time-evolution operator that will play an important role is the fundamental composition law, which states that

\[
\hat{U}(t_b, t_a) = \hat{U}(t_b, t_{t'} \hat{U}(t_{t'}, t_a). \tag{2.4}
\]

This means, if we evolve the state from \( t_a \) to \( t' \) and then evolve from \( t' \) to \( t_b \), it is the same as evolving from \( t_a \) to \( t_b \). With this, we are ready to define the propagator. Suppose the states \( |x\rangle \) are localised states of a particle. We can define:

\[
G(q_b, t_b | q_a, t_a) \equiv \langle q_b | \hat{U}(t_b, t_a) | q_a \rangle. \tag{2.5}
\]

So how can we calculate this amplitude? The brilliant idea of Feynman [6] is to make \( N \) slices, each of width \( \epsilon \), between times \( t_a \) and \( t_b \). We now use the fundamental decomposition law to write the propagator as

\[
G(q_b, t_b | q_a, t_a) = \langle q_b | \hat{U}(t_b, t_N) \hat{U}(t_N, t_{N-1}) \ldots \hat{U}(t_2, t_1) \hat{U}(t_1, t_a) | q_a \rangle. \tag{2.6}
\]
We are translating through time step by step. We will implement a well-known trick in quantum physics: inserting complete sets of states

\[ \int_{-\infty}^{\infty} dq_n |q_n\rangle \langle q_n| = 1 \quad (2.7) \]

between each time-evolution operator in equation (2.6). This way, the propagator becomes a product of tiny evolution amplitudes, from each \( t_n \) to \( t_{n+1} \). At this moment we find that, inserting the definition of equation (2.2):

\[ G(q_b t_b | q_a t_a) = \prod_{n=1}^{N} \left[ \int_{-\infty}^{\infty} dq_n \right] \prod_{n+1}^{N} \langle q_n | \exp \left\{ -i\epsilon \hat{H}(t_n) \right\} | q_{n-1} \rangle, \quad (2.8) \]

where we have \( N \) integrals (slices), and because of that, \( N + 1 \) pieces. This is a formula we can evaluate, because we can find an expression for each tiny evolution amplitude. Due to the \( \epsilon \) involved, the reader might have already guessed that some sort of expansion will come into play. Indeed, we will do that by using the Baker-Campbell-Hausdorff formula. It states:

\[ \exp \left\{ -i\epsilon (\hat{T} + \hat{V})/\hbar \right\} = \exp \left\{ -i\epsilon \hat{V}/\hbar \right\} \exp \left\{ -i\epsilon \hat{T}/\hbar \right\} \exp \left\{ -i\epsilon^2 \hat{X}/\hbar^2 \right\}, \quad (2.9) \]

where

\[ \hat{X} \equiv \frac{i}{2} [\hat{V}, \hat{T}] - \frac{1}{6} \left[ \frac{1}{2} [\hat{V}, [\hat{V}, \hat{T}]] - \frac{1}{3} [[\hat{V}, \hat{T}], \hat{T}] \right] + \ldots. \quad (2.10) \]

For a detailed proof of this formula see [19], appendix 2A. The next step is that for high \( N \), \( \epsilon \) gets very small and we can throw away all terms of order \( \epsilon^2 \) or higher. This basically leaves us with a product of two exponents: one for the kinetic part and one for the potential. If we insert this into equation (2.6) we can evaluate each tiny time-evolution amplitude as

\[ \langle q_n | \exp \left\{ -i\epsilon \hat{V}(\hat{q}, t_n) \right\} \exp \left\{ -i\epsilon \hat{T}(\hat{q}, t_n) \right\} | q_{n-1} \rangle. \quad (2.11) \]

To evaluate the effects of each operator explicitly, we insert a complete set of states between the exponents, in this case a set of coordinates \( |q\rangle \):

\[ \int_{-\infty}^{\infty} dq |q_N\rangle \exp \left\{ -i\epsilon \hat{V}(\hat{q}, t_n) \right\} |q\rangle \exp \left\{ -i\epsilon \hat{T}(\hat{q}, t_n) \right\} | q_{n-1} \rangle. \quad (2.12) \]

For now it is important to keep track of the operators and eigenvalues. We can already evaluate the bracket with the potential term in it. Because it is just a function of \( \hat{q} \) we can simply replace each operator \( \hat{q} \) for the coordinate \( q \): an eigenstate of an operator is also an eigenstate of the exponent of an operator. For the kinetic term it is a bit more difficult, because we are not operating on a basis of eigenstates (yet). However, remember that if \( |p_n\rangle \) is an eigenstate of \( \hat{T} \), then it is also an eigenstate of \( e^{-i\epsilon \hat{T}(\hat{q}, t_n)} \). In other words, inserting yet another complete basis set, now in \( |p_n \rangle > \) will help us out:

\[ \langle q | \exp \left\{ -i\epsilon \hat{T}(\hat{q}, t_n) \right\} | q_{n-1} \rangle = \int_{-\infty}^{\infty} dp_n \langle q | \exp \left\{ -i\epsilon \hat{T}(\hat{q}, t_n) \right\} | p_n \rangle \langle p_n | q_{n-1} \rangle. \quad (2.13) \]
Now we are operating on a basis of eigenstates, and we can replace each operator $\hat{p}$ for a the eigenvalue $p$. Then, using the well-known facts

$$\langle q | p \rangle = \frac{1}{2\pi \hbar} \exp \left\{ \frac{i}{\hbar} \hat{p} q \right\} ; \quad \langle q | q' \rangle = \delta(q - q')$$ \hspace{1cm} (2.14)

we can write down each ‘tiny’ time-evolution amplitude as

$$\langle q_n | \exp \left\{ -i\epsilon \hat{H}(\hat{p}, \hat{q}, t_n) \right\} | q_{n-1} \rangle \approx \int_{-\infty}^{\infty} \frac{dp_n}{2\pi \hbar} \exp \left\{ ip_n(q_n - q_{n-1})/\hbar - i\epsilon (T(p_n, t_n) + V(q_n, t_n))/\hbar \right\} ,$$ \hspace{1cm} (2.15)

which leaves us with the full propagator:

$$G(q_b | q_a) \approx \prod_{n=1}^{N} \left[ \int_{-\infty}^{\infty} dq_n \right] \prod_{n=1}^{N+1} \left[ \int_{-\infty}^{\infty} \frac{dp_n}{2\pi \hbar} \right] \exp \left\{ \frac{i}{\hbar} S^N \right\} ,$$ \hspace{1cm} (2.16)

with $S^N$ being the discrete sum

$$S^N = \sum_{n=1}^{N+1} [p_n(q_n - q_{n-1}) - \epsilon H(p_n, q_n)].$$ \hspace{1cm} (2.17)

The final step is to make the continuum limit, by sending $N \to \infty$, and consequently $\epsilon \to 0$. The sum that makes up $S^N$ turns into an integral which exactly resembles the action as we know it from classical mechanics:

$$S[p, q] = \int_{t_a}^{t_b} [p(t)\dot{q}(t) - H(p(t), q(t), t)]dt$$ \hspace{1cm} (2.18)

The finite products over $n$ that make up the propagator turn into infinite products. Furthermore, when we make infinitely small slices, and integrate over each possible coordinate and momentum on each slice, we are actually integrating over all possible paths!

Because for our purposes all Hamiltonians have a kinetic term which reads $\frac{p^2}{2m(t)}$ and a potential term $V(x, t)$, we can perform the Gaussian momentum integration. This integrates the $p(t)\dot{q}(t)$ term and the $\frac{p^2}{2m(t)}$ term of the Hamiltonian of equation (2.18). We end up with:

$$G(q_b | q_a) = \int \mathcal{D}[q(t)] \exp \left\{ \frac{i}{\hbar} S \right\} ; \quad S = \int \mathcal{L} \, dt ,$$ \hspace{1cm} (2.19)

where $\mathcal{L} = \frac{1}{2} m(t) \dot{x}(t)^2 - V(x, t)$ is the Lagrangian of the system. The notation $\mathcal{D}[q(t)]$ represents the fact that we are integrating over all possible paths $q(t)$.

This is the path-integral formula we set out to look for. So what does it physically mean? It means that if we are interested in finding the amplitude for a particle to propagate from coordinates $(q_a t_a)$ to $(q_b t_b)$, we have to sum all possible paths, assigning a weight of $\exp\left\{ \frac{i}{\hbar} S \right\}$ to each path. Although the formula looks beautiful, this still sounds like a horrific task: summing over all paths! Actually, for some cases, it turns out to be computable, even with time-dependent coefficients. A class of solvable Hamiltonians are the quadratic ones. The next section will treat a way in which to face these problems.
2.2. Quadratic Hamiltonians

Suppose now we would like to find the propagator for a very general time-dependent Hamiltonian:

\[ H = \frac{1}{2} [X(t) p^2 + Y(t) (q p + p q) + Z(t) q^2] + F(t) q, \]  

(2.20)

where \( q \) is a canonical position coordinate with \( p \) its conjugate momentum and \( X(t), Y(t), Z(t) \) and \( F(t) \) are continuously differentiable time-dependent functions. As one can see from equations (2.18) and (2.19) the first step is to transform the Hamiltonian into a Lagrangian. For that purpose we need the Legendre transformation

\[ L(q, \dot{q}) = \dot{q} p - H(q, p), \]  

(2.21)

where \( p = \frac{\partial L}{\partial \dot{q}} \). If you perform this transformation you will find a Lagrangian

\[ L = \frac{1}{2} \left[ \dot{q}^2(t) + \frac{2 Y(t)}{X(t)} q(t) \dot{q}(t) - \left( Z(t) - \frac{Y^2(t)}{X(t)} \right) q^2(t) \right] - F(t) q. \]  

(2.22)

The task is now to integrate the action of this Lagrangian over all possible paths. We employ a method, which one also uses when deriving the propagator of a simple time-independent Hamiltonian [19], we split the path in the classical path plus a fluctuation term

\[ q(t) = q_{cl}(t) + \delta q(t). \]  

(2.23)

The classical path is a fixed path - it is determined by the Euler-Lagrange equation of motion, known from classical mechanics:

\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}, \]  

(2.24)

This results in a classical equation of motion, which in our case reads:

\[ \frac{1}{X(t)} \ddot{q}(t) - \frac{\dot{X}(t)}{X^2(t)} \dot{q}(t) + \left[ Z(t) - \frac{Y^2(t)}{X(t)} + \frac{Y(t) \dot{X}(t)}{X^2(t)} - \frac{\dot{Y}(t)}{X(t)} \right] q(t) + F(t) = 0. \]  

(2.25)

This equation is of great importance for this formalism. It is a second order linear differential equation and depending on the constants \( X(t), Y(t) \) and \( Z(t) \), it is solvable. If we cannot solve it exactly, a numerical solution will be enough to find an approximate propagator.

Because we split the path in a fixed classical part and a fluctuation term, the integral we are left with is over the fluctuation terms: they are the only source of fluctuations left.

Let us first have a look at how we can simplify the action. It turns out that we can write the full action as a sum of the classical part and the fluctuation part, which means that the propagator can be written as:

\[ G(q_b, t_b|q_a, t_a) = \int [D \delta q] \exp \left\{ \frac{i}{\hbar} S_{cl} \right\} \exp \left\{ \frac{i}{\hbar} S_{fl} \right\}, \]  

(2.26)

where \( S_{cl} \) and \( S_{fl} \) are the actions of the classical path and the fluctuations, respectively. Note that \( S_{cl} \) is fixed due to the fact that \( x_{cl} \) is fixed. Here, a note of caution must be addressed: the
fluctuation action does not contain the linear term (the force) of the action. For a detailed proof see appendix A.

At this moment we are left with an integral over the fluctuations. This integral results in the fluctuation factor which can only be a function of the times \( t_a \) and \( t_b \), because the fluctuation at the boundaries \( x_a \) and \( x_b \) is zero due to the boundary conditions. Also, the fluctuation coordinates (deviations from the classical path, which are zero at the boundaries) get integrated out, so this is another sign that the fluctuation factor does not depend on \( x_a \) and \( x_b \).

It has been proven that this fluctuation factor can easily be calculated by use of the Pauli-van Vleck formula [21–23]:

\[
F(t_a, t_b) = \left[ -\frac{1}{2i\pi\hbar} \frac{\partial^2 S_{cl}}{\partial q_b \partial q_a} \right]^{\frac{1}{2}},
\]

(2.27)

where \( F(t_a, t_b) \) is the fluctuation factor, such that

\[
\mathcal{G}(q_b, t_b; q_a, t_a) = \left[ -\frac{1}{2i\pi\hbar} \frac{\partial^2 S_{cl}}{\partial q_b \partial q_a} \right]^{\frac{1}{2}} \exp \left( \frac{i}{\hbar} S_{cl} \right).
\]

(2.28)

A detailed proof of the Pauli-van Vleck formula can be found in appendix B. The next step in our analysis is the computation of the classical action. Because we know the classical path obeys equation (2.25) we can try to employ this property into our computations. We will do this by performing an integration by parts. We integrate one of the \( \dot{q} \) terms, and differentiate the other part of the expression. After these operations we find:

\[
S_{cl} = -\int_{t_a}^{t_b} dt \frac{q(t)}{2} \left[ \frac{1}{X(t)} \ddot{q}(t) - \frac{\dot{X}(t)}{X^2(t)} \dot{q}(t) \right] + \left( \frac{Z(t)}{X(t)} - \frac{Y^2(t)}{X^2(t)} + \frac{Y(t)\dot{X}(t)}{X^2(t)} - \frac{\dot{Y}(t)}{X(t)} \right) q(t) + 2F(t) \left. \right|_{t_a}^{t_b} + \frac{1}{2} \frac{q(t)\dot{q}(t)}{X(t)} \bigg|_{t_a}^{t_b} - \frac{1}{2} \frac{Y(t)}{X(t)} q^2(t) \bigg|_{t_a}^{t_b}.
\]

(2.29)

The term in the square brackets of Eq. (2.29) nearly vanishes due to the equation of motion Eq. (2.25), only a term \( -\frac{1}{2} F(t) q_{cl} \) remains and thus we obtain the simple expression for the classical action:

\[
S_{cl} = \frac{1}{2} \left[ \frac{q_{cl}(t_b) \dot{q}_{cl}(t_b)}{X(t_b)} - \frac{q_{cl}(t_a) \dot{q}_{cl}(t_a)}{X(t_a)} \right] - \frac{1}{2} \left[ \frac{Y(t_b) q_{cl}^2(t_b)}{X(t_b)} - \frac{Y(t_a) q_{cl}^2(t_a)}{X(t_a)} \right] - \int_{t_a}^{t_b} dt \frac{q_{cl}(t)}{2} F(t).
\]

(2.30)

It is worth noticing that for \( X(t) = \text{constant} \), \( Z(t) = \text{constant} \), \( Y(t) = 0 \), and \( F(t) = 0 \) we recover the classical action of an ordinary harmonic oscillator [19]. Equations (2.30), (2.25) represent a closed system of equations that determine the propagator for the Hamiltonian Eq. (2.20). We notice that this result can be trivially extended whenever the Hamiltonian contains an extra time-dependent potential \( c(t) \).
Let us take a moment to realise what this all means. We are now armed with a very powerful formula in which the propagator is fully determined by the classical path! Even more, when \( F(t) = 0 \) it is a closed expression. This way, we have reduced the problem dramatically; the only thing we are left to do with is calculating the classical path by solving a second-order linear differential equation.

A second-order linear differential equation always has two independent solutions. One could picture these solutions as basis vectors of a two-dimensional solution space. Suppose one solves this differential equation and finds two linear independent solutions \( \xi_1(t) \) and \( \xi_2(t) \). One can then write the classical path as a linear combination of these 'basis vectors':

\[
q_{cd}(t) = C_1 \xi_1(t) + C_2 \xi_2(t). \tag{2.31}
\]

Inserting the two boundary conditions \( x_{cd}(t_a) = x_a \) and \( x_{cd}(t_b) = x_b \) we fix \( C_1 \) and \( C_2 \) and write the solution as

\[
q_{cd}(t) = \frac{1}{\xi_2^b \xi_1^a - \xi_2^a \xi_1^b} \times \left[ \left( \xi_2^b x_b - \xi_2^a x_a \right) \xi_1(t) + \left( \xi_1^b x_a - \xi_1^a x_b \right) \xi_2(t) \right], \tag{2.32}
\]

where \( \xi_{1,2} = \xi_{1,2}(t_{a,b}) \).

From now on let us suppose that the force \( F(t) = 0 \) such that we have a closed expression for the action and we do not have to worry about integrals. From equation (2.30) one finds that the action factorises as \( S_{cd} = F_a \dot{q}_a^2 + F_b \dot{q}_b^2 + F_{ab} q_a q_b \).\(^1\) We can insert the classical path (2.32), use the closed expression we know for the action (2.30) and find the following prefactors:

\[
F_a = \frac{1}{2 X_a} \left( \frac{\xi_2^b \dot{\xi}_1^a - \xi_2^a \dot{\xi}_1^b}{\xi_1^b \xi_2^a - \xi_2^a \xi_1^b} + \frac{Y_a}{2 X_a} \right),
\]

\[
F_b = \frac{1}{2 X_b} \left( \frac{\xi_2^a \dot{\xi}_1^b - \xi_2^b \dot{\xi}_1^a}{\xi_1^a \xi_2^b - \xi_2^b \xi_1^a} - \frac{Y_b}{2 X_b} \right),
\]

\[
F_{ab} = \frac{1}{2} \left[ \frac{1}{X_a} \left( \frac{\xi_2^a \dot{\xi}_2^a - \xi_2^b \dot{\xi}_2^b}{\xi_1^a \xi_2^b - \xi_2^b \xi_1^a} \right) + \frac{1}{X_b} \left( \frac{\xi_1^b \dot{\xi}_2^b - \xi_1^a \dot{\xi}_2^a}{\xi_1^b \xi_2^a - \xi_2^a \xi_1^b} \right) \right], \tag{2.33}
\]

where \( \xi_{a,b} = \xi_{1,2}(t_{a,b}) \). \( X_{a,b} = X(t_{a,b}) \) and finally \( Y_{a,b} = Y(t_{a,b}) \). For the fluctuation term, on the other hand, by using Eq. (2.27) we easily get \( F(t_a, t_b) = \sqrt{-F_{ab}/(2\pi i\hbar)} \).

We now have all the ingredients to determine the propagator, because when the classical path is known, the propagator is known. This framework is tremendously powerful, because solving a second-order linear differential equation is all that has to be done. Even when you cannot find an exact solution, numerical approaches will help you out: only 2 linear independent solutions need to be found to know an approximate propagator.

\(^1\)By the way, the force would have given us terms linear in \( q_a \) and \( q_b \).
With the propagator, the time-development of the system is easily calculated. You simply insert an initial state at \( t = 0 \) for example, and propagate this to \( t \) to find the state at that time:

\[
\Psi(q, t) = \int G(q | q', 0) \Psi(q', 0) dq'
\]  

(2.34)

In the next section we would like to determine a set of wave functions. Wave functions are useful as they are a basis and span the Hilbert space. This way, we can always project a certain initial state onto a basis and therefore calculate the time-evolution of this initial state. Already at this point it is important to stress the fact that there are infinitely many sets of wave functions, and we have the freedom to pick a set.

In the time-independent case the eigenfunctions of the Hamiltonian constitute a unique set (up to an irrelevant phase). They are rather special functions as these states have a fixed expectation value for the energy through time. The energy levels are the eigenvalues of the different eigenstates of the Hamiltonian. Furthermore, these states do not change through time, except for the phase. For time-dependent Hamiltonians the story is slightly different: the notion of an eigenstate does not exist.

### 2.3. Wave functions

How do we get a set of wave functions out of a propagator? Actually, there exists a nice formula, the spectral decomposition [19]:

\[
G(q_b, t_b | q_a, t_a) = \sum_n \Psi_n^*(q_a, t_a) \Psi_n(q_b, t_b).
\]  

(2.35)

This formula is quite easily proven by taking the usual definition of the propagator and inserting a discrete complete set of states \( \sum_n |\Psi_n\rangle \langle \Psi_n| \). Using this formula we can calculate a basis set of wave functions. It is important to realise that there are infinitely many sets, but using this expression we can calculate one, which is enough for our purposes.

To find a set of wave functions we have to rewrite the propagator in a way similar to equation (2.35). Once the propagator is written in this format, we can read off a set of wave functions. We stay in the notation of the previous section and introduce the following quantities:

\[
\eta(t) = \frac{\dot{\xi}_2(t)\xi_1(t) - \dot{\xi}_1(t)\xi_2(t)}{\xi_1(t)^2 + \xi_2(t)^2},
\]

\[
\delta(t) = \frac{\xi_1(t)\dot{\xi}_2(t) + \xi_2(t)\dot{\xi}_1(t)}{\xi_1(t)^2 + \xi_2(t)^2},
\]

\[
\phi(t) = \arctan \left( \frac{\xi_2(t)}{\xi_1(t)} \right).
\]  

(2.36)

Firstly, it is important to notice an invariant:

\[
\frac{d}{dt} \left[ \frac{1}{X(t)} \left( \dot{\xi}_1(t)\xi_2(t) - \dot{\xi}_2(t)\xi_1(t) \right) \right] = 0.
\]  

(2.37)
This is proven by using that each $\xi$ separately satisfies the equation of motion. Notice that this quantity can be either positive or negative: if you interchange $\xi_1(t)$ with $\xi_2(t)$, $\eta(t)$ will change sign. Although this sign does not matter for the propagator, it matters for a wave function because only a positive sign will result in a square-integrable wave function, as we will see once we have a closed expression for a wave function.

With this invariant we can rewrite the $F_{ab}$ term in the action in equation (2.33). Notice that the two terms between the brackets are both precisely the invariant! So they are the same and we can add them up and write

$$F_{ab} = \frac{1}{\xi_1^a \xi_2^b - \xi_2^a \xi_1^b} \times \left[ \frac{1}{X(t)} \left( \dot{\xi}_1(t) \xi_2(t) - \dot{\xi}_2(t) \xi_1(t) \right) \right] \tag{2.38}$$

If you then realise that the numerators of

$$\sin(\phi_B - \phi_A) = \frac{\xi_2^B \xi_1^A - \xi_2^A \xi_1^B}{\sqrt{\left(\xi_1^A\right)^2 + \left(\xi_2^A\right)^2} \sqrt{\left(\xi_1^B\right)^2 + \left(\xi_2^B\right)^2}},$$

$$\tan(\phi_B - \phi_A) = \frac{\xi_2^B \xi_1^A - \xi_2^A \xi_1^B}{\xi_1^A \xi_2^B - \xi_2^A \xi_1^B}, \tag{2.39}$$

appear in the factors of (2.33) we can rewrite the propagator into the following form:

$$G(q_b, t_b; q_a, t_a) = \left[ \frac{1}{\pi^2 \hbar^2 X_a X_b} \right]^{1/4} \sqrt{\frac{\eta_a \eta_b}{2i \sin (\phi_b - \phi_a)}} \times \exp \left\{ -\frac{\eta_a q_a^2}{2i \hbar X_a} \tan (\phi_b - \phi_a) - \frac{\eta_b q_b^2}{2i \hbar X_b} \tan (\phi_b - \phi_a) \right\} \times \exp \left\{ \frac{1}{\hbar^2 X_a X_b} i \sin (\phi_b - \phi_a) \right\} \times \exp \left\{ -i \left( \frac{\delta \eta q_a^2}{2\hbar X_a} + i \left( \frac{\delta \eta q_b^2}{2\hbar X_b} \right) \right) \right\} \times \exp \left\{ \frac{i}{2\hbar} \left( \frac{Y_a}{X_a} - \frac{Y_b}{X_b} \right) \right\}. \tag{2.40}$$

This is a very convenient way of writing the propagator, because we can now apply Mehler’s formula [24]. This can be used to express the propagator in terms of the sum of a product of $n$-th order Hermite polynomials $H_n(q)$:

$$\exp \left\{ -\frac{x^2}{2} - \frac{x'^2}{2} \right\} \sum_{n=0}^{\infty} \frac{1}{2^n n!} H_n(x) H_n(x') a^n = \frac{1}{\sqrt{1 - a^2}} \exp \left\{ \frac{(a^2 + 1)(x^2 + x'^2)}{2(a^2 - 1)} + \frac{2xx'}{1 - a^2} \right\} \tag{2.41}$$

Using this formula, we write the propagator exactly in the format demanded by the spectral decomposition (2.35). The propagator is in the format of the right hand side, and the wave
function in the format of the left hand side of Mehler’s formula. To find the right factors $x$, $x'$ and $a$ in Mehler’s formula to match the propagator we have to fulfil:

$$\frac{2xx'a}{1-a^2} = \frac{i}{\hbar} F_{ab},$$

(2.42)

because this mixed term in $x$ and $x'$ cannot be factorised as a product of $\Psi_n^*\Psi_n$ later on. If we get the wrong $F_a$ and $F_b$ that would not matter because we can easily add exponential factors on both sides of equation (2.41). Furthermore, anticipating on Eq. (2.35) we pick $x$ and $x'$ to be the same functions.

With these constraints we find the correct factors in Mehler’s formula. Because we have rewritten $F_{ab}$ we can now put a square root of the term between the brackets in (2.38) in both $x$ and $x'$ (it is an invariant anyway) and find:

$$G(q_b, t_b; q_a, t_a) = \exp\left\{-\frac{\eta_a q_a^2}{2\hbar X_a} - \frac{\eta_b q_b^2}{2\hbar X_b}\right\} \times$$

$$\exp\left\{-i \left[\frac{(\delta_a - Y_a)}{2\hbar X_a} q_a^2 - \frac{(\delta_b - Y_b)}{2\hbar X_b} q_b^2\right]\right\} \times$$

$$\frac{\eta_a \eta_b}{\pi^2 \hbar^2 X_a X_b} \sum_{n=0}^{\infty} \frac{e^{-i(n+1/2)(\phi_b-\phi_a)}}{2^n n!} \times$$

$$H_n\left(\sqrt{\frac{\eta_a}{\hbar X_a}} q_a\right) H_n\left(\sqrt{\frac{\eta_b}{\hbar X_b}} q_b\right).$$

(2.43)

We use the formula of the spectral decomposition now by closely observing how a set of wave functions must look like in order to match (2.43). From equations (2.43), (2.35) we derive a time-dependent set of wave functions:

$$\Psi_n(q, t) = \sqrt{\frac{1}{2^n n!}} \left[\frac{\eta(t)}{X(t)\pi \hbar}\right]^{1/4} e^{-i(n+1/2)\phi(t)} \times$$

$$H_n\left(\sqrt{\frac{\eta(t)}{\hbar X(t)}} q\right) \exp\left\{-\frac{\eta(t)}{2\hbar X(t)} q^2\right\} \times$$

$$\exp\left\{i \left[\frac{\delta(t)X(t) - Y(t)}{2\hbar X(t)^2} - \frac{Y(t)}{2\hbar X(t)}\right] q^2\right\}. \quad (2.44)$$

Notice that we transformed to a general continuous position $q$ and time $t$. We simply found $\Psi_n^*(q_a, t_a)$ and $\Psi_n(q_b, t_b)$ and associated this with a set of wave functions $\Psi_n(q, t)$.

Therefore, Eqs. (2.25), (2.36), (2.44) represent a closed system of equations that exactly solves the quantum theory of a time-dependent harmonic oscillator! But wait a minute, there is still some freedom to pick the $\xi_1$ and $\xi_2$ any way you like. They can be any combination of independent solutions of Eq. (2.25). This does not effect the propagator, but it changes the set of wave functions. This is weird, one might suspect they would be unique, as if they were a set of eigenstates of the Hamiltonian. So what does this mean?
The first question that might rise is whether these wave functions are correct then in the first place. Applying Schrödinger’s equation to the general formula of the wave function (2.44) results in two equations:

\[
\begin{align*}
Z(t) + \frac{1}{X(t)} (\delta(t)^2 - \eta(t)^2) &= \frac{\dot{Y}(t)X(t) - \dot{X}(t)Y(t)}{X(t)^2} - \frac{d}{dt} \left( \frac{\delta(t)}{X(t)} \right), \\
-\frac{\dot{X}(t)}{X(t)} + \frac{\dot{\eta}(t)}{\eta(t)} + 2\delta(t) &= 0,
\end{align*}
\]

where the first one arises from equating the real parts on both sides of Schrödinger’s equation, and the second one from the imaginary parts. Inserting our definitions of \(\eta(t)\) and \(\delta(t)\) and using the fact that \(\xi_1(t)\) and \(\xi_2(t)\) satisfy Eq. (2.25) it is verified that these equations always hold, independent of the particular linear combination. In other words, all wave functions are correct, as long as \(\xi_1(t)\) and \(\xi_2(t)\) satisfy the equation of motion. It is important to realise then that each set represents a complete, orthogonal basis of the Hilbert space.

This means we have found infinitely many wave functions! In the case of a time-dependent Hamiltonian this is not weird at all. There is no such thing as a unique set of eigenstates as we know it from time-independent quantum mechanics. We just found infinitely many states and we found the exact way in which they evolve through time\(^2\).

Something that does matter is the sign of \(\eta(t)\): this should be positive in order to retain normalisability. A wave function must be normalisable, otherwise it is not possible to satisfy the statistical interpretation of it. [20]

Does this result reduce to statics in the static case then? Because we know that with a time-independent Hamiltonian, we must have a unique basis set (again, up to a phase). In this case, the extension of Eq. (2.35) to

\[
G(q_b, t_b; q_a, t_a) = \sum_n \phi_n^*(q_a)\phi_n(q_b)e^{-iE_n(t_b-t_a)/\hbar}
\]

fixes the eigenfunctions uniquely. By restoring time translation symmetry the energy becomes conserved again and is not a function of time anymore. Picking the right \(\xi_1(t)\) and \(\xi_2(t)\) is easy: because \(\frac{\eta(t)}{X(t)}\) must become a constant, and because of the invariant numerator, the denominator \(\xi_1(t)^2 + \xi_2(t)^2\) should be constant. Also the extra position dependent phase factors must vanish, which is another constraint.

This ends our discussion and derivation of a set of wave functions. We found a general procedure with which to find sets of wave functions of time-dependent quadratic Hamiltonians.

Before we move on to the boundary conditions, an interesting question to ask ourselves now is: how do the energy levels of a particular basis set evolve in time? The energy levels of a specific basis can be found by computing the expectation values of the time-dependent Hamiltonian Eq. (2.20) in the basis we chose: \(\langle \Psi_n | H | \Psi_n \rangle\). After a straightforward calculation, which can be

\(^2\)Demanding another constraint could fix the wave functions uniquely. One could for example demand that at certain time \(t_0\) the wave functions coincide with a certain basis, for example the basis of a static Hamiltonian.
found in detail in appendix C, we get:

\[ E_n(t) = h \Omega(t) \left[ n + \frac{1}{2} \right], \quad (2.47) \]

where we introduced the time-dependent frequency:

\[ \Omega(t) = \frac{\eta(t)}{2} + \frac{Z(t)X(t) - Y^2(t)}{2\eta(t)} + \frac{\delta(t)^2}{2\eta} \]

In the case \( X(t) = 1/M = \text{const} \) and \( Z(t) = Z = \text{const} \) and \( Y(t) = 0 \) we recover the ordinary energy levels of an ordinary harmonic oscillator.

To conclude, we have derived the propagator, a set of wave functions and the energy levels of this particular set of wave functions for a generalised time-dependent harmonic oscillator with the path integral method. We find that, independently of the parameter choice, the associated energy spectrum always consists of discrete energy levels. With this basis set of wave functions, one can always project an initial state onto this basis set to find the time evolution of this initial state.

Sometimes the Hamiltonian is not the full story. A physical system can have a boundary condition. The next section will deal with implementing boundary conditions in a system in a classical way.

**2.4. Boundary conditions in the classical way**

We now know how to calculate a set of wave functions. It all relies on finding the classical path that is spanned by two solutions \( \xi_1 \) and \( \xi_2 \). In our physical problem, as will appear in the next chapter, it turns out that we can map the spin-variable \( S \) to a position coordinate \( q \) and some associated momentum \( p \). However, the value of this total spin \( S \) cannot be negative, in other words we need to implement a boundary condition in our problem, namely that \( q_\text{cl} > 0 \). Negative values of our observable are not allowed so we must find some way to avoid them.

It turns out that you can treat this boundary condition in a classical and in a quantum way. We will treat the problem classically in this section and section (2.5) deals with the quantum way.

In this section we treat the classical boundary condition in three different cases of time-dependent Lagrangians. We will compute the classical path for each of them, because the classical path is all we need for the propagator and a set of wave functions. The time-dependent Lagrangians are all of the form:

\[ \mathcal{L} = \frac{1}{2} \left( \frac{1}{X(t)} \dot{q}^2 - Z q^2 \right) - c(t), \quad (2.48) \]

where \( c(t) \) is actually an irrelevant time-dependent shift of the energy-reference level. We will drop it for now, because it does not effect our analysis and we can insert it later on. The time-dependent variable \( X(t) \) will be related to the symmetry breaking magnetic field later on, which can have any shape actually. Finally \( Z \) will be a constant, not related to the symmetry breaking field but to some other system parameters which are not important at this moment.
We will treat three cases in this section. We will kick off with a static field, after that treat an exponentially growing field, and finally consider a linear field.

For this classical approach we also assumed that at certain initial time $t_0$, our spin-variable $q = 0$. With this assumption we are also anticipating on the physical context, in which we start in a singlet $S = 0$ state.

2.4.1. Static field

First of all, we would like to see if we can calculate the classical path for the most simple case: a static field. The Euler-Lagrange equation of motion reduces to

$$\frac{1}{X} \ddot{q}(t) + Zq(t) = 0, \quad (2.49)$$

which has two solutions $\xi_1(t) = \cos\left(\sqrt{XZ}t\right)$ and $\xi_2(t) = \sin\left(\sqrt{XZ}t\right)$. If we insert the initial condition $q(0) = 0$, we pick up the sine:

$$y(t) = C \sin\left(\frac{t}{\tau}\right); \quad \tau = \sqrt{\frac{1}{XZ}}, \quad (2.50)$$

where we inserted a characteristic time $\tau$. We wrote our preliminary solution as $y(t)$ and not as $q(t)$, because this is not the correct solution yet. This is because already in this case, the problem of a negative $y(t)$ arises. We know that we are restrained to solutions where $q > 0$. We can fix this by multiplying $y(t)$ with some other function to make it positive on the whole domain. Suppose that for $t_1, t_2, ..., t_n$, $y(t_i) = 0$. For each time interval $t_i < t < t_{i+1}$ there exists a unique solution:

$$y(t) \equiv \sin\left(\frac{t}{\tau}\right); \quad q(t) = C(t)y(t) \geq 0, \quad (2.51)$$

where $C(t)$ is some kind of step function, which is alternatingly positive and negative in order to make $q(t)$ positive on the whole domain.

The question arises what this function looks like, because it can be any alternating function of constants; the values of the constants are undetermined. There is some physics that helps us out if we realise the goal of this section: we would like to compute the classical path. We know that for this case the action must be at a minimum (that is how the Euler-Lagrange equation is derived in the first place). If we simply calculate the action (and minimise it), from initial time $t_i = 0$ to final time $t = t_f$ using $q(t) = C(t)y(t)$, this might help us out in finding the correct $C(t)$. We start with:

$$S = \int_{t_f}^{t_f} \frac{1}{2X} \dot{q}(t)^2 - \frac{Z}{2} q(t)^2 dt,$$

$$= \int_{t_i}^{t_f} \frac{1}{2X} \left(\dot{C}(t)y(t) + C(t)\dot{y}(t)\right)^2 - \frac{Z}{2} (C(t)y(t))^2 dt, \quad (2.52)$$
where we mention again that the path-independent constant $c(t)$ is left out, because there is no physics in this term. If we decompose the squared term in the brackets we end up with:

$$ S = \int_0^{t_f} \frac{1}{2X} C(t)^2 y(t)^2 - \frac{Z}{2} C(t)^2 y(t)^2 + \frac{1}{X} C(t) \dot{C}(t) y(t) \dot{y}(t) + \frac{1}{2X} \dot{C}(t)^2 y(t)^2 dt. \quad (2.53) $$

The integral of the first two terms in equation (2.53), which we will call $S_{1+2}$ from now on, can be easily evaluated. Noticing that $C(t)$ is a step function, it is a constant $C_i$ on every domain $t_i < t < t_{i+1}$. Inserting our solution for $y(t) = \sin \left( \frac{t}{\tau} \right)$ on each domain we get:

$$ S_{1+2} = \int_{t_i}^{t_{i+1}} \frac{1}{2\tau^2 X} C_i^2 \cos \left( \frac{t}{\tau} \right)^2 - \frac{Z}{2} C_i^2 \sin \left( \frac{t}{\tau} \right)^2 dt, $$

$$ = \int_{t_i}^{t_{i+1}} \frac{Z}{2} C_i^2 \cos \left( \frac{t}{\tau} \right)^2 - \frac{Z}{2} C_i^2 \sin \left( \frac{t}{\tau} \right)^2 dt = 0, \quad (2.54) $$

which is independent of $C_i$. But if we realise that not all contributions between $t_0$ and $t_f$ are exactly between nodes, a non-zero contribution will arise from the last node $t_n$ to $t_f$:

$$ \int_{t_n}^{t_f} \frac{Z}{2} C_n^2 \cos \left( \frac{2t}{\tau} \right) \neq 0. \quad (2.55) $$

The third and fourth term in equation (2.53), which we will call $S_3$ and $S_4$ respectively, require a more careful approach.

We will focus on the contribution around one zero at $t_1$. We can extend this contribution to any number of zeroes later on. We will use a limiting procedure to describe $C(t)$ and its derivative $\dot{C}(t)$. Ideally one would like to use a step-function but this will give rise to derivatives of delta’s that will give infinities in our calculation later on. If we approximate the step function by a hyperbolic tangent, $C(t)$ and $\dot{C}(t)$ will be of the following shape:

$$ C(t) = \lim_{\lambda \to 0} \frac{C_0 + C_1}{2} + \frac{C_1 - C_0}{2} \tanh \left( \frac{t - t_1}{\lambda} \right), $$

$$ \dot{C}(t) = \lim_{\lambda \to 0} \frac{C_1 - C_0}{2\lambda} \text{sech} \left( \frac{t - t_1}{\lambda} \right)^2 \quad (2.56) $$

Upon taking the limit $\lambda \to 0$, the function $C(t)$ will reduce to a step function, and its derivative $\dot{C}(t)$ to a delta function, which is the correct behaviour. If we insert the expressions (2.56) in our third term in equation (2.53) we get:

$$ S_3 = \int_{-t_1/\lambda}^{0} \frac{\lambda}{\tau X} \left( \frac{C_0 + C_1}{2} + \frac{C_1 - C_0}{2} \tanh \left( \frac{\tilde{t}}{\lambda} \right) \right) \frac{C_1 - C_0}{2\lambda} \text{sech} \left( \frac{\tilde{t}}{\lambda} \right)^2 \sin \left( \frac{\lambda \tilde{t} + t_1}{\tau} \right) \cos \left( \frac{\lambda \tilde{t} + t_1}{\tau} \right) d\tilde{t}, \quad (2.57) $$

where we transformed to $\tilde{t} = \frac{t - t_1}{\lambda}$. We perform a Taylor expansion in $\lambda$ around the node $t_1$. We get, omitting all terms of order $\lambda^2$ or higher:

$$ S_3 = \int_{-t_1/\lambda}^{0} \frac{1}{\tau X} \left( \frac{C_0 + C_1}{2} + \frac{C_1 - C_0}{2} \tanh (\infty) \right) \frac{C_1 - C_0}{2} \text{sech}(\infty)^2 \sin \left( \frac{t_1}{\tau} \right) \cos \left( \frac{t_1}{\tau} \right) d\tilde{t}. \quad (2.58) $$
This term vanishes because \( \sin \left( \frac{t_1}{\tau} \right) = 0 \) and all other terms are finite. The argument why the terms of order \( \lambda \) or higher vanish is a bit more subtle. These higher order terms are all proportional to \( \lambda \tilde{t} = t - t_1 \) and they vanish when we are close enough or exactly at \( t_1 \). This is because far from the node, by definition, \( S_3 \) is zero because \( \dot{C}(t) \) vanishes there. If we send \( \lambda \to 0 \), only infinitely close to \( t_1 \), does \( \dot{C}(t) \) not vanish. And we already knew that infinitely close to \( t = t_1 \) all terms of order 1 or higher in \( \lambda \tilde{t} \) vanish. Therefore all higher order terms in \( \lambda \) vanish.

Let us finally look at the fourth term of (2.53). We already know that away from the node \( t_1 \) the term vanishes, for the same reason \( S_3 \) vanished. Taking each step with caution we find:

\[
S_4 = \int_0^{t_f} \frac{1}{2X} y(t)^2 \dot{C}(t)^2 dt,
\]

\[
= \int_0^0 \lim_{\lambda \to 0} \frac{\lambda}{2X} \sin \left( \frac{\lambda \tilde{t} + t_1}{\tau} \right) \left( \frac{C_1 - C_0}{2\lambda} \right) \left( \frac{t_1}{\tau} \right)^2 \sech^4(\tilde{t}) d\tilde{t},
\]

\[
= \int_0^0 \lim_{\lambda \to 0} \frac{(C_1 - C_0)^2}{8\lambda X} \sin \left( \frac{\lambda \tilde{t} + t_1}{\tau} \right) \left( \frac{t_1}{\tau} \right)^2 \sech^4(\tilde{t}) d\tilde{t}. 
\]  

(2.60)

Again we changed the time scale and integration variable to \( \tilde{t} \). This allows us to expand the sine for small \( \lambda \) around the zero of the sine, \( \tilde{t} = 0 \):

\[
S_4 = \int_0^0 \lim_{\lambda \to 0} \frac{(C_1 - C_0)^2}{8\lambda X} \left( \sin \left( \frac{t_1}{\tau} \right) + \lambda \tilde{t} \cos \left( \frac{t_1}{\tau} \right) \right)^2 \sech^4(\tilde{t}) d\tilde{t}
\]  

(2.60)

And once more \( \sin \left( \frac{t_1}{\tau} \right) = 0 \), but the cosine does not vanish. This means we end up with a term first order in \( \lambda \tilde{t} \), which vanishes when \( t \) is close enough to \( t_1 \), which corresponds with the \( \lambda \to 0 \) limit:

\[
S_4 = \lim_{\lambda \to 0} \int_0^0 \frac{(C_1 - C_0)^2}{8\lambda X} \left( \lambda \tilde{t}^2 \cos^2 \left( \frac{t_1}{\tau} \right) \right) \sech^4(\tilde{t}) d\tilde{t} = 0
\]

This procedure did not depend on the specifics of a certain node so we can easily generalise this result to all nodes. So we will find zero action, no matter what the values of \( C_i \) and \( C_{i+1} \) are. If we collect all the terms we find that the action vanishes between the nodes, and that a finite contribution arises from \( S_{1+2} \) between the last node and final time \( t_f \), which is only dependent on the last constant \( C_n \) and some other system parameters. This means that, except for \( C_n \), we can pick each \( C_i \) to be any value: the classical action is degenerate in these constants. We can not determine the constants uniquely at this point so the precise classical path remains unknown as well. We will come back to this point later, as it turns out that with an easy classical analog this all explainable. This ends our discussion of the static field, we move on to consider less trivial cases.

### 2.4.2. Exponential field

We will now investigate an exponentially growing field:

\[
X(t) = X_0 e^{t/\xi}
\]  

(2.61)
We treat the same Lagrangian as before, with this different $X(t)$ inserted. In this case, we will start our classical path at initial time $t = -\infty$, where it again must vanish, so $q(-\infty) = 0$. Solving the Euler-Lagrange equation of motion exactly yields a linear combination of Bessel $J$ and $Y$ functions:

$$q(t) = C_1 e^{\frac{t}{\tau}} J_1 \left( \frac{2\sqrt{Z e^{\frac{t}{\tau}} \xi}}{\sqrt{X_0}} \right) + C_2 e^{\frac{t}{\tau}} Y_1 \left( \frac{2\sqrt{Z e^{\frac{t}{\tau}} \xi}}{\sqrt{X_0}} \right)$$

The Bessel $J$ function goes to zero when $t \to -\infty$, but the Bessel $Y$ function approaches a constant non-zero value. Upon introducing a characteristic time $\sqrt{\frac{1}{X_0Z}} = \tau$, one can normalise the other times to units of characteristic time $t' = t / \tau$ and $\xi' = \xi / \tau$. We find that Bessel $Y$ converges to:

$$\lim_{t \to -\infty} C_2 e^{\frac{t'}{\tau}} Y_1 \left( \frac{2e^{\frac{t'}{\tau}} \xi'}{\sqrt{X_0}} \right) = -\frac{C_2}{\pi} \xi'$$

In order to fulfil the initial boundary condition $q(-\infty) = 0$ we pick $C_2 = 0$. This means we end up with the solution:

$$y(t', \xi') = C e^{\frac{t'}{\tau}} J_1 \left( \frac{2e^{\frac{t'}{\tau}} \xi'}{\sqrt{X_0}} \right)$$

We already discussed that solutions with $q < 0$ are nonphysical. The Bessel function will drop below zero at a certain time, so again, just like the static case, the solution is not correct on the whole domain. We follow the same procedure as we did in the static case. Suppose that for $t_1, t_2, \ldots, t_n, y(t_i) = 0$. For every time interval $t_i < t < t_{i+1}$ there exists a unique solution:

$$y(t', \xi') = e^{\frac{t'}{\tau}} J_1 \left( \frac{2e^{\frac{t'}{\tau}} \xi'}{\sqrt{X_0}} \right) ; \quad q(t', \xi') = C(t')y(t', \xi').$$

Again the constants are alternatingly positive and negative: $C_0 > 0, C_1 < 0$, etc. Again, we are looking for the minimum of the action, because this results in the classical path. So we have to integrate our Lagrangian:

$$S = \int_{-\infty}^{+\infty} \frac{1}{2X(t)} \dot{q}(t)^2 - \frac{Z}{2} q(t)^2 dt,$$

Upon inserting our expression for $q$ our final equation for the action reads:

$$S = \int_{-\infty}^{+\infty} \frac{1}{2X(t)} C(t)^2 y(t)^2 - \frac{Z}{2} C(t)^2 y(t)^2 + \frac{1}{X(t)} C(t) \dot{y}(t) y(t) + \frac{1}{2X(t)} \dot{C}(t)^2 dt$$

Again we start by looking at the first two terms of equation (2.67): $S_{1+2}$. We follow the same procedure as in the static case: we perform the integral on the first two terms at each time interval.
\( t_i < t < t_{i+1} \) in between the nodes. This integral turns out to be zero at each interval. This means that, concerning only these terms, our solution is again degenerate in the constants \( C_i \). One can pick any constant and still find the same result. This is illustrated in figure (2.1) where you can see that \( S_{1+2} \) is exactly zero at each node. In order to evaluate the third (\( S_3 \)) and fourth (\( S_4 \)) term in (2.67), we use an approximation and a limiting procedure to our step function and its derivative again:

\[
C(t) = \lim_{\lambda \to 0} \frac{C_0 + C_1}{2} + \frac{C_1 - C_0}{2} \tanh \left( \frac{t - t_1}{\lambda} \right),
\]

\[
\dot{C}(t) = \lim_{\lambda \to 0} \frac{C_1 - C_0}{2\lambda} \sech \left( \frac{t - t_1}{\lambda} \right)^2.
\]

(2.68)

The procedure must sound familiar. We treat the problem as if there is only one zero, at \( t_1 \), and evaluate our integral considering only this zero. We can extend this solution to any number of zeroes. Consider \( S_3 \) first, leaving out some steps as it is quite similar to the static case:

\[
S_3 = \int_{-\infty}^{\infty} \lim_{\lambda \to 0} \frac{1}{X_0} e^{-t'} \left( \frac{C_0 + C_1}{2} + \frac{C_1 - C_0}{2} \tanh \left( \frac{t' - t_1'}{\lambda} \right) \right) \frac{C_1 - C_0}{2\lambda} \sech \left( \frac{t' - t_1'}{\lambda} \right)^2 y(t) \dot{y}(t) \, dt.
\]

(2.69)

Where all times are written with accents, due to the transformation \( \frac{t}{\tau} = t' \). If we now substitute
\[
\tau^{t'-t_1} = \tilde{t} \text{ we get:}
\]
\[
S_3 = \int_{-\infty}^{\infty} \lim_{\lambda \to 0} \frac{1}{\tau X_0} \left( e^{-\frac{i\lambda}{\tau} e^{-\frac{t_1}{\tau}}} \right) \left( \frac{C_0 + C_1}{2} + \frac{C_1 - C_0}{2} \tanh (\tilde{t}) \right) \left( \frac{C_1 - C_0}{2} \sech (\tilde{t})^2 \right) y(\tilde{t}) \dot{y}(\tilde{t}) d\tilde{t}.
\]

(2.70)

If we now write \( y(\tilde{t}) \) and \( \dot{y}(\tilde{t}) \) as a function of \( \lambda \) as well, and omit all terms of order \( \lambda \) or higher we get:
\[
S_3 = \int_{-\infty}^{\infty} \lim_{\lambda \to 0} \frac{1}{\tau X_0} (\ldots) (\ldots) (\ldots) J_1(2\xi' e^{2\pi i}) (\ldots) \tilde{d}t,
\]

(2.71)

where the terms between brackets have been omitted, except for the \( y(\tilde{t}) = J_1(2\xi' e^{2\pi i}) \) term.

The omitted terms are all finite but \( J_1(2\xi' e^{2\pi i}) = 0 \), which kills the whole expression.

The reason why the full \( S_3 \) is zero is the same as in the previous section: away from the node \( t_1 \) the expression is zero due to the fact that \( \dot{C}(t) \) is obviously zero there and infinitesimally close (because \( \lambda \to 0 \)) to the node \( \lambda \tilde{t} \) is zero.

We now take a look at the fourth term in (2.67): \( S_4 \). If we again insert the correct expression for the derivative of the step-function and make the change in the time variable we get:
\[
S_4 = \int_{-\infty}^{\infty} \lim_{\lambda \to 0} \frac{1}{2\tau X_0} J_1 \left( 2\xi' e^{2\pi i} e^{\frac{i\lambda}{\tau}} \right) \left( \frac{C_1 - C_0}{4\lambda} \right) \sech^4(\tilde{t}) d\tilde{t}
\]

(2.72)

Because \( \lambda \) is small, we expand \( J_1 \) around \( \tilde{t} = 0 \) (where the Bessel function vanishes) in \( \lambda \tilde{t} \):
\[
= \int_{-\infty}^{\infty} \lim_{\lambda \to 0} \frac{1}{2\tau X_0} \left( J_1(0) + \lambda \tilde{t} \left( \frac{\tilde{t}}{\tau} e^{\frac{i\lambda}{2\tau}} e^{\frac{i\lambda}{2\tau}} \right) + \lambda^2 \tilde{t}^2 (\ldots) + \ldots \right) \left( \frac{C_1 - C_0}{4\lambda} \right) \sech^4(\tilde{t}) d\tilde{t}
\]

We can immediately conclude that the \( O(\lambda \tilde{t}) \) and higher order terms vanish when \( \lambda \to 0 \). The \( O((\lambda \tilde{t})^0) \) is zero (because \( \tilde{t} = 0 \)). So again all terms vanish.

This ends our discussion of the exponential field. Also in this case, we only get a contribution from \( t_n \) to \( t_f \) due to \( S_{1+2} \) in (2.67). Just like the static field case, the solution is degenerate in the constants \( C_i \), apart from the last constant \( C_n \).

2.4.3. Linear field

The last case we treat is that of a linear field:
\[
X(t) = X_0 t.
\]

The discussion of this case will be somewhat brief, because of the two preceding cases and the similar method we used. We start by finding a general solution \( y(t) \). Inserting the initial
conditions \( y(0) = 0 \) and zero imaginary part (the general solution is a linear combination of derivatives of Airy functions with complex arguments):

\[
y(t) = (1 + \alpha i) \left[ A_i'(z) + \frac{1}{\sqrt{3}} B_i'(z) \right]
\]

with \( z = \frac{(-1)^{\frac{1}{3}} t}{\xi + \frac{5}{3}} \) and \( \alpha \approx 1.73 \). We multiply this general solution with the usual step function \( C(t) \) to ensure \( q > 0 \) on the whole domain. We return to the familiar action:

\[
S = \int_0^t \frac{1}{2X(t)} C(t)^2 \dot{y}(t)^2 - \frac{Z}{2} C(t)^2 y(t)^2 + \frac{1}{X(t)} C(t) \dot{C}(t) y(t) \dot{y}(t) + \frac{1}{2X(t)} \dot{C}(t)^2 dt.
\]

Again, we have four terms in our action, which we will split up in the first two \( S_{1+2} \) (without delta-like derivatives in \( \dot{C}(t) \)) and the third \( (S_3) \) and fourth \( (S_4) \). We focus on the integration between the nodes \( t_i < t < t_{i+1} \), and then extend this solution to any number of nodes.

As we did in the exponential case, in figure (2.2) it is shown that the integral of the first two terms goes to zero between each node, which only gives us a contribution from the last node \( t_n \) to \( t_f \). Again, we introduce the following approach to a step function:

![Figure 2.2.: Behaviour of the first two terms of the action \( S_{1+2} \) and \( y(t) \). The action vanishes at each node where \( y(t) = 0 \).](image-url)
\[
C(t) = \lim_{\lambda \to 0} \frac{C_0 + C_1}{2} + \frac{C_1 - C_0}{2} \tanh \left( \frac{t - t_1}{\lambda} \right)
\]
\[
\dot{C}(t) = \lim_{\lambda \to 0} \frac{C_1 - C_0}{2\lambda} \text{sech} \left( \frac{t - t_1}{\lambda} \right)^2
\]

We will substitute \( \tilde{t} = \frac{t - t_1}{\lambda} \), expand in \( \lambda \tilde{t} \) around \( \tilde{t} = 0 \). Omitting some steps we find that:

\[
S_3 \sim \int_{-\infty}^{\infty} \text{sech}^2(\tilde{t}) \left[ A_i' \left( \frac{(-1)^{1/3}}{\xi^3 \tau^3} (t_1 + \lambda \tilde{t}) \right) + B_i' \left( \frac{(-1)^{1/3}}{\xi^3 \tau^3} (t_1 + \lambda \tilde{t}) \right) \right] \times
\left[ A_i \left( \frac{(-1)^{1/3}}{\xi^3 \tau^3} (t_1 + \lambda \tilde{t}) \right) + B_i \left( \frac{(-1)^{1/3}}{\xi^3 \tau^3} (t_1 + \lambda \tilde{t}) \right) \right].
\]

Taking the limit \( \lambda \to 0 \), numerically this converges to zero (see figure (2.3)). Analytically we can explain this as well, because near a node

\[
A_i' \left( t_1 + \lambda \tilde{t} \right) \left( \frac{(-1)^{1/3}}{\xi^3 \tau^3} \right) \sim A_i'[t_1] + \lambda \tilde{t} \partial A_i'(\tilde{t}).
\]

This integral is proportional to \( \lambda \tilde{t} \) and approaches zero if \( t \) is close enough to \( t_1 \). Again, this is the case for the \( \lambda \to 0 \) limit.

Finally, consider \( S_4 \). After the same procedure we find:

\[
S_4 \sim \int_{-\infty}^{\infty} \frac{1}{t_1 + \lambda \tilde{t}} \frac{\text{sech}^4(\tilde{t})}{\lambda} \left( A_i' \left( \frac{(-1)^{1/3}}{\xi^3 \tau^3} (t_1 + \lambda \tilde{t}) \right) + \frac{B_i'}{\sqrt{3}} \left( \frac{(-1)^{1/3}}{\xi^3 \tau^3} (t_1 + \lambda \tilde{t}) \right) \right)^2 dt.
\]
Again, numerically we find this to be zero (see figure (2.4)). One can also anticipate this result, because the whole function $A_i' + B_i' \sim \lambda^2 t^2$ which implies that the integral vanishes as we take the limit $\lambda \to 0$.

So also the linear case shows the same behaviour. The classical path cannot be determined uniquely because the values of the constants cannot be determined.

2.4.4. Conclusion and physical analog

We found that for any field the classical path is degenerate in the constants $C_i$. If we try to solve our system in this way one needs more information to uniquely determine the path and the constants. How is that possible?

Well, we did not specify what precisely happens at the boundary. Remember that our system is a harmonic oscillator, but with a boundary condition. One could picture an oscillating mass on a spring just above the table, where the table is located at the equilibrium position of the mass-spring system. Every oscillation the spring hits the table - the boundary condition - and something happens, but what? There could be an elastic or inelastic collision, but this is not determined in this model. Suppose we would know what happens at a ‘bounce’, we could relate $C_i$ to $C_{i+1}$ for example.

It turns out that conservation of energy is the extra physics we need. Because we have infinitely hard boundaries, a bounce is infinitely short and therefore the incoming energy (before the bounce) should equal the outgoing energy (after the bounce). This principle would translate in the fact that the $C_i$’s are alternatingly positive and negative, but have the same absolute value as the $C_i$’s are directly related to the energy.

One might wonder why the action principle did not suffice here. Well, this principle still holds between all nodes, but it breaks down at the boundary: all physics is determined by the characteristics of the boundary at this point, and the action principle will not help us out.
It turns out that we can actually forget about the boundary condition when calculating the propagator and a set of wave functions, and that we can easily insert it later on. This is possible through a pure quantum-mechanical treatment in the next section.

2.5. Boundary conditions in the quantum way: the Kleinert argument

In the previous section we tried to derive the classical path when a boundary condition was already implemented. This was a purely classical approach. In this section we will take another route: we will calculate the classical path and the propagator as if there was no constraint and we implement the boundary condition later on. We follow an approach due to Kleinert [19], although in our case we include more general terms in our Lagrangian. It follows that we can use the same method and machinery as the textbook [19] as long as the potential is symmetric in $x$: $V(x) = V(-x)$.

The following derivation is quite technical, but essential. The first step of this derivation is demanding that $q > 0$. This means that the completeness relation of the position states is modified to:

$$\int_{0}^{\infty} |q\rangle \langle q| \, dq = 1,$$

(2.76)

where the integration is only over half-space, obviously. Another property that the localised states $|q\rangle$ have is that

$$\langle q| q' \rangle = \delta(q - q').$$

(2.77)

With these definitions, we can now calculate the propagator. We simply start with the usual definition that

$$\langle q_b t_b | q_a t_a \rangle = \langle q_b | \hat{U}(t_b, t_a) | q_a \rangle.$$

(2.78)

We follow the same procedure as in section (2.1) and insert $N$ completeness relations to obtain

$$\langle q_b t_b | q_a t_a \rangle = \prod_{n=1}^{N} \int_{0}^{\infty} dq_n \prod_{n=1}^{N+1} \langle q_n | q_{n-1} t_{n-1} \rangle. \quad (2.79)$$

Here of course $q_{N+1} = q_b$ and $q_0 = q_a$. The next step is using the definition of the time-evolution operator.

$$\langle q_b t_b | q_a t_a \rangle = \prod_{n=1}^{N} \int_{0}^{\infty} dq_n \prod_{n=1}^{N+1} \langle q_n | \exp \left\{ \frac{i}{\hbar} \hat{H} \right\} | q_{n-1} \rangle$$

(2.80)

We first take $\hat{H} = 0$. Afterwards we can easily extend it to a Hamiltonian containing a kinetic and a potential term, where the potential must be symmetric. We thus have:

$$\langle q_b t_b | q_a t_a \rangle = \prod_{n=1}^{N} \int_{0}^{\infty} dq_n \prod_{n=1}^{N+1} \langle q_n | q_{n-1} \rangle. \quad (2.81)$$

We have already defined the inner product $\langle q_n | q_{n-1} \rangle = \delta(q_n - q_{n+1})$ but we can extend this definition. We insert the spectral decomposition of this product (we insert a complete set of
wave-like states $|k\rangle$ in between $\langle q|q'\rangle$. Using the fact that because of the half-space the wave function must vanish at $q = 0$, we get:

$$
\langle q|q'\rangle = \frac{2}{\pi} \int_{-\infty}^{\infty} dk \sin kq \sin kq' = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left( e^{ik(q-q')} - e^{ik(q+q')} \right) = \delta(q-q') - \delta(q+q'). \quad (2.82)
$$

The sines appear due to the boundary condition: they vanish at $q = 0$. One sees that another delta function appears. This is the crucial point: the spectral decomposition has an unphysical reflected point at $q = -q'$. We can retain this point and write the inner product as:

$$
\langle q|q'\rangle = \sum_{x=\pm q} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} p(x-q) + i\pi(\sigma(x) - \sigma(q')) \right\}, \quad (2.83)
$$

where $\sigma(x) \equiv \Theta(-x)$, which is defined as

$$
\Theta(x) = \begin{cases} 
1 & x > 0, \\
1/2 & x = 0, \\
0 & x < 0,
\end{cases}
$$

the Heaviside function. So when $x$ and $q'$ have opposite sign we acquire a minus sign, which is precisely what we want. Let us introduce a set of localised states $|x\rangle$ and $|x'\rangle$ which do exist on full space. It is trivial that

$$
\langle x|x'\rangle = \langle q|q'\rangle, \quad (2.84)
$$

whenever $x = q$ and $x' = q'$. With this little trick we come back to the propagator (2.81) and write this in terms of the states $|x\rangle$:

$$
\langle x|x'\rangle = \sum_{x''=\pm x} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp \left\{ \frac{i}{\hbar} p(x''-x') + i\pi(\sigma(x'') - \sigma(x')) \right\},
$$

$$
= \delta(x-x') - \delta(x+x'), \quad (2.85)
$$

where the sum is included because the variables $x$ also take the negative values of $q$. We can now extend the trivial transition amplitude with zero Hamiltonian with the reflected unphysical delta-function:

$$
(q_b t_b q_a t_a) = \delta(q_b - q_a) - \delta(q_b + q_a), \quad (2.86)
$$

and again make many time slices (inserting that $x$ is a sum over $\pm q$, because it is also allowed to be negative):

$$
(q_b t_b q_a t_a) = \prod_{n=1}^{N} \left[ \int_{0}^{\infty} dq_n \right] \prod_{n=1}^{N+1} \left( \sum_{x_n=\pm q_n} (x_n \epsilon|x_{n-1} 0\rangle) \right), \quad (2.87)
$$

33
where of course $q_b = q_{N+1}$ and $q_a = q_0$. If we realise that the amplitude with zero Hamiltonian (depicted by the subscript $0$) is just the inner product and insert (2.85) for that product we get:

$$
(q_b | q_a)_0 = \prod_{n=1}^{N} \left[ \int_{0}^{\infty} dq_n \right] \prod_{n=1}^{N+1} \left( \sum_{x_n=\pm q_n}^{\infty} \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right) \times \exp \left\{ \sum_{n=1}^{N+1} \left[ \frac{i\hbar}{p} (x_n - x_{n-1}) + i\pi (\sigma(x_n) - \sigma(x_{n-1})) \right] \right\}. \tag{2.88}
$$

If we now realise that the sum over $\pm q_n$ (apart from the end points) and the integral $\int_{0}^{\infty} dq_n$ can be combined to the integral $\int_{-\infty}^{\infty} dx_n$ we get:

$$
(q_b | q_a)_0 = \sum_{x_n=\pm q_n}^{\infty} \prod_{n=1}^{N} \left[ \int_{-\infty}^{\infty} dx_n \right] \prod_{n=1}^{N+1} \left( \sum_{x_n=\pm q_n}^{\infty} \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right) \times \exp \left\{ \sum_{n=1}^{N+1} \left[ \frac{i\hbar}{p} (x_n - x_{n-1}) + i\pi (\sigma(x_n) - \sigma(x_{n-1})) \right] \right\}. \tag{2.89}
$$

The path integral now looks really similar to the 'conventional' one, except for the sum $\sum_{x_n=\pm q_n}$ and the extra part in the action. This part is what we will call the 'topological action', because in it, the 'information' on the topology, in this case half-space, is stored:

$$
A^\sigma_{\text{topol}}[x] = \hbar \pi (\sigma(x_b) - \sigma(x_a)). \tag{2.90}
$$

Figure (2.5) shows how the sum together with the topological action takes care of the paths that are not allowed: they get cancelled by a path of equal action which crosses the boundary and ends up at $-x_b$.

The next question is what happens when $\dot{H} = T(p) + V(q) \neq 0$. In this case we have

$$
\langle q_n | \exp \left\{ -\frac{i\hbar}{\epsilon} \hat{H}(p, q) \right\} | q_{n-1} \rangle \tag{2.91}
$$

We can precisely follow all the steps of the derivation of the case when $\dot{H} = 0$ but now we have to be careful when we extend the integral from $\int_{0}^{\infty}$ to $\int_{-\infty}^{\infty}$. This is only possible when $V(q) = V(-q)$. So this trick only holds whenever the Lagrangian is fully quadratic.
We can simply calculate the propagator as if there is no boundary condition, only with a slight modification due to the topological action:

\[
(q_b t_b | q_a t_a)_{\text{with b.c.}} = (q_b t_b | q_a t_a)_{\text{no b.c.}} - (-q_b t_b | q_a t_a)_{\text{no b.c.}},
\]

(2.92)

where the propagator with or without the boundary condition \( q > 0 \) is denoted with the subscript 'with b.c.' and 'no b.c.' respectively.

Within this treatment, in fact we assumed infinitely hard boundaries. This corresponds to energy conservation because the boundaries do not absorb any energy. This way, we are able to connect the quantum treatment with the classical one. By working through the classical case explicitly, we learnt that the boundary behaviour is not so obvious and in fact we found out that energy conservation answers the degeneracy problem.

This ends our discussion of the boundary condition and in the end it means that we can forget about the boundary condition at first and calculate the propagator without the boundary condition. We can insert it later on by using (2.92). This is the easiest approach.

It is instructive to see how this boundary condition works out when calculating wave functions. Let us go back to the spectral decomposition:

\[
G(q_b t_b | q_a t_a) = \sum_n \Psi_n^*(q_a, t_a) \Psi_n(q_b, t_b).
\]

(2.93)

Suppose now that we insert the boundary condition \( q > 0 \) our propagator reads:

\[
G(q_b t_b | q_a t_a) = \sum_n \{ \Psi_n^*(q_a, t_a) \Psi_n(q_b, t_b) - \Psi_n^*(q_a, t_a) \Psi_n(-q_b, t_b) \}.
\]

(2.94)

It is immediately clear that if \( \Psi_n(q_b, t_b) = \Psi_n(-q_b, t_b) \), the propagator becomes zero, which is unphysical. In other words if \( \Psi_n \) is even, the propagator vanishes. \textit{Thus the only allowed wave functions are odd!} This confirms what is known and used before [2] by picking the odd wave functions that vanish at the origin.

### 2.6. Conclusion

We are now armed with a very powerful method. As long as we can determine the classical path by finding two solutions to the classical equation of motion, we are able to calculate the propagator and the wave functions. We can also insert the boundary condition of our spin variable \( S > 0 \), by demanding that all wave functions are odd.

We got the best we could dream of: an exact treatment, as long as the classical path is known. In the next chapter we will employ this machinery to the physical system of the Lieb-Mattis model for an antiferromagnet.
3. Theoretical study of time-dependent symmetry breaking of the Lieb-Mattis model

In this chapter we will investigate the Lieb-Mattis model. This is an infinite-range model for an antiferromagnet where all the spins on a sublattice interact with all the other spins on the other sublattice. The Lieb-Mattis model is very useful because it effectively contains the thin spectrum for the more physical Heisenberg model (with nearest neighbour interactions).

We will start this chapter by explicitly showing in section (3.1) how the Lieb-Mattis Hamiltonian can be derived from the Heisenberg Hamiltonian. After the derivation of this model, we will break the SU(2) spin rotation symmetry of the Lieb-Mattis model in section (3.2) by introducing a staggered magnetic field along the $z$-direction. Although the symmetry was broken by a time-independent field in the literature [2, 26], we will break the symmetry with a time-dependent field.

The symmetry-broken Lieb-Mattis Hamiltonian, which is discrete at first, can be mapped onto a harmonic oscillator Hamiltonian by means of a continuum approximation. We are interested in the time-evolution of a certain initial state of the system. In order to calculate this time-development, we have to find a basis for the symmetry-broken time-dependent Hamiltonian. In section (3.3) we will calculate a basis set of wave functions, compute the evolution of an initial state through time, and compare this result to the statical situation.

3.1. Derivation of the Lieb-Mattis Hamiltonian

The starting point of this section is the Heisenberg Hamiltonian, from which we will derive the Lieb-Mattis Hamiltonian. For more details, see [2] as we will follow their approach. We will consider an antiferromagnet with sublattices $A$ and $B$. Each sublattice contains quantum spins $S$ of size $\sigma$, which have isotropic nearest neighbour interactions of strength $J$. The Hamiltonian reads:

$$H = J \sum_{i,\delta} S_i S_{i+\delta},$$

where $i$ labels the spins on the A sublattice and $\delta$ connects them with its nearest neighbours on the B sublattice. Notice that $J$ is positive in this case, which is essential for the antiferromagnetic behaviour of the system. To analyse the energy spectrum of this Hamiltonian, and in particular its lowest order excitations, one applies linear spin wave (LSW) theory [30]. In this theory one finds, by use of the introduction of bosons, wave-like excitations (spin-waves) in the magnet. These are commonly referred to as magnons. Furthermore, we will discover the existence of a thin spectrum.
Within LSW theory one approximates\(^1\) the spin operators with a linear combination of Holstein-Primakoff bosons \(a\) and \(b\):

\[
S^z_{i \in A} \rightarrow \sigma - a_i^\dagger a_i, \quad S^z_{i \in B} \rightarrow \sigma - b_i^\dagger b_i, \\
S^+_{i \in A} \rightarrow \sqrt{2\sigma} a_i, \quad S^+_{i \in B} \rightarrow \sqrt{2\sigma} b_i^\dagger, \\
S^-_{i \in A} \rightarrow \sqrt{2\sigma} a_i^\dagger, \quad S^-_{i \in B} \rightarrow \sqrt{2\sigma} b_i.
\]

(3.2)

We can insert these relations in the Heisenberg Hamiltonian and then perform a Fourier transform, such that the Hamiltonian to quadratic order in the boson operators reads:

\[
H^{LSW} = \frac{1}{2} J N z \sigma^2 + \sum_k \left( (a_k^\dagger a_k + b_k^\dagger b_k) + \gamma_k (a_k^\dagger b_{-k}^\dagger + a_{-k} b_k) \right),
\]

(3.3)

where \(N\) is the total number of lattice sites, \(z\) is the coordination number of the lattice (the number of nearest neighbours), and \(\gamma_k = \frac{1}{z} \sum_\delta e^{ik\delta}\).

In order to diagonalise the last two terms in \(H^{LSW}\), one uses a Bogoliubov transformation, which we already encountered in the first chapter. However, this transformation is singular at the points where \(e^{ik\delta} = \pm 1\), because then \(\gamma_k^2 \rightarrow 1\).\(^2\) Keeping this in mind, while returning to the notation in terms of spins (instead of the LSW-bosons), the full Hamiltonian in Fourier space reads:

\[
H = J \sum_k \gamma_k S_k \cdot S_{-k}.
\]

(3.4)

The Fourier transform of the spin operator at the singular points is:

\[
S_{k=0} = \frac{1}{\sqrt{2N}} (S_A + S_B),
\]

(3.5)

\[
S_{k=\pi} = \frac{1}{\sqrt{2N}} (S_A - S_B),
\]

(3.6)

where \(S_A\) and \(S_B\) are the total spins of each sublattice. We find that the Heisenberg Hamiltonian (3.4) at these singular points is:

\[
H_{\text{singular}} = \frac{2J}{N} S_A \cdot S_B = \frac{J}{N} (S^2 - S_A^2 - S_B^2),
\]

(3.7)

where \(S = S_A + S_B\). This part of the Heisenberg Hamiltonian turns out to correspond with the Lieb-Mattis Hamiltonian \([26–28]\), which we will denote by \(H_{\text{sym LM}}\).\(^3\) The energy of the Lieb-Mattis Hamiltonian is easily calculated to be

\[
E = \frac{J}{N} \left[ S(S+1) - S_A(S_A+1) - S_B(S_B+1) \right],
\]

(3.8)

---

1Valid for large \(\sigma\).

2The hyperbolic functions blow up for the same reason as they did in the example of the harmonic crystal: \(A_k = \pm B_k\). For details I refer to the text beneath equation (1.5).

3The subscript \(\text{sym}\) is added to distinguish from the asymmetric Hamiltonians, which we will encounter in the next sections, where the symmetry is broken.
and the corresponding eigenfunctions of the Hamiltonian can be expressed in terms of its quantum numbers as $|S_A, S_B, S, M⟩$, where $M$ is the $z$-component of the total spin.

If we observe this energy spectrum, we can conclude that the ground state is a state where $S$ is minimal and $S_A$ and $S_B$ are both maximal. Therefore, the groundstate is a singlet of total spin: $|\frac{N\sigma}{2}, \frac{N\sigma}{2}, 0, 0⟩$. Notice that the minimal value of $S$ is 0, because it cannot be negative. Therefore, $S \geq 0$ is an important constraint throughout the problem.

From now on, we will assume that $S_A$ and $S_B$ are always maximised. If we then, with this assumption, consider the lowest order energy excitations with respect to the ground state singlet, we will find that there are states that differ in $S$ and are separated by energies of order $\frac{J}{N}$. When $N$ is large, the separation is very small and vanishes in the thermodynamic limit where $N \to \infty$. This energy spectrum has the same characteristics as the zero-momentum part of the harmonic crystal and indeed the set of these extremely low energy states with different $S$ is the thin spectrum. Because the Lieb-Mattis Hamiltonian coincides with the singular part of the Heisenberg Hamiltonian (3.7), it displays the effective behaviour of the thin spectrum of the Heisenberg model. This is the only part of the Heisenberg Hamiltonians that is relevant for the symmetry breaking of the antiferromagnet.

3.2. Breaking the symmetry dynamically

In this section we will break the symmetry of the Lieb-Mattis Hamiltonian (3.7) by introducing a time-dependent staggered magnetic field along the $z$-direction. After adding the magnetic field we find the symmetry-broken Lieb-Mattis Hamiltonian to be:

$$H_{LM} = \frac{J}{N}(S^2 - S_A^2 - S_B^2) - B(t)(S_A^z - S_B^z), \quad (3.9)$$

where $S_A^z$ and $S_B^z$ represent the $z$-components of the spin of both sublattices. One observes that the magnetic field couples to both of the sublattice spins with a different sign, which is a result of the staggered field. The symmetry-breaking term does not commute with the Hamiltonian and therefore mixes states with different total spin.

We set out to find the eigenfunctions $|n⟩$ of the symmetry-broken Hamiltonian. They can be expressed in the symmetric $|S⟩$ basis as $\sum_S u^n_S |S⟩$. It turns out that we can map the Hamiltonian onto a harmonic oscillator Hamiltonian, which allows us to find these specific eigenfunctions. If we suppose that $0 \ll S \ll N$ we can use the continuum limit and we express the symmetry-breaking term of $H_{LM}$ as a second derivative to $S$. We will skip the precise derivation here, but the interested reader might want to see [2] for details.

---

4The quantum number corresponding to the operator $S_z$.

5Excitations by lowering $S_A$ or $S_B$ actually correspond to the magnons of the Lieb-Mattis Hamiltonian.

6We will drop the superscript $\text{sym}$ now, for obvious reasons.

7Approximating that $S$ is a continuous variable, instead of a discrete.

8In Ref. [2] a static magnetic field, with $B(t) = \text{const.}$ is used, but this can easily be generalised to time-dependent magnetic fields.
The result of the continuum limit\(^9\) is that the Hamiltonian can be expressed as:

\[
H = \frac{1}{2} \left( -B(t)N\sigma \frac{\partial^2}{\partial S^2} + \frac{2J}{N} S^2 \right) + c(t).
\]  

(3.10)

where \(c(t) = E_{sym}^{LM} - B(t)N\sigma\). This Hamiltonian is a time-dependent harmonic oscillator Hamiltonian. Please notice that, except for the extra term \(c(t)\), it fits in the general formula 2.20, where \(X(t) = \frac{B(t)N\sigma}{\hbar^2}\), \(p = \frac{\hbar}{i} \frac{\partial}{\partial S}\), \(Y(t) = 0\), and \(Z(t) = \frac{2J}{N}\).

In Ref. [2], where the symmetry-breaking field is time-independent (\(B(t) = B\)), the wave functions and energy levels corresponding to the Hamiltonian are computed. The \(u_s^n\) we encountered before, which are the coefficients of the projection of the eigenstate on the \(|S\rangle\)-basis, can be expressed as harmonic oscillator eigenfunctions with a frequency \(\omega = \frac{1}{N}\sqrt{\frac{2J}{\sigma B}}\). The separation of the energy levels can be expressed in a typical energy scale \(E_{thin} = \sqrt{2\sigma J B}\) such that the energy levels read:

\[
E_0^n = E_{sym}^{LM} - B N\sigma + \left( n + \frac{1}{2} \right) E_{thin}.
\]  

(3.11)

It is important to realise the consequences of the boundary condition \(S \geq 0\) at this moment. Remember from chapter (2) that such a boundary condition results in the fact that only the odd wave functions are allowed (so \(n = 1, 3, \text{etc.}\)).

Furthermore, one can prove that the spin rotation symmetry SU(2) is broken spontaneously by an infinitesimally small symmetry-breaking field \(B\) [2,29]. The way one proceeds is to calculate the order parameter, which in the antiferromagnet is represented by the staggered magnetisation

\[
\langle S^z_A - S^z_B \rangle.
\]  

(3.12)

In Ref. [2, 29] it is shown, that the ordering of the limits \(N \to \infty\) and \(B \to 0\) matters for the outcome of this order parameter. This non-commuting limit proves that the spin rotational symmetry is spontaneously broken.

We will now return to our study of the time-dependent symmetry-breaking. From now on we will drop the \(c(t)\) term. All it does is adding a time-dependent 'reference' value to the energy levels\(^10\), which can easily be taken into account later on. It does not effect any of our upcoming analysis.

In the time-dependent case we cannot simply insert \(B(t)\) in these parameters, we have to use the path integral approach. However, it will prove to be useful to define a set of parameters that represent the value of \(\omega\) and \(E_{thin}\) at initial time \(t_{in}\) (when we switch on the time-dependent symmetry-breaking field) and final time \(t_f\) (when we switch off the time-dependent symmetry-breaking field).

\(^9\)Actually, requiring that \(S_A\) and \(S_B\) are maximal is also essential in this derivation but we already made this assumption in the first section.

\(^10\)In the same way as it does in the static case.
If we then denote the time-dependent symmetry breaking field at $t_{in}$ by $B_{in}$, and at $t_f$ by $B_f$, we can define this set of parameters as follows:

$$E_{in}^{th} = \sqrt{2\sigma J B_{in}}; \quad E_{in}^{f} = \sqrt{2\sigma J B_{f}}$$

$$\omega_{in} = \frac{1}{N} \sqrt{\frac{2J}{\sigma B_{in}}}; \quad \omega_f = \frac{1}{N} \sqrt{\frac{2J}{\sigma B_{f}}}$$

(3.13)

It is useful to refer to dimensionless physical quantities. A first simplification is to make the Hamiltonian dimensionless by dividing through an energy scale $E_{in}^{f}$, therefore measuring all energies in units of $E_{in}^{f}$ from now on:

$$\frac{H}{E_{in}^{f}} \equiv \mathcal{H} = \frac{1}{2} \left( -\frac{B(t)}{B_{f}} \frac{1}{\omega_f} \frac{\partial^2}{\partial S^2} + \omega_f S^2 \right).$$

(3.14)

From this expression one can see that if we define $S = \sqrt{\omega_f} S$, therefore measuring the spin in units of $\frac{1}{\sqrt{\omega_f}}$, the expression simplifies to:

$$\mathcal{H} = \frac{1}{2} \left( -\frac{B(t)}{B_{f}} \frac{\partial^2}{\partial S^2} + S^2 \right).$$

(3.15)

At this point we cannot simplify it any further, without specifying $B(t)$.

### 3.3. Theoretical study of a linear symmetry-breaking field

Ideally, we would like to find out what would happen with the exact singlet state, the ground state of the symmetric ($B = 0$) Lieb-Mattis Hamiltonian, when the symmetry gets broken in a particular time-dependent way. We would like to find an answer to the question: what happens if the system starts in a singlet state ($S = 0$), and at some initial time $t_{in}$ the field starts to increase?

It turns out that starting from an exact singlet is impossible within our treatment. Remember that we assumed that $S \gg 0$, which allowed us to write the Hamiltonian as a harmonic oscillator. However, at $S = 0$ this assumption cannot be made, as we are neglecting an important term linear in $S$. Furthermore, it turns out that we cannot propagate the state away from the singlet: when we start at $S = 0$, we stay at $S = 0$. This is due to the boundary condition $S \geq 0$.

Therefore, we choose our initial state ($t < t_{in}$) to be very close to a singlet. It is the ground state of the time-independent symmetry-broken Hamiltonian with a small initial static field $B_{in}$.

We project the initial state onto a basis in the regime where $B(t)$ is time-dependent ($t \geq t_{in}$), and find the time-evolution of the state. To calculate the basis of the dynamical regime, we will use the developed path integral formalism.

We know what the evolution of the state looks like after the projection onto the dynamical basis. It is simply a superposition of dynamical basis states, where the projection determines the coefficient (weight) of each basis state. This leads to the first result we are interested in: the time-evolution of the state, which we will call $\Psi(S, t)$ from now on.
We can compare this *dynamical* state (due to the dynamical field) with the *instantaneous* state that we would have found if we would have forgotten about dynamics and would have considered the field to be static at every moment in time with the system in its ground state. This way we learn something about the difference the dynamics make.

With this dynamical state, we can calculate other parameters we are interested in. We calculate the energy of our dynamical solution, and compare this to the instantaneous solution. We will define a density of defects, which is related to the difference between the correct dynamical result and the instantaneous result. The defects are differences between the symmetry-broken dynamical ground state we find and the one we would have expected in an instantaneous approach. We can summarise the behaviour of the defect density in different regimes by introducing a phase diagram. Finally, we will generalise the obtained results for different shapes of the symmetry breaking field.

### 3.3.1. Shape of the symmetry-breaking field and the equations of motion

The first step is to specify the shape of the symmetry breaking field, which is illustrated in figure (3.1).

![Figure 3.1: The behaviour of $B(t)$. For $t < t_{in}$, the field is static and very small, in order to represent a singlet initial state. At $t_{in}$ we switch the field on linearly, until we reach a value of $B_f$ at the final time $t_f$. $B_f$ can be expressed in terms of a characteristic time $\tau$.](image)

We already mentioned that for $t < t_{in}$ the field is $B_{in}$. For $t \geq t_{in}$ the field increases linearly.
so the field $B(t)$ can be written as:

$$B(t) = \begin{cases} 
B_f \frac{t_{in}}{t_f} & t < t_{in}, \\
B_f & t_{in} \leq t \leq t_f, \\
B_f \frac{t}{t_f} & t > t_f,
\end{cases}$$

where we used the fact that $B_f t_{in} = B_{in} t_f$ to rewrite $B_{in}$ in terms of the other parameters. Furthermore, we introduce a time:

$$\tau \equiv \frac{\hbar}{E_{thin}^f},$$

(3.16)

which is the typical time associated to the thin spectrum of the time-independent symmetry-broken Lieb-Mattis model when $B = B_f$.

With this shape of the symmetry-breaking field, we can simplify (3.15) to:

$$\mathcal{H} = \begin{cases} 
\frac{1}{2} \left( -\frac{t_{in}}{t_f} \frac{\partial^2}{\partial t^2} + S^2 \right) & t < t_{in}, \\
\frac{1}{2} \left( -\frac{t}{t_f} \frac{\partial^2}{\partial t^2} + S^2 \right) & t_{in} \leq t \leq t_f, \\
\frac{1}{2} \left( -\frac{\partial^2}{\partial S^2} + S^2 \right) & t > t_f.
\end{cases}$$

Notice that the Hamiltonian fully describes the system and that it is governed by two time parameters: $t_{in}$, the time at which the symmetry breaking field $B(t)$ is switched on and $t_f$, the time after which $B(t)$ stays constant.

The Hamiltonian for $t < t_{in}$ is time-independent and we take the ground state of it to be our initial state $\Psi(t_{in})$. At this point it is important to remember from section (3.2) that $S$ is constrained to be positive. In chapter (2) we saw that such a constraint for time-dependent Hamiltonians results in the fact that only odd (basis) wave functions are allowed. Therefore, the ground state of the Hamiltonian for $t < t_{in}$ is not an even $n = 0$ state but an odd $n = 1$ state, and thus reads:

$$\Psi(S, t_{in}) = \left( \frac{t_f}{\pi^2 t_{in}} \right)^{1/8} \exp \left\{ -\sqrt{\frac{t_f}{t_{in}}} S^2 / 2 \right\} H_1 \left( \left( \frac{t_f}{t_{in}} \right)^{1/4} S \right),$$

(3.17)

where $H_1$ is the first Hermite polynomial, and where we chose the phase in such a way that $\Psi(S, t_{in})$ is real. This is our initial state, illustrated in figure (3.3.1). In this figure also the final static state at $B_f$ is shown. Note that in the limit $t_{in} \to 0$, the initial state becomes infinitesimally close to a singlet.

We project the initial state onto the basis of wave functions for $t \geq t_{in}$ to study the time-evolution of this state. Therefore, our goal for the next section is to find a basis of wave functions for the Hamiltonian when $t_{in} \leq t \leq t_f$. Remember from chapter 2 that this comes down to solving the classical equation of motion. After a short derivation, which can be found in detail in appendix D, the classical equation of motion reads:

$$\frac{t_f}{t} \frac{\partial^2 S(t)}{\partial t^2} - \frac{t_f}{t^2} \frac{\partial S(t)}{\partial t} + \frac{1}{\tau^2} S = 0.$$
Figure 3.2.: The initial state of $\Psi(S,t_{in})$ at $t_{in}/t_f = 10^{-4}$ (blue curve) and the final instantaneous state $t_{in}/t_f = 1$ (red curve). Further decreasing of $t_{in}/t_f$ for the blue curve would result in a state that resembles a singlet even more.

We now make a final variable change, by measuring each time in units of $\tau$ (e.g. $t = t/\tau$), and find the dimensionless equation of motion:

$$\frac{t_f}{\tau} \frac{\partial^2 S(t)}{\partial t^2} - \frac{t_f}{\tau^2} \frac{\partial S(t)}{\partial \tau} + S = 0.$$  \hfill (3.19)

Our problem has now been reduced to two time parameters: $t_{in}$ and $t_f$. But if we pause for a moment, we remember that we had three parameters that determined our symmetry-breaking field (and therefore our system): the time at which we start increasing the field $t_{in}$, the time at which we stop increasing the field $t_f$, and the amount by which we increase the field $B_f - B_{in}$. So where is $B_{in}$?\footnote{One might wonder what happened to $B_{in}$, but it is determined by $B_f$, $t_{in}$, and $t_f$, so this variable is not hidden.}

This parameter is in fact hidden inside the $\tau$’s. Remember that $\tau = t/\tau$ and that $\tau$ is a function of $B_f$. Furthermore, this parameter is hidden inside $S$ as well, because $S = \sqrt{\omega_f}S$, and $\omega_f$ also contains a $B_f$. At this point we reduced the problem to the easiest formulation, with as few parameters as possible.

### 3.3.2. The dynamical basis

Now that we found a dimensionless equation of motion, the first step in obtaining a basis set of wave functions for $t_{in} \leq t \leq t_f$, is solving this equation of motion. Remember that it does not matter which solutions of the equation of motion we use for the calculation of a basis set of
wave functions, as long as the solutions are independent and span the solution space. It turns out that it is convenient to write the solutions, with the use of Ref. [32], in terms of real Bessel functions of the same order:

\[
\xi_1(t) = t J_{-2/3} \left( \frac{2}{3} \frac{t^{3/2}}{\sqrt{t_f}} \right), \\
\xi_2(t) = t Y_{-2/3} \left( \frac{2}{3} \frac{t^{3/2}}{\sqrt{t_f}} \right).
\]  

(3.20)

Before we move on, we stress the importance of the asymptotic expansion of general Bessel functions:

\[
J_\alpha(x) \approx \sqrt{\frac{2}{\pi x}} \cos \left( x - \frac{\alpha \pi}{2} - \frac{\pi}{4} \right), \\
Y_\alpha(x) \approx \sqrt{\frac{2}{\pi x}} \sin \left( x - \frac{\alpha \pi}{2} - \frac{\pi}{4} \right),
\]  

(3.21)

for arguments \( x \gg |\alpha^2 - \frac{1}{4}| \). We will use this asymptotic expansion quite frequently, as it allows us to simplify expressions for large \( t \). In our case we can use the expansion when \( t \gg t_c \), where

\[ t_c = t_f^{1/3}. \]  

(3.22)

We can now calculate the functions \( \eta(t) \), \( \delta(t) \) and \( \phi_d(t) \), as defined in chapter 2. It is simply a matter of inserting \( \xi_1 \) and \( \xi_2 \) into their definitions. We will omit the extensive exact expressions here.

With these parameters, a dynamical basis set of wave functions is known. So the work of chapter 2 paid out: we only needed to solve the classical equation of motion!

If one takes a look at the general formula for a basis set of wave functions (2.44), one immediately sees that our dynamical basis wave functions can be written in terms of a dynamical frequency \( \omega_d \):

\[
\omega_d(t) = \frac{t_f}{t} \eta(t),
\]  

(3.23)

a dynamical phase:

\[
\Delta_d(t) = \frac{t_f}{t} \delta(t),
\]  

(3.24)

and \( \phi_d(t) \). We will discuss the behaviour of these parameters later on, when we introduced similar instantaneous functions.

As we announced before, we could have also forgotten about dynamics and just use the static eigenfunctions of the harmonic oscillator Hamiltonian, inserting the time-dependence instantaneously at each point in time. This way, the state knows nothing about the past and it reacts to the external field as if it is static.

---

12In that case the functions \( \eta(t) \) and \( \delta(t) \), as defined in chapter 2, do not oscillate. If we would have picked a different set of solutions, in general these quantities will oscillate.

13We insert an extra subscript \( d \) here in order to avoid confusions later on.
Remember that we defined an $\omega$ in section (3.2), in which the eigenfunctions of the time-independent symmetry-broken Lieb-Mattis Hamiltonian could be expressed. We naively insert the time-dependence now, and find that the instantaneous frequency $\omega_i(t)$ reads: \begin{equation} \omega_i(t) = \sqrt{\frac{t}{\tau_f}}. \tag{3.25} \end{equation}

In a similar way, the instantaneous phase factor can be found:

$$\phi_i(t) = t\sqrt{\frac{t}{\tau_f}}. \tag{3.26}$$

As we do not have a $\delta$-term in the instantaneous case, we define:

$$\Delta_i(t) \equiv 0. \tag{3.27}$$

The static eigenfunctions and the dynamic basis are very similar. It is useful to define the harmonic oscillator eigenfunctions:

$$\chi_n(S, \omega) = \sqrt{\frac{1}{2^n n!}} \left( \frac{\omega S^2}{2\pi} \right)^{1/4} H_n \left( \sqrt{\omega S} \right) \exp \left\{ -\omega S^2/2 \right\}, \tag{3.28}$$

such that we can write the bases as:

$$\psi_{in}(S, t) = \chi_n(S, \omega_i(t)) \exp \left\{ -i(n + 1/2)\phi_i(t) \right\} \exp \left\{ i\Delta_i(t)S^2/2 \right\},$$

$$\psi_{dn}(S, t) = \chi_n(S, \omega_d(t)) \exp \left\{ -i(n + 1/2)\phi_d(t) \right\} \exp \left\{ i\Delta_d(t)S^2/2 \right\}. \tag{3.29}$$

So the parameters $\omega$, $\phi$ and $\Delta$ completely specify the problem! Furthermore, the difference between the dynamic and instantaneous versions of these parameters fully describes the difference between the dynamic and instantaneous bases.

We will now compare the dynamic and the instantaneous parameters that entered the basis wave functions. With that, we are actually comparing the basis states $\psi_{in}$ and $\psi_{in}$ and therefore observing the differences dynamics make.

Figure (3.3) shows the behaviour of both $\omega_d$ and $\omega_i$. One observes that for small times, the instantaneous frequency $\omega_i$ diverges, while the dynamic one $\omega_d$ approaches a finite value. The divergence of the instantaneous frequency is related to the singlet we approach in the limit $\tau_{in} \to 0$: the exact singlet has an infinite frequency.

The fact that the dynamic frequency is finite for $t = 0$ is due to the specifics of $\eta(t)$ and the specifics of the classical solution we used. This results in the fact that the dynamical basis states do not approach a singlet in the limit $\tau_{in} \to 0$.

Furthermore, after a critical time $t_c = (\tau_f)^{1/3}$, both frequencies are converging to each other. This critical time is related to the fact that for $t \gg t_c$, the Bessel functions are approximated by the asymptotic expansion. When $t \gg t_c^2$:

$$\eta(t) \approx \sqrt{\frac{t}{\tau_f}}, \tag{3.30}$$

\[14\] The $\omega$ of section (3.2) was not dimensionless yet, here we use the dimensionless form, which is in fact $\omega_i/\omega_f$. 45
Figure 3.3.: Comparison of the dynamic frequency $\omega_d(t)$ (red curve) and the instantaneous frequency $\omega_i(t)$ (blue curve) for $t_f = 300$. One sees that both frequencies converge when $t \gg t_c$. Furthermore, the instantaneous frequency diverges in the limit $t \to 0$, while the dynamical one has a finite value.

and therefore

$$\omega_d(t) = \frac{t_f}{t} \eta(t) \approx \sqrt{\frac{t_f}{t}} = \omega_i(t). \quad (3.31)$$

So we find that the frequencies are the same in this limit. If $t \ll t_c$, the difference between both the frequencies is substantial and therefore, the basis sets of wave functions are quite different.

There are two more sources of difference between the instantaneous basis and the dynamical basis. First of all, the phases $\phi_d(t)$ and $\phi_i(t)$, illustrated in figure (3.4(a)). When $t \gg t_c$, using the asymptotic expansion of the Bessel functions, we find that:

$$\phi_d(t) \approx 2 \frac{t^{3/2}}{3 \sqrt{t_f}} = \frac{2}{3} \phi_i(t). \quad (3.32)$$

In other words, the difference between the dynamic and instantaneous phase in this limit is just a multiplicative factor. When $t \ll t_c$, the phases have a different shape as well, due to a different power-law behaviour.

Secondly, the dynamical basis contains an extra $S$-dependent phase term due to $\Delta_d(t)$, which is illustrated in figure (3.4(b)). It vanishes for large $t$, therefore converging to the instantaneous case in which $\Delta_i(t) \equiv 0$. Furthermore, it approaches a finite value when $t \to 0$.

We have now found and investigated the dynamical basis. Furthermore, we defined an instantaneous basis with which we can compare dynamics with statics. We found the existence of a critical time $t_c$. When $t \gg t_c$, the only difference between the dynamic and instantaneous bases is a multiplicative factor in the phases $\phi_i(t)$ and $\phi_d(t)$. When $t \ll t_c$, the bases are different regarding all parameters.
Figure 3.4.: Figure (a) shows the dynamical phase term $\phi_d(t)$ (red curve), the instantaneous one $\phi_i(t)$ (blue curve), and $2/3 \phi_i(t)$ (green curve). Figure (b) shows the behaviour of the extra phase $\Delta_d(t)$ in the dynamical basis state for $t_f = 50$. It converges to a finite value when $t \to 0$ and it vanishes after the critical time $t_c$.

With the dynamical basis, we can calculate the time-evolution of the dynamical state $\Psi(t)$. The first thing that needs to be done is calculating the overlaps between the initial state and the dynamical basis.

3.3.3. The overlaps and the dynamical state

Remember from chapter (2) that we find the time-development of a state by using the propagator:

$$\Psi(S,t) = \int G(S \mid S', t_{in}) \Psi(S', t_{in}) dS'.$$

(3.33)

However, as we can rewrite the propagator as:

$$G = \sum_n \Psi_n^*(S', t_{in}) \Psi_n(S, t),$$

(3.34)

we find that the dynamical state can be written as an infinite sum of products of overlaps at the initial time and basis states:

$$\Psi(S,t) = \sum_{n=2k+1}^{\infty} c_n \phi_n^d(S,t),$$

(3.35)

$$c_n = \langle \chi_n^d(t_{in}) \mid \Psi(t_{in}) \rangle,$$

where $k = 0, 1, 2, \text{etc.}$ We will rewrite this equation using (3.29) as this will reduce notational confusions later on:

$$\Psi(S,t) = \sum_{n=2k+1}^{\infty} \tilde{c}_n \chi_n^d(t) \exp \left\{ i \Delta(t) S^2 / 2 \right\} \exp \left\{ -i \left( \phi(t) - \phi(t_{in}) \right) \right\},$$

$$\tilde{c}_n = \langle \chi_n^d(t_{in}) \mid \Psi(t_{in}) \rangle \exp \left\{ i \Delta(t_{in}) S^2 / 2 \right\} \mid \Psi(t_{in}) \rangle.$$  

(3.36)
The difference with (3.35) is that we did not include the n-dependent phase term in the definition of the overlap, and therefore it appears as an extra term in the state \( \Psi(S, \tau) \).

We calculate the overlaps, which are all Gaussian integrals of Hermite polynomials, and are proportional to:

\[
\tilde{c}_n \sim \int \exp \left\{ -\omega_d(t_{in})S^2/2 \right\} H_n \left( \sqrt{\omega_d(t_{in})} \right) \exp \left\{ -i\Delta(t_{in})S^2/2 \right\} S \exp \left\{ -\omega_i(t_{in})S^2/2 \right\} dS.
\]

(3.37)

If we now change to integration variables \( S' = \omega_i(t_{in})S \), one observes that the integral only depends on ratios:

\[
R = \frac{\omega_d(t_{in})}{\omega_i(t_{in})},
\]

\[
R_{\Delta} = \frac{\Delta(t_{in})}{\omega_i(t_{in})}.
\]

(3.38)

With these definitions we find the following analytical expression for the overlaps:

\[
\tilde{c}_n = \frac{2i^{n-1}\sqrt{2}}{\left( -1 + \frac{1}{R} + \frac{iR_{\Delta}}{R} \right)^{1/2}} \left\{ 1 + \frac{1}{R} + \frac{iR_{\Delta}}{R} \right\}^{-1/2} \frac{n}{2 \sqrt{\frac{2^{1-n}}{n!} n!}} \left( \frac{1}{2} \right) \left( -1 + n \right)!
\]

(3.39)

Figure (3.5) shows the behaviour of the overlaps. The plot on the left shows that by increasing \( t_{in} \), the real part of the overlaps tend to a delta peak at \( n = 1 \). The plot on the right shows that the imaginary part vanishes. This can be explained with the fact that by increasing \( t_{in} \), eventually \( t_{in} > t_c \). In this limit the dynamic and instantaneous bases are very similar. As the initial state is a \( n = 1 \) state of the instantaneous basis, the dynamic state will converge to a \( n = 1 \) state in this limit. If \( t_{in} < t_c \), the basis are different and the overlaps get increasingly spread out.

With the exact expressions for the overlaps and the dynamical basis, we reached an exact expression for the full dynamical state \( \Psi(S, \tau) \). At this point it is still an infinite sum but we can try to simplify the dynamical state by defining:

\[
\Psi(S, \tau) = \gamma_1(S, \tau) + \gamma_2(S, \tau),
\]

(3.40)

where \( \gamma_1(S, \tau) \) and \( \gamma_2(S, \tau) \) are defined as:

\[
\gamma_1(S, \tau) = \sum_{n=2k+1}^{\infty} \tilde{c}_n \chi_n^d(\omega_d(S, t)) \exp \left\{ i\Delta(t)S^2/2 \right\} \exp \left\{ -i(\phi(t) - \phi(t_{in}))3/2 \right\}
\]

\[
\gamma_2(S, \tau) = \sum_{n=2k+1}^{\infty} \tilde{c}_n \chi_n^d(\omega_d(S, t)) \exp \left\{ i\Delta(t)S^2/2 \right\} \exp \left\{ -i(\phi(t) - \phi(t_{in}))3/2 \right\} \\
\times \left( \exp \left\{ -i(n-1)(\phi(t) - \phi(t_{in})) \right\} - 1 \right).
\]

(3.41)
This way we split the wave function in two parts. Notice that $\tilde{\gamma}_1(S, t)$ reduces to $\Psi(S, t)$ when the $n$-dependent phase term vanishes. This will be very convenient as we can find a more clever way to write $\tilde{\gamma}_1(S, t)$. For a detailed derivation see appendix E. Upon using:

$$\chi_1(\omega_i(t_{in})) = \sum_{n=2k+1}^{\infty} \tilde{c}_n \left( \frac{\omega_d(t_{in})}{\omega_i(t_{in})} \right) \left( \frac{\Delta(t_{in})}{\omega_i(t_{in})} \right) \chi_n(\omega_d(t_{in})) \exp \left\{ i \frac{\Delta(t_{in})}{2} \right\}, \quad (3.42)$$

we find that:

$$\gamma_1(t) = \chi_1(\omega_r(t)) \exp \left\{ i(\Delta(t) - \Delta_r(t)) \frac{S^2}{2} \right\} \exp \left\{ -i(\phi(t) - \phi(t_{in})) \frac{3}{2} \right\} \quad (3.43)$$

where,

$$\omega_r(t) = \frac{\omega_d(t)}{\omega_d(t_{in})} \omega_i(t_{in}),$$

$$\Delta_r(t) = \frac{\omega_r(t)}{\omega_i(t_{in})} \Delta(t_{in}) \quad (3.44)$$

are rescaled parameters. We find that, apart from phase factors, $\gamma_1$ is a $n = 1$ state with a rescaled frequency $\omega_r$.

**Behaviour and meaning of $\gamma_1$ and $\omega_r$**

We learnt that our dynamical state is a sum of a $n = 1$ part, $\gamma_1(S, t)$, and a 'perturbing' contribution, $\gamma_2(S, t)$. We can now use the fact that we are in half-space and $n$ is always some odd
number (so \( n - 1 \) is always an even number). Therefore one can immediately conclude that when the phase \( \phi(t) - \phi(t_{in}) \) is an integer number \( k \) times \( \pi \), the perturbing part \( \gamma_2(S, t) \) vanishes and \( \Psi(S, t) \) reduces to \( \gamma_1(S, t) \).

This simplifies our problem enormously, as \( \gamma_1(S, t) \) is easily computed because it is not an infinite sum anymore, but simply an \( n = 1 \) state of a rescaled frequency. So at least we know the exact behaviour of \( \Psi(S, t) \) at points where the phase is \( k\pi \).

By definition, \( \gamma_1(S, t) \) is fully determined by \( \omega_r \). We can compare the behaviour of \( \omega_r \) with that of \( \omega_i \), and therefore, compare the behaviour of \( \gamma_1(S, t) \) to the instantaneous case wave function. The critical time \( t_c \) in relation to the initial time \( t_{in} \) plays an important role here, as this gives us information about how different the basis states are (due to the difference in \( \omega_d \) and \( \omega_i \)) at initial time. We already encountered this behaviour at the overlaps: when \( t \gg t_c \) the overlaps converge to a delta at \( n = 1 \). When \( t \ll t_c \) the overlaps spread out over an increasing amount of higher order states.

When \( t_{in} \ll t_c \), the frequencies \( \omega_r \) and \( \omega_i \) are quite different, illustrated in figure (3.6(a)). This is related to the fact that in this limit, the dynamic and instantaneous basis are very different at initial time. As we saw, this translates into the fact that a lot of overlaps are nonzero at initial time. Therefore a lot of higher order states are entering the dynamical state. This will cause \( \omega_r \) and the dynamical state to be very different. One should also notice that \( \omega_r \) does not really change in this limit while \( \omega_i \) does. However, both \( \omega \)'s get closer to each other as time increases.

When \( t_{in} \gg t_c \), the frequencies \( \omega_r \) and \( \omega_i \) are quite the same, which means the dynamical state \( \Psi(t) \) is approximately the same as the instantaneous state - the symmetry broken ground state. In this limit the dynamic and instantaneous basis are very similar at \( t_{in} \) and only the \( n = 1 \) state enters the dynamical state, as we saw in the behaviour of the overlaps. Therefore,
the dynamical state is very similar to the instantaneous state. This behaviour is illustrated in figure (3.6(b)).

We will discuss the effects of $\gamma_2$ in detail in section (3.3.7). For now, it is important to know that $\gamma_2$ is a perturbing contribution that does not alter the qualitative behaviour of the system. Therefore we will neglect this contribution for the moment.

### 3.3.4. Energy of the dynamical state

In this section the energies of both the dynamical and the instantaneous state will be computed. When we treat the field instantaneously at every point the energy levels must be the usual static ones with the time-dependency inserted afterwards:

$$E_i^n(t) = (n + \frac{1}{2}) \frac{t}{\tau_f}. \quad (3.45)$$

Therefore the energy of the instantaneous state, a $n = 1$ state, reads:

$$E_i^1(t) = \frac{3}{2} \frac{t}{\tau_f}. \quad (3.46)$$

The reader might wonder what happened with the dimensions of these energies, but by making the substitutions to dimensionless units, the energies changed as well: they are divided by $E_{\text{fin}}^f$.

Again, computing the dynamic energy for the full $\Psi(S, t)$ state can only be done numerically. However, for the periodically correct part $\gamma_1(S, t)$ the energy is given by:

$$\langle \gamma_1(S, t) | \mathcal{H} | \gamma_1(S, t) \rangle. \quad (3.47)$$

If one computes the integrals over Hermite polynomials and Gaussian-shaped pre-factors, one finds:

$$E_d^d(t) = \frac{3\tau}{4\tau_f} \omega_p(t) + \frac{3}{4\omega_p} + \frac{3\tau}{4\tau_f} \frac{\Delta(t) - \Delta_r}{\omega_p}. \quad (3.48)$$

The time-dependent energies are shown in figure (3.3.4). The energy of the dynamical state is always higher than the energy of the instantaneous state. This makes sense as the instantaneous state represents an adiabatic evolution, which follows the lowest possible energy development.

One could wonder why there are three terms entering the analytical expression of the energy $E_d^d$. The first two terms can be associated with ‘normal’ potential and kinetic terms, quite similar to the instantaneous ones. The third contribution is purely created by the dynamics: there is a phase term in the dynamical state (due to $\Delta(t)$) that depends on $S$ as well. This phase term modifies the kinetic energy.

### 3.3.5. Density of defects

After breaking the symmetry, one would expect to recover the symmetry-broken ground state, the $n = 1$ instantaneous basis state. The defect density is a measure of how much the dynamical ground state $\Psi(S, t)$ is different from that expected $n = 1$ instantaneous ground state. The
order parameter of the system, the staggered magnetisation (3.12), is maximal in the instantaneous ground state: the system is maximally ordered. In the dynamical ground state, the order parameter is reduced due to the presence of the defects.

With density, we are referring to the fact that we are assigning a defect value 'per spin'. If we would like to find the total number of defects, we would have to multiply the defect density with the number of spins. The density of defects should be maximal (1) when the dynamical state is maximally different, and minimal (0) when there is no difference. Therefore we define the density of defects as:

$$\rho(t) = 1 - |\langle \psi_i^1(t) | \gamma_1(t) \rangle|^2.$$ \hspace{1cm} (3.49)

We are able to calculate the periodically correct density of defects $\rho_\pi(t)$, by inserting $\Psi(S, t) = \gamma_1(S, t)$ and, after a calculation which is very similar to that of the overlaps, we find the analytical result:

$$\rho_\pi(t) \equiv 1 - |\langle \psi_i^1(t) | \gamma_1(t) \rangle|^2 = 1 - \left| \left( \frac{\omega_i}{\omega_r} \right)^{3/4} \frac{2}{\sqrt{2}} \left( 1 + \frac{\omega_i}{\omega_r} + i \left( \frac{\Delta(t) - \Delta_r}{\omega_r} \right) \right)^{-3/2} \right|^2.$$ \hspace{1cm} (3.50)

This analytical formula allows us to explore the characteristics of the defect density. Of course, the formula only reduces to the exact defect density when $\gamma_2 = 0$, but as we will find out later, the ‘true’ defect density oscillates around the smooth evolution of $\rho_\pi(t)$. Figures (3.8) and (3.9) illustrate the behaviour of the defect density.

In figure (3.8(a)) $t_{in} < t_c < t_f$. This means that at initial time the dynamical and instantaneous bases are very different. Therefore $\omega_r$ is very different from $\omega_i$ and thus the defect density is big because the overlap between the $\gamma_1$ state (which is controlled by $\omega_r$) and $\psi_i^1$ (which is controlled by $\omega_i$) is small. This is related to the fact that a large number of overlaps is nonzero

Figure 3.7.: Behaviour of $E_i^1(t)$ (green curve) and $E_\pi^1(t)$ (red curve) for $t_f = 100$ and $t_{in} = 1$.

The instantaneous energy is lower as it is an ‘adiabatic’ evolution of the energy through time.
Figure 3.8.: Figure (a) shows the defect density in the defects saturating regime as well as the behaviour in the \( t_{in} \rightarrow 0 \) limit. The final time \( t_f = 10 \) and \( t_{in} = 10^{-4} \) (red curve), \( t_{in} = 10^{-3} \) (blue curve), and \( t_{in} = 10^{-2} \) (green curve). One observes that reducing \( t_{in} \) increases the density of defects, eventually to 1 when \( t_{in} = 0 \). Figure (b) shows the defect density in the defects saturating regime as well as the behaviour in the \( t_f \rightarrow \infty \) limit. The initial time is \( t_{in} = 0.1 \) and the final times are \( t_f = 100 \) for the red curve, \( t_f = 1000 \) for the blue curve, and \( t_f = 10000 \) for the green curve. Increasing \( t_f \) even further will result in a defect density that is even closer to 1. This is counterintuitive, but is related to the fact that increasing \( t_f \) at a fixed \( t_{in} \), results in decreasing \( B_{in} \) as well. Therefore we are approaching a singlet initial state.

and higher-order states enter the dynamical state. At the final time \( t_f \), the bases are similar again and the difference between the frequencies is constant. Therefore, the density of defects saturates.

The figure shows three curves for different \( t_{in} \) at fixed \( t_f \). Decreasing \( t_{in} \) increases the density of defects because then, the bases are even more different at initial time. Increasing \( t_{in} \) has the opposite effect, of course. It might not surprise the reader that the moment at which the density of defects saturates is precisely related to the critical time \( t_c \). At this point, the frequencies \( \omega_r \) and \( \omega_d \) are different, but the difference remains the same until the final time, and therefore the density of defects saturates.

In figure (3.8(b)) \( t_{in} < t_c < t_f \) as well, and therefore we recognise identical features. In this plot the density of defects saturates as well, again after a critical time. This figure shows three curves for different \( t_f \) at fixed \( t_{in} \) and allows us to study the effects of \( t_f \) on the defect density. Increasing \( t_f \) increases the critical time \( t_c \), therefore removing the initial time even further from \( t_c \). This results in a bigger difference between \( \omega_r \) and \( \omega_i \), and therefore a bigger density of defects. In terms of overlaps this means that by increasing \( t_f \), the number of higher order overlaps increases. Decreasing \( t_f \) of course has the opposite effect. A subtle effect that can be noticed is the moment at which saturation occurs. This is of course related to the critical time \( t_c \).

Figure (3.9(a)) is in the regime where \( t_{in} > t_c \), and shows a very different behaviour: there
are practically no defects! The fact that the initial time is bigger than the critical time is the reason for this. From figure (3.6(b)) it is clear that in this regime the frequencies $\omega_r$ and $\omega_i$ are very similar. Therefore, the instantaneous and dynamical state are very much the same and the defects vanish.

If one increases $t_{in}$ in this regime, the defect density becomes even smaller. The higher the initial time, the more similar the frequencies $\omega_r$ and $\omega_i$ become. Therefore the bases are increasingly similar as well and the defects vanish. Also in this plot the defect density increases at first, and then saturates. This is due to the fact that any difference in $\omega_r$ and $\omega_i$, as small as it may be, gets created in the beginning and saturates after some time.

Figure (3.9(b)) is in the regime where $t_{in} < t_f < t_c$. Not only are the frequencies $\omega_r$ and $\omega_i$ very different in this regime, they are still different at $t_f$, because the system has not reached the critical time yet. Therefore the defect density keeps increasing until the final time, and has not yet saturated at final time.

This plot was made at a fixed final time and shows that decreasing $t_{in}$ in this regime, increases the defect density. Once more, this is related to the relationship between the initial time and the critical time: a decreasing $t_{in}$ moves the initial time further away from the critical time, therefore increasing the difference between $\omega_r$ and $\omega_i$, resulting in a higher density of defects.

These figures gave us a lot of information and hinted at the existence of three different regimes. First of all a defect creation regime exists, where the defects have not yet saturated. Secondly a defect saturation regime can be found, where we encounter a substantial nonzero defect density which has already saturated. Finally there exists a defect free regime, where practically no
Defects can be found. In the next section we will condense all our observations into one single figure: the phase diagram.

The phase diagram

Figure 3.10.: The phase diagram displays the behaviour of the defect density in three different regions. First of all, the region where \( t_{in} > t_f \) is unphysical, as the initial time cannot be bigger than the final time \( t_f \). In the region 'Defect creation', the density of defects keeps increasing and does not saturate. When the system is in the saturating region, the density of defects is saturated at the final time, and in the defect free region, there are practically no defects at final time.

We can summarise the knowledge of \( \rho_{\pi} \) in a phase diagram (3.10), in which all the observed features can be recognised. First of all, the triangle where \( t_{in} > t_f \), is the unphysical regime: the initial time cannot be bigger than the final time. Secondly, in the bottom left corner, when \( t_f < 1 \) and \( t_{in} < t_f \), defects are being created from initial time until the final time, corresponding to figure (3.9(b)). This is the defect creation regime. In this regime the frequencies \( \omega_r \) and \( \omega_i \) are very different at initial time, and the difference keeps increasing until the final time. Therefore the defects keep on being created. The closer one gets to the line \( t_{in} \) in this regime, the higher the number of defects is.

The bottom right corner, when \( t_f > 1 \) and \( t_{in} < t_c \), shows the region where the density of defects is saturated, corresponding to figure (3.8). In this regime, the defects are being created when \( t < t_c \), because at these times the frequencies \( \omega_r \) and \( \omega_i \) are different. After the critical time \( t_c \), the difference between both frequencies remains constant and the density of defects no longer increases, but saturates. Once more, the closer one gets to the line \( t_{in} = 0 \), the higher the density of defects gets. This represented by the grayscale in the figure: the darker it is, the higher the density of defects is.

And finally, in the upper right corner one finds the defect free regime. Already from the
beginning, the dynamical state is very close to the instantaneous symmetry-broken ground state in this regime, corresponding to figure (3.9(a)). In this regime, \( t_{in} > t_c \), and therefore \( \omega_f \approx \omega_i \).

Increasing \( t_{in} \) in this regime decreases the defect density. Notice that if one increases \( t_f \) at a fixed initial time \( t_{in} \), one cannot stay in the defect free regime but moves into the defect saturation regime: defects appear when taking this limit. This might sound counterintuitive, but increasing \( t_f \) means increasing \( t_c \). Then, eventually \( t_{in} < t_c \) and the bases are different at initial time, which results in defects. Another way to understand it, is to realise that by increasing the final time \( t_f \) at a fixed initial time \( t_{in} \), we are in fact decreasing the initial field \( B_{in} \).

One might wonder why we call the different regimes phases, as there is no clear phase transition where a certain parameter diverges. The density of defects changes smoothly when one crosses the boundary between two regions. This behaviour is represented by the 'smooth' broad lines in figure (3.10). In a sense there is no phase transition, but we expect that the defect density shows different power-law behaviour in all three regimes. In that case, crossing a boundary in the phase diagram means changing from one power-law behaviour of the density of defects to another power-law behaviour of the density of defects. This still has to be studied though.

Another interesting aspect for future research is the behaviour of the order parameter in these three regimes. In principle, the higher the density of defects is, the lower the order parameter should be. A calculation still has to be made to confirm this.

We can generalise the results of this phase diagram. Notice that it is built up by just two curves. The \( t_f = t_{in} \) line is trivial and the same for any time-dependent symmetry breaking field. The \( t_c \) curve depends on the specifics of the symmetry-breaking field. So if we know the behaviour of \( t_c \) corresponding to some time-dependent symmetry-breaking field, we can immediately write down the phase diagram, and therefore know the qualitative behaviour of the system for any given \( t_{in} \) and \( t_f \). We will try to find a way of generalising \( t_c \) in the next section.

### 3.3.6. Generalisation to other time-dependent symmetry-breaking fields

After extensively analysing the consequences of one specific shape of the symmetry-breaking field, one might wonder if the results can be generalised to other shapes of the symmetry-breaking field. Precise knowledge of \( t_c \) allows us to make a phase diagram. In this section we will try to find a general formula for \( t_c \) with a symmetry breaking field \( B(t) = B_f \left( \frac{t}{t_{in}} \right)^{\alpha} \).

The first step in solving a system with such a symmetry-breaking field, would be to solve the equation of motion, which reads:

\[
\left( \frac{t_f}{t} \right)^{\alpha} \frac{\partial^2 S}{\partial t^2} - \alpha \left( \frac{t_f}{t} \right)^{\alpha} \frac{1}{t} \frac{\partial S}{\partial t} + S = 0. \tag{3.51}
\]

By trial and error, one finds that a general set of solutions to this differential equation reads:

\[
\xi_1(t) = t^{\frac{\alpha+1}{2}} J_{\frac{\alpha+1}{2}} \left( \frac{2}{\alpha+2} t \left( \frac{t}{t_f} \right)^{\frac{\alpha}{2}} \right),
\]

\[
\xi_2(t) = t^{\frac{\alpha+1}{2}} Y_{\frac{\alpha+1}{2}} \left( \frac{2}{\alpha+2} t \left( \frac{t}{t_f} \right)^{\frac{\alpha}{2}} \right). \tag{3.52}
\]
We mentioned before, that in order to find the critical time \( t_c \), an asymptotic expansion needs to be made, with which the Bessel functions are expressed in terms of simple sines and cosines. The critical time is defined to be at this point, because here the dynamical and instantaneous basis converge. The asymptotic expansion holds when:

\[
\frac{2}{\alpha + 1} t \left( \frac{t}{t_f} \right)^{\frac{\alpha}{2}} \gg \left| \left( \frac{\alpha + 1}{\alpha + 2} \right)^2 \frac{1}{4} \right|. 
\]  

(3.53)

We pick the critical time in such a way that when \( t \gg t_c \), the asymptotic expansion is allowed. Simplifying the equation leads us to find:

\[
t_c \approx t_f^{\frac{\alpha}{\alpha + 2}} \left( \frac{\alpha + 1}{2} \left| \left( \frac{\alpha + 1}{\alpha + 2} \right)^2 - \frac{1}{4} \right| \right)^{\frac{2}{\alpha + 2}} .
\]  

(3.54)

One can immediately see that, neglecting the positive prefactor in front:

\[
t_c \approx t_f^{\frac{\alpha}{\alpha + 2}} .
\]  

(3.55)

Figure 3.11.: Figure (a) shows \( \omega_d \) (red curve) and \( \omega_i \) (blue curve) for \( \alpha = 1/2 \) at a final time \( t_f = 100 \). The corresponding critical time \( t_c \approx 2.5 \) and this plot confirms that both \( \omega \)'s converge after this critical time. Figure (b) shows \( \omega_d \) (red) and \( \omega_i \) (blue) for \( \alpha = 3 \) at a final time \( t_f = 100 \). The corresponding critical time \( t_c \approx 16 \) and this plot confirms that both \( \omega \)'s converge after this critical time.

This precisely coincides with what we found for \( \alpha = 1 \). Figures (3.11(a)) and (3.11(b)) show that for different values of \( \alpha \) the critical time \( t_c \) indeed represents the point where the frequencies start to converge. Furthermore, the instantaneous frequency for a general \( \alpha \) is easily found to be:

\[
\omega_i = \left( \frac{t}{t_f} \right)^{\frac{\alpha}{2}} \right).
\]  

(3.56)
We can conclude that, for symmetry-breaking fields represented by power-laws, $t_c$ is always a power of $t_f$ between 0 and 1. Therefore, the shape of the $t_c$ line in the phase diagram is quite similar in the sense that the $t_c$ line is above the $t_f = t_{in}$ line when $t < 1$, and below it when $t > 1$. For each power $\alpha$, a phase diagram, containing all the regions we found, can be drawn.

3.3.7. Influence of the perturbing state $\gamma_2(S, t)$ on the dynamical state $\Psi(S, t)$, energy $E(t)$, and the density of defects $\rho(t)$.

Figure 3.12.: Figure (a) shows an oscillating behaviour in $|\Psi(S, t)|^2$, with $t_{in} = 0.4$ and $t_f = 4$. Figure (b) shows the evolution of the fully correct defect density $\rho(t)$ (blue) around the trend governed by $\rho_{\pi}(t)$ (red), for $t_{in} = 0.01$ and $t_f = 10$. The oscillations tend to vanish for larger times. Figure (c) shows the evolution of the fully correct energy $E(t)$ (blue) on top of the trend governed by $E_{\pi}(t)$ (red), for $t_{in} = 1$ and $t_f = 10$.

In the previous section, we considered only the first part, $\gamma_1(S, t)$ (which periodically reduces to the full dynamical state), of the dynamical ground state wave function. In this section, we would like to find out what the effects of the perturbing part $\gamma_2(S, t)$ are on the state $\Psi(S, t)$,
the defect density $\rho(t)$, and the energy $E(t)$. It is important to find out whether it is allowed to neglect $\gamma_2(S,t)$.

We start by analysing the effects on $\Psi(S,t)$. If we consider one particular value of $t_{in}$ and another one for $t_f$, and we observe the time-evolution of a particular wave function from $t_{in}$ to $t_f$, one finds that each wave function spreads out through time. If we also take $\gamma_2(S,t)$ into account we observe small oscillations in this smooth evolution: the wave function sometimes moves a bit back and forth. This is illustrated in figure (3.12(a)).

The effect of $\gamma_2(S,t)$ on the behaviour of $\rho(t)$ is similar: it causes oscillations around the smooth evolution governed by $\gamma_1(S,t)$. The $\gamma_1(S,t)$ governs the trend, the $\gamma_2(S,t)$ state makes it oscillate a bit around this trend. Figure (3.12(b)) is in agreement with this. At first, the oscillations are quite large, later on, they become smaller and increasingly fast.

The effect on the energy of the state is nearly identical, except for the fact that the oscillations are not around the smooth evolution caused by $\gamma_1(S,t)$, but on top of it, as can be seen in figure (3.12(c)).

The influences of $\gamma_2(S,t)$ are governed by the phase term of $\phi_d(t)$. If we return to figure (3.4(a)), we see that for high $t_f$, the phases grow increasingly faster. This will result in the fact that the oscillations of the full state $\Psi(S,t)$ around $\gamma_1(S,t)$ are becoming smaller and faster. For low $t_f$, the phase increases slower and therefore the importance of $\gamma_2(S,t)$ increases.

We can conclude that $\gamma_2(S,t)$ causes perturbations which are most important in the regime where $t$ is small. The perturbations do not alter the general trend of the parameters $\Psi(S,t)$, $E(t)$, and $\rho(t)$, and do not change the qualitative behaviour.

3.4. Conclusion

In this chapter we added a time-dependent symmetry breaking field to the Lieb-Mattis Hamiltonian for an antiferromagnet. We extensively treated a linear symmetry-breaking field, but we can generalise the treatment to any power-law behaviour of the symmetry breaking field. Therefore we can also generalise the conclusions we draw to these types of symmetry-breaking fields.

The question we tried to answer is: suppose you start from a symmetric ground state, what happens if you switch on a symmetry-breaking field in a particular way?

It turns out that we cannot start from an exact ground state, but we can approximate it by starting from a symmetry-broken ground state at a very small symmetry-breaking field. At a certain time, we switch on the field. At this point, we project the initial state on a dynamical basis. We found this basis by using the path integral formalism. We defined an instantaneous basis as well, which corresponds to the basis we would have found if we would have considered the symmetry-breaking field to be static at every moment in time.

We found the existence of a critical time $t_c$, which turns out to be very important to our system. When $t \ll t_c$, the dynamical and instantaneous basis are very different. When $t \gg t_c$, they are very similar.

We found the evolution of the state and it turns out that the dynamical state can be expressed as a sum of a $n = 1$ state with a rescaled frequency, and a perturbing part. The perturbing part causes some oscillations but does not change the qualitative behaviour of the state.

We defined a density of defects which represents the difference between the dynamical ground
state we found, and the instantaneous ground state. The defects reduce the ordering of the system.

All the important conclusions that can be drawn from this chapter are summarised in the phase diagram (3.10). It turns out that there are three different regions, determined by the values of $t_{in}$ and $t_f$, that show different behaviour of the defect density. First of all, there exists a defect creation regime when the initial time $t_{in}$ is smaller than the critical time $t_c$. In this regime, the defect density increases and does not saturate. The defects are created because of the difference in the frequency $\omega_r$ that describes the dynamical state and the frequency $\omega_i$ that describes the instantaneous state. In this limit the dynamic and instantaneous basis are very different at initial time $t_{in}$, and therefore we end up with a lot of defects. The bases are still different at the final time $t_f$, and therefore the number of defects keeps increasing.

Secondly, there is a defect saturation regime where the defects have been increasing for some time, but are saturated at some value between 0 and 1. Again, this is connected to the frequencies as in this regime the difference between the frequencies $\omega_r$ and $\omega_i$ converges to a constant value. Finally, the system contains a defect free regime in which no defects are observed. This is related to the fact that in this regime, where $t_{in} > t_c$, the frequencies $\omega_r$ and $\omega_i$ are always more or less the same and therefore, no defects are being created.

When there are no defects observed, the dynamical ground state completely overlaps with the instantaneous one. The more defects there are present in the system, the more localised and closer to the singlet initial state the dynamical ground state is.

With the phase diagram, we can assess the limiting behaviour of our system. In the limit $t_{in} \rightarrow 0$, we will always end up with a maximal number of defects. Actually, taking this limit is not allowed within our treatment. If we take a closer look at the discrete Lieb-Mattis model, this is explainable. Remember that, in order to solve this problem, we made a continuum approximation. This approximation relies on the fact that $0 \ll S \ll N$. But if we are very close to a singlet, $S \approx 0$, and this approximation obviously breaks down. We cannot use the continuum approximation when considering a pure singlet initial state. One has to take the discrete model and use computer calculations to investigate the behaviour there. Furthermore, the boundary condition $S \geq 0$ forces our dynamical basis states to be odd and vanishing at $S = 0$. Therefore, we cannot project a pure singlet state onto the dynamical basis.

We can also increase the initial time. When $t_{in} \gg t_c$, we end up in the defect free regime. The dynamic and the instantaneous bases are very similar in this limit, resulting in a very similar state and a vanishing number of defects.

We can also consider the limiting behaviour of $t_f$. When $t_f \rightarrow \infty$, at a fixed $t_{in}$, the number of defects keeps increasing, eventually reaching 1. This is related to the fact that we keep increasing the critical time $t_c$, therefore removing $t_{in}$ further away from the critical time, and increasing the difference between $\omega_r$ and $\omega_i$, resulting in a maximal defect density. We cannot take the $t_f \rightarrow 0$ limit, because the constraint $t_{in} < t_f$ forces us to take the limit $t_{in} \rightarrow 0$ as well, and we already discussed the problems with that limit.

We found out that we can generalise this treatment to other shapes of the symmetry breaking field. We studied symmetry-breaking fields that can be written as power-laws. For any power-law shape of the symmetry-breaking field, we can find the shape of the critical time and therefore immediately draw the phase diagram and appoint the different regions.

We now try to answer our question from the introduction: does the precise way in which a
**symmetry is broken matter?** The answer is yes, the way in which we break a symmetry matters. Not only does it matter within the class of linear fields, as can be seen in the phase diagram, but different symmetry-breaking field give rise to different phase diagrams and therefore, different behaviour of the system.
4. Summary

We can split the research work and the thesis in two parts: the method, and its application to the physical model. We can draw important conclusions from both of them. In the first part of this thesis, we investigated the method with which to attack this problem: the path integral formalism. First of all, we found a procedure for solving the path integral for a general quadratic Lagrangian. It comes down to solving a second-order linear differential equation: the Euler-Lagrange equation of motion. Once the solutions of this equation are known, the path integral is easily solved. One can compute the propagator, and with that, one can find a basis set of wave functions.

It is important to realise that there is no such thing as a set of eigenstates in the time-dependent case. This is not necessarily a problem. For our physical system, for instance, we can specify a precise initial state, project this onto a dynamical basis, and calculate the time-development of the state.

Furthermore, we investigated a boundary condition problem, by limiting the solution space to the positive half, say $q > 0$. With the classical approach, we found that if one only uses the action principle, the solution becomes degenerate in between each node (except for the last one). However, if one imposes infinitely hard boundaries, in other words, energy conservation, one finds that the degeneracy vanishes.

The boundary condition problem can also be treated by a quantum mechanical approach. A topological action can be defined, which in itself includes the energy conservation. It turns out, that with this formulation, we can forget about the boundary conditions until the very end: we find a set of wave functions of a specific problem without the boundary condition and then select only the odd ones, which vanish at the boundary, to constitute the correct basis.

After this extensive treatment of the methods necessary to attack the real problem, we turned to the physical model. We studied the Lieb-Mattis model for an antiferromagnet, which is an infinite range model. It has a wide range of applications as it contains the thin spectrum of Heisenberg Hamiltonians. We started, as an introduction to the system and all its parameters, with the case of static symmetry breaking.

We introduce a staggered magnetic field to the Lieb-Mattis Hamiltonian, which will break the SU(2) spin rotational symmetry. One can map the problem of the symmetry-broken Lieb-Mattis Hamiltonian onto a harmonic oscillator, and use time-independent quantum mechanics to find the eigenstates. One finds that the $u^n_S$, which represent the coefficients of the projection of the symmetry broken eigenstates $|n\rangle$ onto the symmetric Lieb-Mattis Hamiltonian eigenstates $|S\rangle$, correspond to harmonic oscillator eigenfunctions. Therefore, the symmetry broken ground state, projected onto the symmetry-unbroken $|S\rangle$-basis, is a $n = 1$ harmonic oscillator eigenstate.

Furthermore, it turns out that the spin rotational symmetry is in fact broken spontaneously, by considering the order parameter and the way it behaves when interchanging the limits $N \to \infty$ and $B \to 0$. 
After this, we turned our attention to the dynamical situation, which was our main point of interest. One can make the same mapping to a harmonic oscillator problem. We find a dynamical set of basis wave functions with the use of the path integral mechanism. Because starting from a singlet corresponds to starting from $S = 0$, where each of our basis set wave functions vanishes by definition (because they are odd), we have to start from a very small symmetry broken ground state with an initial field $B_{in}$. Starting from an exact singlet is impossible within this treatment.

We project this initial state onto our dynamical basis set and study the ground state wave function we find. We can compare this dynamical state with a state that we would have found if we would have treated the symmetry breaking field instantaneously. For this instantaneous state, we use the known result for static symmetry breaking and simply insert the time-dependence afterwards. The system contains a critical time $t_c$ that is related to the differences between the dynamical and instantaneous states. When $t > t_c$, both bases are similar, when $t < t_c$, they are different.

It turns out that the dynamical state is a sum of an analytically known state, governed by a rescaled frequency, which forms a trend, and a perturbing state, which causes the full wave function to oscillate around the trend. We can neglect the perturbing state as it only causes oscillations in physical observables, but it does not change the smooth evolution.

We compare the dynamical state with the instantaneous state. With these two states, we define a density of defects. The defects represent the difference between the dynamical symmetry broken ground state and the instantaneous state, which is the symmetry broken ground state we would have found by using a statical approach. The defects reduce the maximal ordering of the instantaneous ground state.

We introduce a phase diagram in which three regions with different behaviour of the density of defects can be found. The regions are determined by three parameters of the system: the initial time $t_{in}$ at which we switch on the field, the final time $t_f$ at which we switch it off, and the critical time $t_c$. When the initial time $t_{in}$ and the final time $t_f$ are both smaller than a critical time of the system $t_c$, the system is in the defect creation phase: the amount of defects is growing. When $t_f > t_c$, but $t_{in} < t_c$, the defect density has grown in the past, but saturates after $t > t_c$. The third phase, where $t_{in} > t_c$, contains no defects: at the initial time the bases are very similar and therefore no defects are being created.

In this thesis we extensively studied the case in which the symmetry-breaking field was switched on linearly. However, we showed that we can generalise this treatment to any power-law-shaped field. Each case of those class of symmetry-breaking fields is solvable and contains the same regions in the phase diagram. The specific critical time depends on the characteristics of the symmetry-breaking field.

The density of defects shows that the way in which a symmetry broken matters and that dynamical symmetry breaking creates defects in the sense that the symmetry broken ground state is different than we would expect from an instantaneous approach.
Acknowledgements

This thesis reflects the work done in cooperation with Carmine Ortix and Jeroen van den Brink at the Lorentz institute, at Leiden University. This work would obviously not have been possible without them.

First of all, I owe a lot to Carmine, who is responsible for a great deal of on-the-job coaching. I learnt a lot from his experience the past year and it was great to be working with him.

Secondly, I would like to thank Jeroen for his excellent guidance. I also thoroughly enjoyed the opportunity of breathing in the special academic atmosphere in Stanford, where his hospitality was amazing.

I would like to thank Jasper van Wezel, who gave me invaluable advice on writing my thesis. And finally I would like to thank Peter Denteneer, who was willing to act as a second reviewer of my work.
A. Factorisation

We start with a full Lagrangian
\[ S = \int dt \left\{ \frac{1}{2} \left[ \dot{q}(t) \frac{q(t) q(t)}{X(t)} - \frac{2 Y(t)}{X(t)} q(t) \dot{q}(t) - \left( Z(t) - \frac{Y^2(t)}{X(t)} \right) q^2(t) \right] - F(t) q \right\} \] (A.1)
and write \( q(t) = q_{cl}(t) + \delta q(t) \). Implementing this in each term we get:
\[ S = \int dt \left\{ \frac{1}{2} \left[ \left( \dot{q}_{cl}(t) + \delta q(t) \right)^2(t) - \frac{2 Y(t)}{X(t)} \left( q_{cl}(t) + \delta q(t) \right) \left( \dot{q}_{cl}(t) + \delta \dot{q}(t) \right) (t) \right. \right. \\
- \left. \left. \left( Z(t) - \frac{Y^2(t)}{X(t)} \right) \left( q_{cl}(t) + \delta q(t) \right)^2(t) \right] - F(t) \left( q_{cl}(t) + \delta q(t) \right) \right\}. \] (A.2)

We now get three types of terms: one with elements linear and quadratic in \( q_{cl} \) (the classical action \( S_{cl} \)), one with elements quadratic in \( \delta q \) (the fluctuation term \( S_{fl} \)) and one with mixed terms \( q \delta q \) (only quadratic). We can write this as \( S_{cl} + S_{fl} + S_{mixed} \).
\[ S = S_{cl} + S_{fl} + \int dt \left\{ \frac{\dot{q} \delta q}{X(t)} - \frac{Y(t)}{X(t)} \left( q_{cl} \delta \dot{q} + \dot{q}_{cl} \delta q \right) - \left( Z(t) - \frac{Y^2(t)}{X(t)} \right) q \delta q - F(t) \delta q \right\}, \] (A.3)
where
\[ S_{cl} = \int dt \left\{ \frac{1}{2} \left[ \frac{\dot{q}_{cl}^2(t)}{X(t)} - \frac{2 Y(t)}{X(t)} q_{cl}(t) \dot{q}_{cl}(t) - \left( Z(t) - \frac{Y^2(t)}{X(t)} \right) q_{cl}^2(t) \right] - F(t) q_{cl} \right\} \] (A.4)
\[ S_{fl} = \int dt \left\{ \frac{1}{2} \left[ \frac{\dot{q}_{fl}^2(t)}{X(t)} - \frac{2 Y(t)}{X(t)} q_{fl}(t) \dot{q}_{fl}(t) - \left( Z(t) - \frac{Y^2(t)}{X(t)} \right) q_{fl}^2(t) \right] \right\}. \] (A.5)

If we now perform an integration by parts on the integral term, integrating each \( \delta \dot{x} \), we get
\[ S = S_{cl} + S_{fl} + \left[ \frac{\dot{q}_{cl}(t)}{X(t)} \delta q(t) - \frac{Y(t)}{X(t)} q_{cl}(t) \delta q(t) \right]_{t_a}^{t_b} \right. \\
- \int_{t_a}^{t_b} dt \left. \delta q(t) \left\{ \frac{\dot{q}(t)}{X(t)} + \left( \frac{Y(t)}{X(t)} - \frac{X(t)}{X^2(t)} \right) \dot{q}_{cl}(t) - \left( \frac{Z(t) - Y^2(t)}{X(t)} - \frac{X(t)Y(t)}{X^2(t)} \right) q_{cl}(t) + F(t) \right\}. \] (A.6)

The evaluation of the boundary terms of the integration by parts drops out because we know that \( \delta q(t_a) = \delta q(t_a) = 0 \). The integral becomes zero because of equation (2.25). Thus, we end up with:
\[ S = S_{cl} + S_{fl}, \] (A.7)
where the fluctuation part takes only the quadratic terms in the action. In the next appendix we will calculate precisely these fluctuation terms.
B. Pauli-van Vleck formula

In this section we will derive the Pauli-van Vleck formula for the fluctuation term of the action $S_{fl}$. The following proof will be for quadratic actions only and is based on the books [19, 31]. The extension to include linear terms is quite easy, because they do not enter in the fluctuation term. They do alter the classical action, but not the fluctuation term (see appendix A). Anticipating on the result of this section, the general formula for $S_{fl}$ does not take these terms into account.

Firstly, realise that the fluctuation factor $F(t_a, t_b)$, the integral over the fluctuations $\delta x$ of the exponent $\exp \left\{ \frac{i}{\hbar} S_{fl} \right\}$, is a function of the times $t_a$ and $t_b$ only, because the fluctuations are zero at the boundaries. It is essentially the propagator from coordinates $(0, t_a)$ to $(0, t_b)$.

Before we start, I will use the notation by [31] and denote the fluctuations $\delta x(t)$ as $\eta(t)$. Without loss of generality, I will also take a Lagrangian $L = \frac{1}{2} a(t) \dot{\eta}^2 - b(t) \eta^2 + \gamma \eta(t) \dot{\eta}(t)$. We are left with calculating:

$$G(0 t_b | 0 t_a) = [D \eta(t)] \exp \left\{ \frac{i}{\hbar} \int \frac{1}{2} a(t) \dot{\eta}^2 - b(t) \eta^2 + \gamma \eta(t) \dot{\eta}(t) dt \right\}. \quad (B.1)$$

If we integrate the $\gamma$ term by parts, this vanishes because at the end points $\eta(t) = 0$. So we are only left with quadratic terms. Following [31]:

$$G(0 t_b | 0 t_a) = [D \eta(t)] \exp \left\{ \int \frac{1}{2} a(t) \dot{\eta}^2 - b(t) \eta^2 dt \right\}. \quad (B.2)$$

We will slice the infinite sum over paths $N$ times again, such that the action reads:

$$S_N = \frac{1}{2\epsilon} \sum_{k=1}^{N} \left[ a_k (\eta_k - \eta_{k-1})^2 - \epsilon^2 b_k \eta_k^2 \right], \quad (B.3)$$

where the subscript $k$ refers to the values of the constant at that particular time. With this, we can write the propagator as

$$G_N(0 t_b | 0 t_a) = A_N \int \exp \left\{ i \alpha \eta \cdot P \eta \right\}, \quad (B.4)$$

where $P$ is a Hermite matrix with elements defined by equation (B.3), $\alpha = (2\hbar\epsilon)^{-1}$ and $\eta$ a vector with components representing the value of $\eta$ at a particular time. This matrix can be diagonalised by a unitary matrix $A$. Define $\eta = A \mu$, perform the Gaussian integrals and we find

$$G_N(0, t_b | 0, t_a) = \left( \frac{D_N}{i \pi} \right)^{1/2}; \quad D_N = \left( \prod_{k=1}^{N} a_k \right) \frac{\alpha}{\det P}. \quad (B.5)$$
We will now take a continuum limit: send $N \to \infty$ and consequently $\epsilon \to 0$. In order to evaluate $\det P$ we use that the matrix is tridiagonal and that the $k$-th minor (determinant of a small space of a matrix, $2 \times 2$ for instance) $\Delta_k$ must satisfy a recurrence relation

$$\Delta_k = (a_k + a_{k+1} - b_k \epsilon^2)\Delta_{k-1} - a_k^2 \Delta_{k-2}. \quad (B.6)$$

Using the continuum analogue of this (which transforms into a differential equation) and defining $\Delta_k = \frac{1}{\epsilon} \left( \prod_{j=1}^{k+1} a_j \right) \psi_{k+1}$ we get

$$\frac{d}{dt}(a \dot{\psi}) + b \psi = 0, \quad (B.7)$$

with initial conditions $\psi(t_a) = \psi^a = 0$ and $\dot{\psi}(t_a) = 1/\sqrt{a}$. We can solve an associated differential equation for variables $v = \psi \sqrt{a}$. With this one can calculate the value of $D_N$ with $N \to \infty$ to be

$$D = \frac{((\dot{\psi}_1^a)^2 a(t_a) a(t_b))^{1/4}}{\sqrt{2 \hbar \psi_1^b}}, \quad (B.8)$$

such that the propagator can be written as

$$G(x_b, t_b | x_a, t_a) = \left( \frac{(\dot{\psi}_1^a)^2 a(t_a) a(t_b)}{2 \pi \hbar \psi_1^b} \right)^{1/4} \exp \left\{ \frac{i}{\hbar} S_{cl} \right\}. \quad (B.9)$$

If we now calculate the value of the classical action, we can first express the classical path as

$$x_{cl}(t) = \frac{1}{\sqrt{a}} \left( \frac{\sqrt{a(t_a)} x^a v_2}{v_2^a} + \frac{\sqrt{a(t_b)} x^b v_1}{v_1^b} \right). \quad (B.10)$$

Then we use this path to calculate the classical action, which (using that it can be written as $S_{cl} = F_a x_a^2 + F_b x_b^2 + F_{ab} x_a x_b$) has a term

$$F_{ab} = -\frac{\sqrt{a(t_a)} a(t_b) \dot{\psi}_1^a}{v_1^b}. \quad (B.11)$$

And now, one can conclude that:

$$F(t_a, t_b) = \left[ -\frac{1}{2i\pi \hbar} \frac{\partial^2 S_{cl}}{\partial x_b \partial x_a} \right]^{1/2}, \quad (B.12)$$

which is the Pauli-van Vleck formula. Note that also for a force this holds: a force changes the classical action only linearly and does not change the second derivative. This is precisely what we want, because in appendix A it is shown that such a force term does not enter the fluctuation part. For a more detailed proof or further reading on the Pauli-van Vleck formula see [19, 21–23, 31].

67
C. Energy levels

In this appendix we would like to calculate the energy levels of a basis set of a general Hamiltonian:

\[ H = \frac{1}{2} \left[ X(t)p^2 + Y(t)(qp + pq) + Z(t)q^2 \right]. \]  

(C.1)

We know the specific set of wave functions, so calculating the energy is just a matter of calculating:

\[ \langle \Psi_n | H | \Psi_n \rangle. \]  

(C.2)

Which can be split in three contributions: \( \langle V \rangle \) is the potential part of the Hamiltonian, \( \langle T \rangle \) the kinetic and \( \langle M \rangle \) comes from the 'mixed term' \( \langle qp + pq \rangle \). We know that a set of wave functions can be written as:

\[ \Psi_n(q,t) = \sqrt{\frac{1}{2^n n! \pi \hbar}} \eta(t) \frac{X(t)}{X(t)} \frac{1}{2} \left[ \frac{Z(t)}{X(t)} - \frac{Y(t)q^2}{2 \hbar X(t)} \right] e^{-i(n+1/2)\phi(t)} \times \]

\[ H_n \left( \frac{\eta(t)}{\hbar X(t)} q \right) \times \exp \left\{ - \frac{\eta(t)}{2\hbar X(t)} q^2 \right\} \]

\[ \exp \left\{ i \left[ \frac{\delta(t) - \gamma(t)}{2\hbar X(t)} - \frac{\gamma(t)}{2\hbar} \right] q^2 \right\}. \]  

(C.3)

So we have to calculate integrals over products of exponents and Hermite polynomials. We use the following properties:

\[ \int_{-\infty}^{\infty} \exp(-x^2)H_n(x)H_m(x)dx = \delta_{n,m}n!2^n \sqrt{\pi}, \]

\[ \frac{\partial H_n(x)}{\partial x} = 2nH_{n-1}(x), \]

\[ H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \]

\[ \int_{-\infty}^{\infty} x^2 \exp(-x^2)H_n(x)^2dx = (n+1/2)\sqrt{\pi}2^n n!, \]  

(C.4)

to find that:

\[ \langle V \rangle = \frac{\hbar X(t)}{\eta(t)} \left( \frac{1}{2} \left[ \frac{Z(t)}{X(t)} - \frac{Y^2(t)}{X(t)} \right] \right), \]

\[ \langle T \rangle = \left( \frac{\eta(t)}{\eta(t)} + \frac{\delta(t)^2}{\eta(t)} - \frac{2Y(t)\delta(t)}{\eta(t)} + \frac{Y(t)^2}{\eta(t)^2} \right) \frac{\hbar}{2}(n+1/2), \]

\[ \langle M \rangle = \frac{\hbar Y(t)}{\eta(t)} (\delta(t) - Y(t)) (n+1/2). \]  

(C.5)
And if we combine those we find the energy spectrum to be:

\[ E_n(t) = \hbar \Omega(t) \left[ n + \frac{1}{2} \right], \]

where we introduced the time-dependent frequency:

\[ \Omega(t) = \frac{\eta(t)}{2} + \frac{X(t)Z(t) - Y^2(t)}{2\eta(t)} + \frac{\delta(t)^2}{2\eta} \]

(C.6) (C.7)
D. Derivation of the equation of motion

The equation of motion is most easily derived by starting from the original Hamiltonian (3.10). Starting from the dimensionless Hamiltonian would complicate matters enormously, although the result will be the same. We perform a Legendre transform on (3.10) and find:

\[ L = \frac{1}{2} \left( \frac{\hbar^2}{B(t) N \sigma} \dot{S}^2 - \frac{2J}{N} S^2 \right). \]  
(D.1)

Dividing by \( E_{\text{thin}} \) and inserting that \( B(t) = B_f \frac{t}{t_f} \) we find that:

\[ \frac{L}{E_{\text{thin}}} \equiv \mathcal{L} = \frac{1}{2} \left( \frac{t^2}{t_f} \omega_f \dot{S}^2 - \omega_f S^2 \right). \]  
(D.2)

Now substituting \( S = \sqrt{\omega_f} S \) and \( t = \frac{t}{\tau} \) results in:

\[ \mathcal{L} = \frac{1}{2} \left( \frac{t}{t_f} \left( \frac{\partial S}{\partial \tau} \right)^2 - S^2 \right) \]  
(D.3)

And by using the Euler-Lagrange equation we find the Euler-Lagrange equation of motion to be:

\[ \frac{t_f}{t} \frac{\partial^2 S(t)}{\partial \tau^2} - \frac{t_f}{t^2} \frac{\partial S(t)}{\partial \tau} + S = 0. \]  
(D.4)
E. Derivation of $\omega_r$ and the $\gamma_1(S, t)$ state

We set out to find an easier expression for:

$$
\gamma_1(t) = \sum_{n=2k+1}^{\infty} \tilde{c}_n \chi_n^d(\omega_d(t), \Delta(t)) \exp \left\{ i\Delta(t)S^2/2 \right\} \exp \left\{ -i(\phi(t) - \phi(t_{in}))3/2 \right\}, \quad (E.1)
$$

where $k = 0, 1, etc.$ We should now realise that the coefficients $\tilde{c}_n$ are defined by:

$$
\Psi(t_{in}) = \sum_{n=2k+1}^{\infty} \tilde{c}_n(R, R_{\Delta}) \chi_n(\omega_{id}(t_{in})) \exp \left\{ i\Delta(t)S^2/2 \right\}.
$$

We can generalise this formula to:

$$
\chi_1(\omega_0) = \sum_{n=2k+1}^{\infty} \tilde{c}_n(\omega_1, \omega_0, \omega_i) \chi_n(\omega_0) \exp \left\{ i\Delta_1S^2/2 \right\}, \quad (E.2)
$$

for any function $\omega_1, \omega_0, \Delta_1$. If we now choose the proper values of $\omega_1, \omega_0, \Delta_1$, by observing the definition of $\gamma_1(t)$:

$$
\omega_1 = \omega_d(t), \\
\omega_0 = \omega_1 \frac{\omega_d(t)}{\omega_d(t_{in})}, \\
\Delta_1 = R \Delta_0 = \frac{\Delta(t_{in})}{\omega_d(t_{in})},
$$

we will find that:

$$
\gamma_1(t) = \chi_1(\omega_r(t)) \exp \left\{ i(\Delta(t) - \Delta_r(t))S^2/2 \right\} \exp \left\{ -i(\phi(t) - \phi(t_{in}))3/2 \right\} \quad (E.5)
$$

with,

$$
\omega_r(t) = \frac{\omega_d(t)}{\omega_d(t_{in})}, \\
\Delta_r(t) = \frac{\omega_r(t)}{\omega_i(t_{in})} \Delta(t_{in})
$$

rescaled parameters.
Bibliography


[22] W. Pauli, Ausgewalte Kapitel der Feldquantisierung (Lecture notes), pp. 139-52.


