Quantum Phase Transitions In Spin Models

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Abstract

This work focuses on the concept of Quantum Phase Transitions (QPT) applied to the Ising model in a transverse field. After a discussion on what QPT are and why they are useful, an exact derivation of QPT on the Ising model is provided, as well as an extension to the continuum space. A discussion of the Schwinger bosons mean-field theory (SBMTF) applied to the same Hamiltonian is also given. The SBMFT method proves unsuccessful to predict the quantum phase transition present in the Ising model, but the same approximation applied to the antiferromagnetic Heisenberg model in one dimension is found to give qualitatively correct results.

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Foreword

This Master of Science Thesis is dedicated to the world of Quantum Phase Transitions; what they are, how to deal with them. The work is basically divided into two parts: the first one covers chapters 1 and 2 and is focused on introducing the reader to the concept of QPT, and the second part, chapter 3, gives an introduction to the Schwinger boson mean-field theory as an approximate method to calculate QPT.

In part one, the main idea is to give a general impression of what QPT are, by giving a definition and making a comparison with classical phase transitions. It is also shown that QPT need a new theory to treat them, since applying classical methods is not possible. Chapter 2 gives then an example of a quantum phase transition, the one present in the Ising model in a transverse field. This part basically follows the work by Sachdev, [1], but it is aimed towards a more detailed understanding of the concepts, and a thorough and complete derivation of the formulas, so that for example undergraduate students can follow their way throughout the book. The exact spectrum for the Ising Hamiltonian with a transverse field is given, together with the recipe for how to draw the quantum phase diagram for this model, a necessary step if one wants to visualize the physics behind the numbers.

Part two is focused on Schwinger boson mean-field theory as an example of an approximate theory to calculate quantum phase transitions. It is *a priori* not the best choice, because mean-field theories are known to work properly only around well-behaved points, but it is also a good chance to learn about this powerful approximate method and, besides, some qualitatively correct results are found. This second part is not as rich in details as the first one, since otherwise this thesis would be twice as big as it is now, but further details can be found in the literature given in the Bibliography.

Contents

Chapter 1

Introduction

1.1 What is a Quantum Phase Transition?

The notion behind a phase transition in classical physics is, as we know, a rapid change in the properties of a material, triggered by the variation of some physical parameter, such as temperature. Easily comes to one's mind the vapour that goes out of a bowl when we boil water: at atmospheric pressure, as temperature increases up to 373 K, water undergoes a phase transition from liquid to vapour.

A convenient way to characterise a phase transition is by using an *order parameter*, ϕ. It is a quantity constructed from some of the physical variables describing the system, and it has the particularity that it is non-zero in one of the phases and zero in the other[1]. For the example above, this is

$$\phi = \rho_l - \rho_g \tag{1.1}$$

where ρ is the density and the subindices l and g refer to the liquid and the gaseous phase, respectively. Other phase transitions are not so quotidian. In the case of a ferromagnet, where the transition to a paramagnetic phase is driven by the increase of spin flipping as the temperature goes up, the order parameter is the magnetisation.

Quantum phase transitions (QPT) are analogous to their classical counterparts, but taking place at $T = 0$, when the system is in its ground state.

[1] This is the Landau order parameter; other combinations are possible: positive in one phase and negative in the other, etc. For our further purposes, it is important to follow Landau's definition.

We say that a quantum phase transition is present when the ground state energy diverges or has some other kind of non-analiticity[1]. For instance, the Ising model in a transverse field, with the Hamiltonian

$$H_I = -Jg\sum_i \hat{\sigma}_i^x - J\sum_{<ij>} \hat{\sigma}_i^z \hat{\sigma}_j^z \,, \tag{1.2}$$

has a parameter g that can be "tuned" up and down and, as we will see, the system undergoes a phase transition at g=1 (Let us not worry about the details of the Hamiltonian at this point; we will get back to it soon). The phase transition, though, is a little strange in this case compared to its classical relatives: the phase space in which the transition appears is composed of a physical magnitude, the temperature, and a *dimensionless* quantity g. Since the value of g determines the phase at T=0, an order parameter can be constructed from g for this quantum phase transition:

$$\phi = \theta(\mathrm{g} - 1) \,. \tag{1.3}$$

Here, θ is the theta function, which is equal to 1 for a positive argument and equal to 0 if the argument is negative.

Another characteristic of QPT is, as explained above, that they occur at T=0. This may sound strange: why should we deal with something so unphysical, then? The answer to this question is that, as we will see in chapter 2, *the phase transition at T=0 has an influence on the system at higher temperatures.*

1.2 Classical mapping of quantum phase transitions

Classical and quantum phase transitions have much more in common than what one could expect *a priori* after having seen the two examples given in the previous section. Actually, QPT in N dimensions can be mapped onto ordinary, classical, N+1-dimensional phase transitions [1, 2].

Let us start with the classical partition function

$$Z(\beta) = \mathrm{Tr}\, \mathrm{e}^{-\beta H} = \sum_n \langle n|\mathrm{e}^{-\beta H}\,|n\rangle \,, \tag{1.4}$$

with

$$\beta = \frac{1}{k_B T} \,.$$

Notice that the (classical) density matrix operator, $e^{-\beta H}$, is the same as the (quantum) time evolution operator $e^{-iH\tau/\hbar}$ if we set

$$\tau = -i\hbar\beta \tag{1.5}$$

as the considered time interval. This implies that (1.4) can be regarded either as a classical partition function or as a quantum time evolution, provided that we use the *imaginary time* (1.5) in this latter case.

Suppose now that we take (1.4) to be a quantum expression in imaginary time. By virtue of the Feynman path integral formalism [3, 4], we can interpret the exponent in the rightmost expression in (1.4) as the transition amplitude to go from $\langle n|$ to $|n\rangle$. Also, the same formalism tells us that this amplitude can be calculated by summing all the amplitudes for all possible paths starting and ending at $|n\rangle$. Thus we take a very small time interval, $\delta\tau$, and a very large integer, N, such that $N\delta\tau = \hbar\beta$, and expand the exponential in N terms; formally,

$$e^{-\beta H} = \left(e^{-\frac{1}{\hbar}\delta\tau H}\right)^N . \tag{1.6}$$

Let $|m_1\rangle, ..., |m_N\rangle$ be the states at points 1,..., N respectively, in which we have divided the trajectory between the starting and ending kets. We insert (1.6) into (1.4) and use the resolution of the identity at each point 1,..., N to get:

$$Z = \sum_n \sum_{m_1 ... m_n} \langle n| e^{-\frac{1}{\hbar}\delta\tau H} |m_1\rangle \langle m_1| e^{-\frac{1}{\hbar}\delta\tau H} |m_2\rangle \langle m_2| ... |m_N\rangle \langle m_N| e^{-\frac{1}{\hbar}\delta\tau H} |n\rangle . \tag{1.7}$$

This is then the ordinary quantum expression for the time evolution of an N-dimensional system. Now, if we insert the expression $\tau \to it$ for the imaginary time[2] into (1.7), we recover an ordinary N+1-dimensional classical partition function, with one exception: the N+1-th dimension, the imaginary time, has a finite extent: $\hbar\beta$ units of time. This looks strange, but things get better as we set T tending to zero: this way, β tends to infinity and the once "anomalous" dimension goes to infinite size as the rest. Therefore, there exists a mapping of quantum, N-dimensional systems into classical, N+1-dimensional systems.

[2]Notice that this is the same expression as (1.5) if we set $\tau = 1/k_B T$. This suggests that the temperature plays the role of an inverse imaginary time in this formalism.

1.3 Why study QPT?

If we can map quantum systems onto classical mechanics, why bother trying to learn QPT from scratch?

This question was answered by the first physicists that dealt with QPT in this fashion: we shouldn't [5]. Anything we can learn is already contained in the classical formalism. Subir Sachdev was one of the first who realised [1] that this is, by far, not true:

- Our mapping between classical and quantum transitions is made possible by introducing imaginary time. This seems very reasonable if we look at (1.6), but this does not mean that going back to real time after getting the results in the classical, N+1-dimensional mapping will produce a real, physical results for the quantum system. Actually, this strategy has proven to fail for most systems when we take $T > 0$.

- Quantum critical points usually map onto classical critical points that are very hard to treat. In many cases, the classical problem has complex-valued Boltzmann weights, which is a consequence of the quantum mechanics that lies behind the problem. This makes the classical mapping very difficult because the solution found may have no analogy with any well-known classical problem.

- Even if the critical point has a good classical analogue, the geometry for the problem is quite difficult to handle for $T > 0$: as we may recall from section 1.2, the phase space in this case has N infinite-length dimensions and one (the imaginary time) that is finite; so, if $N = 1$, we would have a kind of rectangle as the phase space, with a certain, finite heigth, but infinite length. This is, at least, unusual, and it is quite difficult to find any existing results in this geometry, so we are often forced to work out everything from scratch.

So *we do need to learn QPT*. This does not mean that certain simple systems cannot be solved using the mapping to classical statistical physics (for instance, a 1-D array of Josephson junctions; see [2]), but more powerful methods are required in general.

Now that we are familiar with the concepts of QPT, we shall introduce a particular method that has proven useful to study QPT. This will be done in the next chapter, where we will see the way it operates by applying it to the Ising model in a transverse field.

Chapter 2

The 1-D Ising model in a transverse field

2.1 Generalities

This chapter will follow Sachdev's calculations [1] for the Ising model in one dimension, but thoroughly filling in the numerous gaps present in the cited book. We will derive the (T=0) quantum phase transition present in the Ising model when a magnetic field is present, and see that it also influences the physics at finite ($T > 0$) temperatures.

We have already mentioned the Ising model in section 1.1, as an example of a model with a quantum phase transition. Let us now take a deeper look at it.

The Ising model was introduced by Ernst Ising, who further developed an idea [6] of his teacher Lenz. This model is an attempt to describe the microscopic behaviour of magnetic materials [7, 8]. It assumes that every site in the system has only two possible orientations for its spin (either "up" or "down") and that there is an interaction only between nearest neighbours. Despite the simplicity of this model, it gives fairly good results for some problems and it is still nowadays a tool-of-the-trade for physicists.

By adding a field perpendicular to the spin orientation (that is, in the "transverse" direction) we obtain the 1-D *quantum Ising Hamiltonian*, already encountered in equation (1.2):

$$H_I = -Jg \sum_i \hat{\sigma}_i^x - J \sum_{<ij>} \hat{\sigma}_i^z \hat{\sigma}_j^z \,. \tag{2.1}$$

To be more specific, this is *one* of the possible representations of the Ising Hamiltonian with a transverse field, depending on the way we have defined the spin axes. This particular choice will simplify the calculations later on. In contrast to the ordinary Ising Hamiltonian (with g=0), equation (2.1) defines a *quantum* model since it contains non-commuting operators.

The coefficient g has already been presented; it is a parameter that can be tuned from zero to infinity and that presents a criticality for a certain value – this is what we will derive soon. J is a positive number that, as can be seen from dimensional analysis, depends on the energy available to the system, and $\hat{\sigma}^{x,z}$ are the ordinary Pauli matrices. The subindices i, j refer to the sites in the lattice, and the notation $< ij >$ indicates nearest-neighbour pairs.

First of all, let us rewrite (2.1) in a more practical way:

$$H_I = -J \sum_i \left(g\hat{\sigma}_i^x + \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z \right). \tag{2.2}$$

The idea of "sum over nearest-neighbours" might seem a little concealed in (2.2) because of the single sum, but it is not difficult to see that (2.2) is in fact equivalent to (2.1).

Now we are ready to begin.

2.2 Limiting cases at T=0

As the parameter g in (2.2) ranges from zero to infinity, it is convenient to take a quick look at the limiting cases $g \ll 1$ and $g \gg 1$, to see what the spectrum is in these limits. This is useful because it will give an intuitive physical picture of what happens with this model at T=0 .

2.2.1 g≫1

If g is very big, then the sum over nearest neighbours in (2.2) can be neglected, so that the Hamiltonian becomes:

$$H_I \simeq H_{I\gg} \equiv -J \sum_i g\hat{\sigma}_i^x \,. \tag{2.3}$$

Here is a reminder of how the eigenvectors of $\hat{\sigma}_i^x$ look in the basis of $\hat{\sigma}_i^z$:

$$|\rightarrow\rangle_i = \frac{(|\uparrow\rangle_i + |\downarrow\rangle_i)}{\sqrt{2}}\,,$$

$$|\leftarrow\rangle_i = \frac{(|\uparrow\rangle_i - |\downarrow\rangle_i)}{\sqrt{2}}\,.$$

One sees immediately that (2.3) has

$$|0\rangle = \prod_i |\rightarrow\rangle_i \tag{2.4}$$

as the ground state[1]. The first excited states are also evident:

$$|i\rangle = |\leftarrow\rangle_i \prod_{j\neq i} |\rightarrow\rangle_j\,. \tag{2.5}$$

We will define the *particle number* as the number of flipped sites in a state, that is, the number of times that $|\leftarrow\rangle_i$ appears in the ket. For example, $|0\rangle$ has particle number zero, $|i\rangle$ has particle number one, and it is apparent from (2.5) that we can analogously construct states with any particle number, up to N, the number of sites in the lattice.

A quick peek indicates that, since all kets, regardless of their particle number, are proper vectors of $H_{I\gg}$, these kets will remain static for ever and ever. To make things more interesting, we must allow $\hat{\sigma}_i^z$ to intervene[2].

As g$\gg$1, we will neglect order $1/g$ and smaller ($1/g^2$, etc.), which can be achieved by not taking into consideration mixing of states with different particle numbers. This assertion can be easily proven by looking at perturbation theory. Let us set $H_I = H_0 + H_1$, with

$$H_0 = -Jg \sum_i \hat{\sigma}_i^x\,, \tag{2.6}$$

$$H_1 = \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z\,. \tag{2.7}$$

[1]Notice that, although apparently (2.4) could also have been constructed with the other eigenvector of $\hat{\sigma}_i^x$,$|\leftarrow\rangle_i$, this ket has eigenvalue -1 and this would *maximise* the energy in (2.3), thus not leading to a ground state.

[2]$\hat{\sigma}_i^z\,|\rightarrow\rangle_i = |\leftarrow\rangle_i\,,\hat{\sigma}_i^z\,|\leftarrow\rangle_i = |\rightarrow\rangle_i$, hence mixing of states with different particle number is made possible by this operator.

According to second-order perturbation theory, the eigenvalues E_n of H_I can be approximated by

$$E_n \simeq E_n^0 + \langle n \left| H_1 \right| n \rangle + \sum_{m \neq n} \frac{\left| \langle n \left| H_1 \right| m \rangle \right|^2}{E_n^0 - E_m^0} \,, \tag{2.8}$$

where $|n\rangle$ and $|n\rangle$ are one-particle eigenkets of H_0 and E_n^0 are the eigenvalues of H_0.

It is clear from (2.6) that the eigenvalues of H_0, E_n^0, are proportional to g, whereas from (2.7) we see that the matrix elements of H_1 do not depend on g. Therefore, the sum over m in (2.8) is proportional to $1/g$. This sum mixes states with different particle number, thus our assertion that this mixing would lead to order $1/g$ is proven.

Let us go back to our main problem. Now that we have finally brought $\hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$ to the scene, an off-diagonal matrix term appears. Taking $|\rightarrow\rangle_{j \neq i}$ as a shorthand for $\prod\limits_{j \neq i} |\rightarrow\rangle_j$, we have:

$$\begin{aligned} \langle i | - J \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z \left| i+1 \right\rangle &= -J \left\langle \rightarrow \right|_{j \neq i} \left\langle \leftarrow \right|_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z \left| \leftarrow \right\rangle_{i+1} \left| \rightarrow \right\rangle_{k \neq i+1} \\ &= -J \left\langle \rightarrow \right|_{j \neq i} \left\langle \rightarrow \right|_i \left| \rightarrow \right\rangle_{i+1} \left| \rightarrow \right\rangle_{k \neq i+1} = -J \left\langle 0 \right| \left. 0 \right\rangle = -J \,. \end{aligned} \tag{2.9}$$

Hence,

$$\langle i | \, H_I \left| i+1 \right\rangle = -J \tag{2.10}$$

since $\langle i | \, \hat{\sigma}_j^x \left| i+1 \right\rangle = 0$ for all j.

We can recover a diagonal form for H_I if we go to momentum space:

$$|k\rangle = \frac{-J}{\sqrt{N}} \sum_j \mathrm{e}^{ikx_j} \left| j \right\rangle \tag{2.11}$$

(remember that N is the number of lattice sites).

Let us now introduce a notation to further simplify the formulae: a Pauli eigenket symbol with no subindex appearing together with indexed eigenkets means that the rest of the single-site kets not specified are of the kind indicated by the ket without subindex. For example,

$$\left| \rightarrow \right\rangle_i \left| \rightarrow \right\rangle_{i+1} \left| \leftarrow \right\rangle \equiv \left| \rightarrow \right\rangle_i \left| \rightarrow \right\rangle_{i+1} \prod_{j \neq i,\, i+1} \left| \leftarrow \right\rangle_j \,. \tag{2.12}$$

Thus, in our new notation, $|j\rangle \equiv |\leftarrow\rangle_j |\rightarrow\rangle$.

If H_I acts on $|k\rangle$, we get:

$$H_I |k\rangle = \frac{-J}{\sqrt{N}} \sum_{i,j} \left(g\hat{\sigma}_i^x + \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z \right) \mathrm{e}^{ikx_j} |\leftarrow\rangle_j |\rightarrow\rangle$$

$$= \frac{-J}{\sqrt{N}} \sum_{i,j} \left(g(N-1) |k\rangle + (-g) |k\rangle \right) \mathrm{e}^{ikx_j}$$

$$+ \frac{-J}{\sqrt{N}} \sum_j \mathrm{e}^{ikx_j} \left(\sum_{i \neq j, j+1} |\leftarrow\rangle_j |\leftarrow\rangle_i |\leftarrow\rangle_{i+1} |\rightarrow\rangle + |\leftarrow\rangle_{j+1} |\rightarrow\rangle + |\leftarrow\rangle_{j-1} |\rightarrow\rangle \right). \tag{2.13}$$

The term $|\leftarrow\rangle_j |\leftarrow\rangle_i |\leftarrow\rangle_{i+1} |\rightarrow\rangle$ has particle number 3 and, since to $\mathcal{O}(1/g)$ we do not have to consider mixing of states with particle numbers 1 and 3, we shall neglect it.

Let a be the lattice constant. Then, up to order 1/g, we have:

$$H_I |k\rangle = -Jg(N-2) |k\rangle + \frac{-J}{\sqrt{N}} \mathrm{e}^{-ika} \sum_j \mathrm{e}^{ik(x_j+a)} |j+1\rangle$$

$$+ \frac{-J}{\sqrt{N}} \mathrm{e}^{ika} \sum_j \mathrm{e}^{ik(x_j-a)} |j-1\rangle = -Jg\,(N-2) |k\rangle - J\,\mathrm{e}^{-ika} |k\rangle - J\,\mathrm{e}^{ika} |k\rangle\,.$$

Using that $x_j + a = x_{j+1}$, $x_j - a = x_{j-1}$, we obtain

$$H_I |k\rangle = (-Jg(N-2) - 2J\cos ka) |k\rangle\,. \tag{2.14}$$

It is convenient to set the energy of the ground level to zero; this amounts to add JgN to the eigenvalue of H_I. This is of course permitted, since it only means that we change the zero for the energy. So we finally get

$$\epsilon_k = Jg \left(2 - \frac{2}{g} \cos ka + \mathcal{O}\left(\frac{1}{g^2} \right) \right) \tag{2.15}$$

as the eigenvalues for H_I when $g \gg 1$.

2.2.2 g≪1

This limit corresponds to neglecting the sum over $\hat{\sigma}_i^x$ in (2.2):

$$H_I \simeq H_{I\ll} \equiv -J \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z \,. \tag{2.16}$$

Now there are two possible ground states: $|\uparrow\rangle = \prod_i |\uparrow\rangle_i$ and $|\downarrow\rangle = \prod_i |\downarrow\rangle_i$, because both give a minimum for the energy. This suggests that it is not important whether the spins point up or down; what really matters is if two neighbouring spins are of the same kind or not. If they are, the energy is minimised, just as in the ground state. But if we want to flip a spin, extra energy is needed. Notice also that the state

$$|a\rangle_i \equiv |\uparrow\rangle_1 |\uparrow\rangle_2 \cdots |\uparrow\rangle_{i-1} |\downarrow\rangle_i |\downarrow\rangle_{i+1} \cdots |\downarrow\rangle_N \tag{2.17}$$

is more energetically favourable than

$$|b\rangle_i \equiv |\uparrow\rangle_1 |\uparrow\rangle_2 \cdots |\uparrow\rangle_{i-1} |\downarrow\rangle_i |\uparrow\rangle_{i+1} \cdots |\uparrow\rangle_N \,, \tag{2.18}$$

because in $|b\rangle_i$, going from left to right, the spins are flipped twice, whereas in $|a\rangle_i$ only once. The site where there is a transition from a spin of one type to the other is called a *domain wall*. Domain walls act as quasi-particles; one just has to apply H_I to $|a\rangle_i$ to see it: when $\hat{\sigma}^x$ acts on a spin next to a domain wall, the spin is flipped and thus the domain wall moves.

The Hamiltonian can be diagonalised in the same way as for $g \gg 1$, that is, passing to momentum space:

$$|k\rangle = \frac{-J}{\sqrt{N}} \sum_j \mathrm{e}^{ikx_j} |a\rangle_j \,, \tag{2.19}$$

$$H_I |k\rangle = \frac{-J}{\sqrt{N}} \sum_{i,j} \left(g\hat{\sigma}_i^x + \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z \right) \mathrm{e}^{ikx_j} \prod_{l=1}^{j-1} \prod_{m=j}^{N} |\uparrow\rangle_l |\downarrow\rangle_m$$

$$= (N-2)|k\rangle + \frac{-J}{\sqrt{N}} \sum_j \mathrm{e}^{ikx_j} \left(\prod_{l=1}^{j-2} \prod_{m=j-1}^{N} + \prod_{l=1}^{j} \prod_{m=j+1}^{N} \right) g\, |\uparrow\rangle_l |\downarrow\rangle_m + O(g^2) \,,$$

where all the terms that give extra domain walls have been ignored. So

$$H_I |k\rangle = -J \left((N-2) + g(\mathrm{e}^{ika} + \mathrm{e}^{-ika}) \right) |k\rangle \,,$$

hence the eigenvalue (having added JN to make the energy of the ground state zero) is:

$$\epsilon_k = 2J(1 - g\cos ka) \tag{2.20}$$

if we neglect orders higher than g.

Notice that the presence of domain walls implies that there is a correlation between the spins of two sites that are very far away; depending on the number of domain walls in between, the spins will point in the same or opposite directions.

2.3 Exact spectrum

After having obtained a general picture of what happens in some limiting cases, now it is time to deal with the full problem. This requires a lot more work, but the bounty waiting at the end of the road is a quantum phase transition for g=1.

All steps will be carried out with great detail, except those that are simple substitutions and hence should cause no further problems.

2.3.1 Jordan-Wigner transformation

The Jordan-Wigner transformation is a mapping between a model with spin-1/2 per site and another model describing the hopping of spinless fermions between sites with single orbitals. It is based on the following observation: if we have a lattice of spinless atoms that have an orbital which can be full or empty, we can *assign* the state $|\uparrow\rangle_i$ to represent an empty orbital at the i-th site and the state $|\downarrow\rangle_i$ if the i-th atom has an occupied orbital.

Since, $|\uparrow\rangle_i$ and $|\downarrow\rangle_i$ have eigenvalues +1 and -1 respectively when acted upon by σ_i^z, the mapping

$$\hat{\sigma}_i^z = 1 - 2N = 1 - 2c_i^\dagger c_i\,, \tag{2.21}$$

where c_i is the annihilation operator for the spinless state, will do the job, because it has value 1 if N=0 and -1 if N=1. Furthermore, since c_i flips the spin from down to up, and $c_i^\dagger$ does the opposite, we can identify

$$\left.\begin{array}{l} c_i \rightarrow \hat{\sigma}_i^+ = \frac{\hat{\sigma}_i^x + i\hat{\sigma}_i^y}{2} \\ c_i^\dagger \rightarrow \hat{\sigma}_i^- = \frac{\hat{\sigma}_i^x - i\hat{\sigma}_i^y}{2} \end{array}\right\}\,. \tag{2.22}$$

There is a problem, though: this works for one site, but not for several, because the spinless fermionic operators on two different sites anticommute, whereas the spin operators commute. The solution was found by Jordan and Wigner [9], who showed that the following transformation works also for two different sites :

$$\begin{aligned} \hat{\sigma}_i^+ &= \prod_{j<i} (1 - 2c_j^\dagger c_j) c_i \\ \hat{\sigma}_i^- &= \prod_{j<i} (1 - 2c_j^\dagger c_j) c_i^\dagger . \end{aligned} \tag{2.23}$$

Using (2.21) and (2.22), it is easy to see that the inverse transformation is:

$$\begin{aligned} c_i &= \left(\prod_{j<i} \hat{\sigma}_j^z \right) \hat{\sigma}_j^+ \\ c_i^\dagger &= \left(\prod_{j<i} \hat{\sigma}_j^z \right) \hat{\sigma}_j^- . \end{aligned} \tag{2.24}$$

The usual (anti)commutation relations are fulfilled both by (2.23) and (2.24), as required.

The Jordan-Wigner transformation is often presented as in (2.23), but it is more convenient for our purposes to rotate the spin axes by 90° about the y axis, so that $z \to x$, $x \to -z$, and in this configuration the mapping becomes:

$$\begin{aligned} \hat{\sigma}_i^x &= (1 - 2c_i^\dagger c_i) \\ \hat{\sigma}_i^z &= - \prod_{j<i} (1 - 2c_i^\dagger c_i)(c_i + c_i^\dagger) . \end{aligned} \tag{2.25}$$

Substituting this into H_I in (2.1), leads to our first important result[3]:

$$H_I = -J \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i - 2g c_i^\dagger c_i + g \right) . \tag{2.26}$$

2.3.2 Bogoliubov transformation

There is one bad thing about the Hamiltonian in (2.26): it contains some terms that do not conserve the fermion number. It would be desirable to get rid of these terms, and the method that accomplishes this is called the Bogoliubov transformation [10].

[3]First edition (year 1999) of Sachdev's book has a misprint in the corresponding formula, (4.30). It has been corrected in the paperback edition from year 2001.

To use this transformation, we pass to momentum space, and write

$$c_k = \frac{1}{\sqrt{N}} \sum_j c_j \mathrm{e}^{-ikx_j} \tag{2.27}$$

with the inverse relation

$$c_j = \frac{1}{\sqrt{N}} \sum_k c_k \mathrm{e}^{ikx_j} \,. \tag{2.28}$$

We have to substitute (2.28) into (2.26), but this is not exactly straightforward, so let us take a close look at the process.

Using $x_{j+1} = x_j + a$, the first term becomes:

$$\begin{aligned} \sum_j c_j^\dagger c_{j+1} &= \sum_j \tfrac{1}{\sqrt{N}} \tfrac{1}{\sqrt{N}} \left(\sum_k c_k^\dagger \mathrm{e}^{-ikx_j} \right) \left(\sum_{k'} c_{k'} \mathrm{e}^{ik'x_{j+1}} \right) \\ &= \sum_j \tfrac{1}{N} \left(\sum_{k,\,k'} c_k^\dagger c_{k'} \mathrm{e}^{i(k'-k)x_j} \mathrm{e}^{ika} \right) = \sum_k c_k^\dagger c_k \mathrm{e}^{ika} \,, \end{aligned} \tag{2.29}$$

where the representation of the delta function, $\delta_{k\,k'} = \frac{1}{N} \sum_j c_k^\dagger c_{k'} \mathrm{e}^{i(k'-k)x_j}$ has been used to get rid of one of the summations.

Similarly, the second term is:

$$\sum_j c_{j+1}^\dagger c_j = \sum_j \frac{1}{N} \left(\sum_{k,k'} c_k^\dagger c_{k'} \mathrm{e}^{i(k-k')x_j} \mathrm{e}^{-ik'a} \right) = \sum_k c_k^\dagger c_k \mathrm{e}^{-ika} \tag{2.30}$$

so that the first two terms lead to

$$\sum_j \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) = \sum_k (2 \cos ka) c_k^\dagger c_k \,. \tag{2.31}$$

The third term is a little trickier. Let us begin with the identity

$$\begin{aligned} \sum_j c_j^\dagger c_{j+1}^\dagger &= \tfrac{1}{2} \sum_j \left(c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1}^\dagger \right) \\ = \tfrac{1}{2N} \sum_{j,k,k'} &\left(c_k^\dagger c_{k'}^\dagger \mathrm{e}^{-i(k+k')x_j} \mathrm{e}^{ik'a} + c_k^\dagger c_{k'}^\dagger \mathrm{e}^{-i(k+k')x_j} \mathrm{e}^{ik'a} \right) . \end{aligned} \tag{2.32}$$

The last equality contains two terms summed over k and k'; we make the substitution $k \to -k$ in the first of these terms, and $k' \to -k'$ in the second[4]:

$$\begin{aligned}\sum_j c_j^\dagger c_{j+1}^\dagger &= \sum_{j,k,k'} \tfrac{1}{2N} \left(c_{-k}^\dagger c_{k'}^\dagger \mathrm{e}^{-i(-k+k')x_j} \mathrm{e}^{ik'a} + c_k^\dagger c_{-k'}^\dagger \mathrm{e}^{-i(k-k')x_j} \mathrm{e}^{ik'a} \right) \\ &= \tfrac{1}{2} \sum_k \left(c_{-k}^\dagger c_k^\dagger \mathrm{e}^{ika} + c_k^\dagger c_{-k}^\dagger \mathrm{e}^{-ika} \right) . \end{aligned} \tag{2.33}$$

Since $\left\{ c_i^\dagger, c_j^\dagger \right\} = 0$, also $\left\{ c_{-k}^\dagger, c_k^\dagger \right\} = c_{-k}^\dagger c_k^\dagger + c_k^\dagger c_{-k}^\dagger = 0$, so that

$$c_{-k}^\dagger c_k^\dagger = -c_k^\dagger c_{-k}^\dagger . \tag{2.34}$$

Inserting this into (2.33) gives

$$\sum_j c_j^\dagger c_{j+1}^\dagger = \frac{1}{2} \sum_k c_{-k}^\dagger c_k^\dagger (\mathrm{e}^{ika} - \mathrm{e}^{-ika}) = \sum_k c_{-k}^\dagger c_k^\dagger i \sin ka . \tag{2.35}$$

And finally, the fourth term is analogously:

$$\sum_j c_{j+1} c_j = \sum_k c_{-k} c_k i \sin ka \tag{2.36}$$

So, (2.31), (2.35) and (2.36) inserted into (2.26) lead to:

$$H_I = J \sum_k \left(2[g - \cos ka] c_k^\dagger c_k - i \sin ka [c_{-k}^\dagger c_k^\dagger + c_{-k} c_k] - g \right) . \tag{2.37}$$

We have not yet got rid of the terms that do not conserve the fermion number. To do so, it is now time to introduce the Bogoliubov transformation:

$$\gamma_k = u_k c_k - i v_k c_{-k}^\dagger , \tag{2.38}$$

where u_k, v_k are real numbers such that $u_k^2 + v_k^2 = 1$, $u_{-k} = u_k$ and $v_{-k} = -v_k$.

The new operators defined by the transformation are also fermionic operators, since they fulfil the canonical anticommutation relations.

The inverse of (2.38) is

$$c_k = u_k \gamma_k + i v_k \gamma_{-k}^\dagger . \tag{2.39}$$

[4]This is possible because the sums over k and k' run over positive and negative values, so even after the substitution, the sums will go over all possible values.

This is to be inserted into (2.37), but choosing u_k, v_k so that the terms that violate fermion number conservation are killed off. We define

$$\left.\begin{aligned} u_k &= \cos\tfrac{\theta_k}{2} \\ v_k &= \sin\tfrac{\theta_k}{2} \end{aligned}\right\}. \tag{2.40}$$

A value for θ_k has to be found so that the undesired terms vanish. We should write down the explicit formula that results from inserting (2.40) into (2.37), set the coefficients that multiply the unwanted terms to zero and hence find the value that makes them disappear. This is in principle straightforward, but since the procedure is somewhat cumbersome, we will simply verify that the choice

$$\tan\theta_k = \frac{\sin ka}{(\cos ka) - g} \tag{2.41}$$

gives the desired result.

First things first. To avoid unnecessary pomposity, it is better to drop the subindex k, so that $c \equiv c_k, c_- \equiv c_{-k}$ and so on. With this notation, we substitute (2.39) into (2.37) and take a look at the individual terms inside the summation:

$$c^\dagger c = (u\gamma^\dagger - iv\gamma_-)(u\gamma + iv\gamma_-^\dagger) = u^2\gamma^\dagger\gamma + v^2\gamma^\dagger\gamma_-^\dagger - iuv(\gamma^\dagger\gamma_-^\dagger + \gamma_-\gamma). \tag{2.42}$$

Using $\left\{\gamma, \gamma^\dagger\right\} = 1$ and $\sum\limits_k \gamma^\dagger\gamma = \sum\limits_k \gamma_-^\dagger\gamma_-$ together with (2.40), we get

$$\begin{aligned} c^\dagger c &= (u^2 - v^2)\gamma^\dagger\gamma + v^2 - iuv(\gamma^\dagger\gamma_-^\dagger + \gamma_-\gamma) \\ &= (\cos\theta)\gamma^\dagger\gamma + \sin^2\tfrac{\theta}{2} - i\sin\tfrac{\theta}{2}(\gamma^\dagger\gamma_-^\dagger + \gamma_-\gamma)\,. \end{aligned} \tag{2.43}$$

Similarly,

$$c_-^\dagger c^\dagger + c_- c = u^2(\gamma_-^\dagger\gamma^\dagger + \gamma_-\gamma) + v^2(\gamma\gamma_- + \gamma^\dagger\gamma_-^\dagger) + i\sin^2\frac{\theta}{2}(2 - 4\gamma^\dagger\gamma)\,. \tag{2.44}$$

Inserting (2.41), (2.43) and (2.44) into (2.37) yields

$$\begin{aligned} H_I = J\sum_k 2(g - \cos ka)\left[\cos\theta\left(\gamma^\dagger\gamma - \tfrac{1}{2}\right) + \tfrac{1}{2}\right] + i\sin ka\cos\theta(\gamma^\dagger\gamma_-^\dagger + \gamma_-\gamma) + \\ i\sin ka\cos\theta\left(\gamma_-^\dagger\gamma^\dagger + \gamma\gamma_-\right) - g - 2\sin ka\sin\theta\left(\gamma^\dagger\gamma - \tfrac{1}{2}\right)\,. \end{aligned} \tag{2.45}$$

We group the terms containing the fermionic operators so that we can write some of them as anticommutators:

$$\begin{array}{c} H_I = J\sum\limits_k 2(g-\cos ka)\left[\cos\theta\left(\gamma^\dagger\gamma-\frac{1}{2}\right)+\frac{1}{2}\right]+ \\ i\sin ka\cos\theta\left(\left\{\gamma_-^\dagger,\gamma^\dagger\right\}+\{\gamma_-,\gamma\}\right)-g-2\sin ka\sin\theta\left(\gamma^\dagger\gamma-\frac{1}{2}\right)\ . \end{array} \tag{2.46}$$

Since the anticommutators vanish, we get rid of the unwanted terms:

$$H_I = 2J\sum_k\left[\left[(g-\cos ka)\cos\theta-\sin ka\sin\theta\right]\left(\gamma^\dagger\gamma-\frac{1}{2}\right)-\frac{1}{2}\cos ka\right]. \tag{2.47}$$

The sum $\sum\limits_k \cos ka$ also vanishes, since it runs over all possible k's. Hence,

$$H_I = \sum_k \epsilon_k\left(\gamma^\dagger\gamma-\frac{1}{2}\right), \tag{2.48}$$

where

$$\epsilon_k \equiv 2J\left((g-\cos ka)\cos\theta-\sin ka\sin\theta\right)\ . \tag{2.49}$$

Using (2.41) to express (2.49) as a function of k only, we obtain:

$$\begin{array}{c} \epsilon_k = 2J\cos\theta(g-\cos ka-\sin ka\tan\theta) \\ = -2J\cos\theta\left(\frac{\sin ka}{\tan\theta}+\sin ka\tan\theta\right) = -2J\frac{\cos\theta}{\tan\theta}\sin ka\left(1+\tan^2\theta\right) \\ = 2J\frac{\sin ka}{\cos\theta\tan\theta} = -2J\frac{\cos ka-g}{\cos\theta} = |-2J|\,|\cos ka-g|\sqrt{1+\tan^2\theta} \\ = 2\,|J|\sqrt{(\cos ka-g)^2+\sin^2 ka}\,, \end{array} \tag{2.50}$$

whence we get the final result[5]:

$$\epsilon_k = 2\,|J|\sqrt{1+g^2-2g\cos ka}\,. \tag{2.51}$$

We have taken J to be positive, so that the absolute value in (2.51) is actually redundant, but it is better to leave the formula like this for further purposes.

Notice that (2.51) is consistent with the limiting cases for g, (2.15) and (2.20).

[5]Formula 4.38 in Sachdev's book [1], that corresponds to this result, has an evident misprint, since it gives cos k, which is not dimensionally correct.

2.4 Physical interpretation and the quantum transition

Although (2.48) is expressed in terms of fermionic operators, it is more convenient to consider the particles as hard-core bosons, because the physical interpretation is easier in this case. Hard-core bosons are simply bosonic particles that can be regarded as "hard balls", so that the centres of two of these particles cannot be brought closer to each other than the distance of two radii. In other words, hard-core bosons cannot be "deformed" in any way, and the space that is occupied by one of them cannot be occupied by another at the same time. In this respect they behave like fermions.

We have already seen some limiting cases in section 2.2 where the bosonic case can be easily applied: if $g \gg 1$, the bosons are spins oriented in the $|\leftarrow\rangle$ direction; if $g \ll 1$, they are domain walls. So from now on we will treat the quasi-particles as bosons.

Now let us get back to (2.51). The energy-momentum relation ϵ_k is non-negative for all k. The energy gap is always at k=0 and its value is $2J|1-g|$. We can see here that, when g=1, the gap is zero and any excited particle can carry arbitrarily low energy, so that it should dominate near T=0, when there is not a large amount of energy available for the particles. This suggests that the considered state at g=1 must be critical.

This is so far just an intuition, of course, but at least our results suggest that we are on the right track. To see that a quantum phase transition does take place, we should study the vicinity of the possible critical point, g=1. For this, it is convenient to use a continuum theory.

2.5 Continuum theory

2.5.1 Grassmann variables

First of all, we need to define a new set of variables that represent the old annihilation operators c_i:

$$\Psi(x_i) = \frac{1}{\sqrt{a}}\, c_i \,. \tag{2.52}$$

This new set of variables describes the continuum Fermi field, since the definition in (2.52) implies the canonical anti-commutation relation

$$\left\{\Psi(x), \Psi^{\dagger}(x')\right\} = \delta(x - x')\,. \tag{2.53}$$

The term $a^{-1/2}$ takes care of dimensional considerations when we take the continuum limit of the Hamiltonian, as we will see shortly.

This means that (2.52) is a good candidate for the role of continuum theory variable, but is it good enough? Here is a reminder of another anti-commutation relation for the Fermi field:

$$\{\Psi(x), \Psi(x')\} = 0\,. \tag{2.54}$$

In particular, when x=x', we have the astonishing result $2\Psi^2 = 0$, which should imply that Ψ=0, in contradiction with (2.52).

The solution is that Ψ is not an ordinary number, but a *Grassmann variable* [11, 12]. These entities have the property that their square is always equal to zero. Once we accept this, we can work with Grassmann variables to get useful results in the same fashion as we work with complex numbers although they do not exist as anything countable. For example, integration of functions of Grassmann variables can be carried out, as explained in [12], and we will use it (at least implicitly) to find some results in the next section.

2.5.2 Excitation energy in the continuum case

After this short acquaintance with Grassmann variables, it is now time to see them in action. As the whole problem reduces to a small region around k=0 when the quantum transition comes to stage, we can Taylor-expand the variables near the point considered:

$$\Psi(x_{i+1}) \simeq \Psi(x_i) + a\frac{\partial\Psi(x_i)}{\partial x_i}\,. \tag{2.55}$$

Inserting (2.52) and (2.55) into (2.26) yields, term by term:

$$\begin{gathered} c_i^{\dagger}c_{i+1} = \sqrt{a}\Psi^{\dagger}(x_i)\sqrt{a}\Psi(x_{i+1}) = a\Psi^{\dagger}(x_i)\left(\Psi(x_i) + a\tfrac{\partial\Psi(x_i)}{\partial x_i}\right) = \\ a\Psi^{\dagger}(x_i)\Psi(x_i) + a^2\Psi^{\dagger}(x_i)\tfrac{\partial\Psi(x_i)}{\partial x_i}\,. \end{gathered} \tag{2.56}$$

From now on, all Grassmann variables are to be evaluated at x_i, to avoid carrying this symbol *ad nauseam*.

$$c_{i+1}^\dagger c_i = a\Psi^\dagger\Psi + a^2\frac{\partial\Psi^\dagger}{\partial x}\Psi\,, \tag{2.57}$$

$$c_i^\dagger c_{i+1}^\dagger = a\Psi^\dagger\Psi^\dagger + a^2\Psi^\dagger\frac{\partial\Psi^\dagger}{\partial x} = a^2\Psi^\dagger\frac{\partial\Psi^\dagger}{\partial x}\,, \tag{2.58}$$

$$c_{i+1}c_i = a\Psi\Psi + a^2\frac{\partial\Psi}{\partial x}\Psi = -a^2\Psi\frac{\partial\Psi}{\partial x}\,, \tag{2.59}$$

where, in the last two equations, we have used that Grassmann variables squared are zero.

Using (2.56)-(2.59) in (2.26) and taking the continuum limit $\sum_i \to \frac{1}{a}\int dx$ gives

$$H_F = -Jg - \int dx\left[\left(\frac{c}{2}\left(\Psi^\dagger\frac{\partial\Psi^\dagger}{\partial x} - \Psi\frac{\partial\Psi}{\partial x}\right) + \Delta\Psi^\dagger\Psi\right) + a\frac{\partial}{\partial x}\left(\Psi^\dagger\Psi\right)\right], \tag{2.60}$$

where the constants Δ and c have a value

$$\begin{aligned} c &\equiv 2Ja\,, \\ \Delta &\equiv 2J(1-g) \end{aligned} \tag{2.61}$$

and the notation H_F has been introduced to distinguish the continuum Fermi field Hamiltonian (2.60) from the discrete one, (2.26), denoted H_I.

Since $\frac{\partial}{\partial x}(\Psi^\dagger\Psi)$ can be readily integrated to give only a constant value, we finally obtain[6]

$$H_F = E_0 - \int dx\left[\left(\frac{c}{2}\left(\Psi^\dagger\frac{\partial\Psi^\dagger}{\partial x} - \Psi\frac{\partial\Psi}{\partial x}\right) + \Delta\Psi^\dagger\Psi\right)\right], \tag{2.62}$$

where E_0 is a constant that we can set at will, since it only defines the zero of energy.

Via a Legendre transformation, we can immediately get the Lagrangean density that corresponds to (2.62):

$$\mathcal{L} = \Psi^\dagger\frac{\partial\Psi}{\partial\tau} + \frac{c}{2}\left(\psi^\dagger\frac{\partial\Psi^\dagger}{\partial x} - \Psi\frac{\partial\Psi}{\partial x}\right) + \Delta\Psi^\dagger\Psi\,, \tag{2.63}$$

[6]There is another misprint in [1] when it comes to the analogous formula, 4.41: the sign after E_0 is a plus in that book.

where $\tau = it$ is the imaginary time that we introduced in section 1.2.

The Lagrangean density can be used to determine the partition function [11]:

$$\mathcal{Z} = \int D\Psi D\Psi^\dagger \exp\left(-\int_0^{1/T} d\tau dx \mathcal{L}\right), \tag{2.64}$$

where the integration limits for τ are set taking into consideration the relationship between imaginary time and temperature discussed in section 1.2: if τ_i and τ_f are the initial and final times respectively, then $\tau_f - \tau_i = \beta\hbar$, so that the final limit will be 1/T (setting k=$\hbar$=1) and the initial limit, τ_i - τ_i = 0.

After this, it is now time to diagonalise (2.63) or, equivalently, the Hamiltonian density

$$\mathcal{H} = \mathcal{L} - \Psi^\dagger \frac{\partial \Psi}{\partial \tau} = \frac{c}{2}\left(\Psi^\dagger \frac{\partial \Psi^\dagger}{\partial x} - \Psi \frac{\partial \Psi}{\partial x}\right) + \Delta \Psi^\dagger \Psi \,. \tag{2.65}$$

This is completely analogous to the procedure seen in section 2.3, but fortunately shorter. As we have a certain practice in carrying out this kind of analysis, less details are necessary.

The Jordan-Wigner transformation is not needed because (2.65) already has a quadratic form, so that we can directly go to Fourier space:

$$\phi_k = \frac{1}{2\pi}\int dx_j \; \Psi(x_j) e^{-ikx_j}\,, \tag{2.66}$$

with the inverse:

$$\Psi(x_j) = \int dk \; \phi_k e^{ikx_j}\,. \tag{2.67}$$

Hence, (2.65) becomes

$$\mathcal{H} = \frac{c}{2}\left(\int dk \; dk' \left(\phi_k^\dagger e^{ikx_j} ik' \phi_k^\dagger e^{ik'x_j} - \phi_k e^{ikx_j} ik' \phi_{k'} e^{ik'x_j}\right)\right) + \Delta \int dk \; \phi_k^\dagger \phi_k =$$

$$\int dk \left(\frac{c}{2} ik \left(\phi_k \phi_{-k} - \phi_k^\dagger \phi_{-k}^\dagger\right) + \Delta \int dk \; \phi_k^\dagger \phi_k\right). \tag{2.68}$$

We now use the Bogoliubov transformation

$$\Psi = u\gamma + iv\gamma_-^\dagger\,, \tag{2.69}$$

with u= cos $(\theta/2)$, v= sin $(\theta/2)$ and combine (2.68) and (2.69). Then, term by term:

$$\phi\phi_- = (u\gamma + iv\gamma_-^\dagger)(u\gamma_- + iv\gamma^\dagger) = u^2\gamma\gamma_- + v^2\gamma_-^\dagger\gamma^\dagger + iuv(\gamma_-^\dagger\gamma_- - \gamma\gamma^\dagger)\,, \quad (2.70)$$

$$\phi^\dagger\phi_-^\dagger = u^2\gamma^\dagger\gamma_-^\dagger + v^2\gamma_-\gamma^\dagger + iuv(\gamma^\dagger\gamma_- - \gamma_-\gamma_-^\dagger)\,, \quad (2.71)$$

$$\phi^\dagger\phi = u^2\gamma^\dagger\gamma + v^2\gamma\gamma^\dagger + iuv(\gamma^\dagger\gamma_-^\dagger + iuv(\gamma^\dagger\gamma_-^\dagger - \gamma\gamma_-)\,. \quad (2.72)$$

We should now recall from section 2.3 that we can change both subindices in a term containing two γ factors at will; for example, $\gamma_-^\dagger\gamma = \gamma^\dagger\gamma_-$, because all possible k's are covered in the sum or, in this case, the integral. Also, remember the canonical relation

$$\left\{\gamma^\dagger, \gamma_-\right\} = 0\,. \quad (2.73)$$

We realise that, when we insert (2.70)-(2.73) into (2.68), many terms vanish or can be grouped together:

$$\mathcal{H} = \int dk \left[i\left(\frac{ck}{2}\cos\theta - \frac{\Delta}{2}\sin\theta\right)\left(\gamma\gamma_- + \gamma_-^\dagger\gamma^\dagger\right) + \Delta\gamma^\dagger\gamma\cos\theta\right]. \quad (2.74)$$

Clearly, we must set

$$\tan\theta = \frac{ck}{\Delta} \quad (2.75)$$

so that the unwanted terms vanish. This yields

$$\mathcal{H} = \int dk\, \varepsilon_k(\gamma^\dagger\gamma)\,, \quad (2.76)$$

where

$$\varepsilon_k = \Delta\cos\theta = \Delta\sqrt{1+\tan^2\theta} = \Delta\sqrt{1+\left(\frac{ck}{\Delta}\right)^2} = \sqrt{\Delta^2 + c^2k^2}\,. \quad (2.77)$$

This result is very interesting: Firstly, it has a form that reminds us of a relativistic theory, although we have not explicitly used relativistic invariance; the reason is that $\mathcal{L}$ is in fact invariant under Lorentz transformations. Secondly, it also shows that the two parameters Δ and c can be given a physical interpretation: Δ is the gap at k=0, and c is the velocity of the excitations, in analogy with relativity (where Δ is a mass and c is the velocity of light).

2.6 Quantum phase diagram

To finish with this first example of a quantum phase transition, we have to construct the phase diagram.

Instead of presenting every mathematical detail, this time we will concentrate on the physics that lies behind the formulae, and refer to the literature for the actual derivation of these formulae.

First of all, let us introduce an important quantity that characterises the system: the two-point correlator of the order parameter $\hat{\sigma}^z$:

$$C(x_i, t) \equiv \langle \hat{\sigma}^z(x_i, t)\hat{\sigma}^z(0,0)\rangle \ . \tag{2.78}$$

For our specific problem at $T > 0$, we have [13]:

$$\lim_{|x|\to\infty} C(x,0) = z\, T^{1/4} G_I\left(\frac{\Delta}{T}\right) \exp\left(\frac{-T\,|x|}{c} F_I\left(\frac{\Delta}{T}\right)\right) , \tag{2.79}$$

with z a non-universal constant, and with F_I and G_I functions defined by

$$F_I(s) = |s|\,\theta(-s) + \frac{1}{\pi}\int_0^\infty dy \ln\coth\frac{\sqrt{y^2+s^2}}{2} , \tag{2.80}$$

$$\ln G_I(s) = \int_s^1 \frac{dy}{y}\left[\left(\frac{dF_I(y)}{dy}\right)^2 - \frac{1}{4}\right] + \int_1^\infty \frac{dy}{y}\left(\frac{dF_I(y)}{dy}\right)^2 , \tag{2.81}$$

where $s = \frac{\Delta}{T}$ and θ is the theta function already encountered in (1.3).

Firstly, it can be proven that the exponential decay in (2.79) leads to a correlation length that has the following form:

$$\xi^{-1} = \frac{T}{c} F_I\left(\frac{\Delta}{T}\right) . \tag{2.82}$$

Secondly, also from (2.79), we see that the correlation disappears for x large enough, so that, for $T > 0$, if we take two sites that are very distant from each other, their spins are not correlated, in contrast with what happens when T=0, that we proved that they are correlated (cf. § 2.2.2).

Another consideration that will help us in drawing our phase diagram is that, if T is high enough, the supposition that we are near the quantum critical point, where k=0 (as explained in §2.4), is not fulfilled because the momenta become too high. This means that, above a certain temperature, we go back to the "classical" regime.

The key step in establishing the quantum phase diagram is to study the limiting cases for (2.82). These are [1, 13]:

- For $\Delta \gg T \quad (s \to \infty)$:

$$\xi = c \sqrt{\frac{\pi}{2\Delta T}\, e^{\Delta/T}}\,. \tag{2.83}$$

- For $\Delta \ll -T \quad (s \to -\infty)$:

$$\xi = \frac{c}{|\Delta|}\,. \tag{2.84}$$

- For $|\Delta| \ll T \quad (s \to 0)$:

$$\xi = \frac{4c}{\pi T}\,. \tag{2.85}$$

Let us not spend time trying to derive these three limits, as it can easily be done with a computer program, taking the arguments of F_I and G_I tending to the values indicated by s for each of the three cases. What is more important here is to try to interpret these limits.

First of all, (2.83) shows an exponential divergence of ξ as $T \to 0$. This agrees with the regime previously discussed in § 2.2.2, where there is a magnetic long-range order for $T \to 0$, but not for $T > 0$, as quoted above when examining (2.79).

Furthermore, (2.84) shows a finite correlation length, so that there is no long-range order. This corresponds to a quantum paramagnet case, as in section 2.2.1.

Finally, (2.85) has no analogoue for $T \to 0$, and there is no semi-classical interpretation of this regime. To see this, we must now introduce the key concept of *phase coherence time,* τ_φ. It can be naively defined as the time the system retains memory of its phase, so that there will be interference effects for times shorter than τ_φ. In this case, it is [1] $\tau_\phi \sim \frac{1}{T}$, as opposed to the two preceding cases, in which τ_φ was much bigger than $\frac{1}{T}$.

Whereas in the other cases it was possible to find a classical analogue because of the big phase coherence time, in this latter case this time is not big enough compared to the available energy, hence things go incoherent and there is definitely a quantum behaviour lying behind.

These qualitative considerations finally allow us to draw the desired quantum phase diagram, which is shown in figure 2.1.

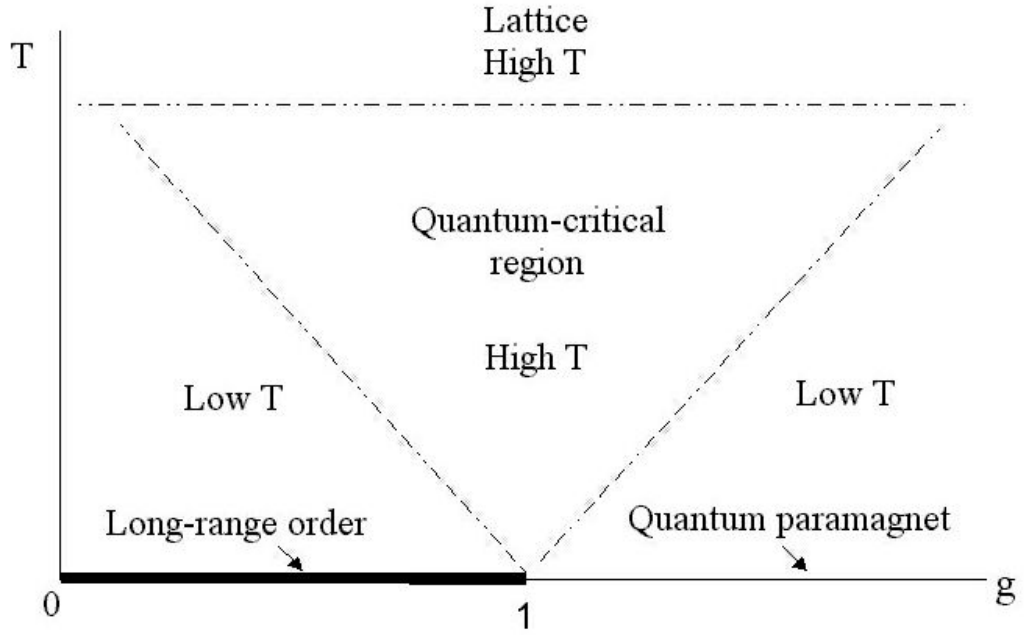

Figure 2.1: Phase diagram of the quantum Ising model in one dimension. The dashed lines are cross-overs at $T \sim |\Delta|$ that separate the different phases for $T > 0$; the solid lines are phases at T=0, which influence the region above them, thus leading to the two low temperature phases; at $g = 1$, there is a quantum critical point that leads to the quantum critical region at high T. Above them, there is a region where $T \gg J$ and hence its properties are determined by the ordinary lattice model, not by continuum theory.

2.6.1 Anti-ferromagnetic Ising model

To finish this chapter, we will take a look at the antiferromagnetic Ising Hamiltonian with a transverse field. We would like to see if there is also a phase transition in the quantum Ising model for the antiferromagnet. Fortunately, the antiferromagnetic Hamiltonian is very similar to that of the ferromagnet:

$$H_{A-F} = -Jg \sum_i \hat{\sigma}_i^x + J \sum_{<i,j>} \hat{\sigma}_i^z \hat{\sigma}_j^z \,. \tag{2.86}$$

Comparing it with (2.1), we see that the change

$$\begin{array}{c} J \to -J \,, \\ g \to -g \end{array} \tag{2.87}$$

transforms the ferromagnetic Hamiltonian (2.1) into the antiferromagnetic one, (3.35). Hence we can use all the results found previously for the antiferromagnet just by making the aforementioned substitution.

In particular, the energy spectrum is, from (2.51) and (2.87),

$$\epsilon_k = 2\,|J|\,\sqrt{1 + g^2 + 2g\cos ka}\,. \tag{2.88}$$

This gives g=-1 as the point where the quantum phase transition occurs. But g=-1 implies that the positive term in (2.86) turns to negative, so that we end up with the transition found before for the ferromagnetic case. This means that there is no phase transition in the antiferromagnetic Ising model: if we try to find it, we are "pushed back" into the ferromagnetic model.

Chapter 3

Schwinger Bosons Approach

When we want to study a phase transition, one approach is obviously to try to find the exact result, as we did in Chapter 2 for the Ising model. No doubt this is the preferrable way to proceed, but sometimes things are much more complicated and the exact solution is enormously difficult to find. Then we turn to approximate solutions.

For instance, our results in chapter 2 were all for $S = 1/2$. We might also want to investigate what happens for arbitrary spin, but our derivations cannot easily be generalised to arbitrary S. Therefore, an approximate method might be necessary. This is the reason why we will investigate one of the many possible approaches to the solution for arbitrary spin by introducing an approximate method, the Schwinger Boson mean-field theory.

In this chapter, we will apply the Schwinger Boson mean-field theory (SBMFT) to the Ising model in a transverse field. Our purpose is to find the differences between the solution that this technique gives and the exact result found previously, thus gaining knowledge on the features and limitations of this particular approach to the problem. This will permit us to determine when this method is likely to succeed in dealing with our problems.

The last part of this chapter is devoted to SBMFT for the more sophisticated Heisenberg model, where we will get an approximate result that also predicts a quantum phase transition.

3.1 Schwinger Bosons

Schwinger bosons are mathematical entities introduced by Julian Schwinger that have properties of bosonic particles. The basic idea behind them is that we can completely describe a spin-N operator with $2N$ *independent* spin-$\frac{1}{2}$ bosons, the so-called Schwinger bosons. Proceeding this way, certain problems are simplified, like for example the calculation of matrix elements between Fock states [14].

Here is the definition of the two Schwinger bosons a and b in terms of the spin operator $\mathbf{S}$:

$$\begin{aligned} S^x + iS^y &= a^\dagger b\,, \\ S^x - iS^y &= b^\dagger a\,, \\ S^z &= \frac{1}{2}(a^\dagger a + b^\dagger b)\,, \end{aligned} \tag{3.1}$$

with the constraint $n_a + n_b = 2S$ (n_a and n_b are the eigenvalues of the number operators for both Schwinger bosons). This can be generalised to N different Schwinger bosons, but two is enough for our purpose.

The constraint $n_a + n_b = 2S$ implies that the two Schwinger bosons are related to the eigenvalue of $\mathbf{S}^2$. Since the Schwinger bosons are represented bytwo commuting operators, we can relate them to the eigenvalue of S_z at the same time, so that they can together characterise the state $|S, m\rangle$. By defining [4]

$$\begin{aligned} S &= \tfrac{n_a + n_b}{2}\,, \\ m &= \tfrac{n_a - n_b}{2}\,, \end{aligned} \tag{3.2}$$

we see that the relations

$$|a\rangle = \frac{(a^\dagger)^{n_a}}{\sqrt{n_a!}}\,|0\rangle$$

and

$$|b\rangle = \frac{(b^\dagger)^{n_b}}{\sqrt{n_b!}}\,|0\rangle$$

together imply that:

$$|S, m\rangle = \frac{(a^\dagger)^{S+m}(b^\dagger)^{S-m}}{\sqrt{(S+m)!(S-m)!}}\,|0\rangle\ , \tag{3.3}$$

which is the expression that relates spin states to Schwinger bosons.

3.2 Mean-field theory

As outlined above, mean-field theory is an approximate method to investigate phase transitions. The name itself gives a clue to how this approach works: we substitute the field present in our problem with a homogeneous, "mean" field that is much smoother hence easier to work with. Intuitively, what we do is to disregard all fluctuations of the field, hoping that they will compensate each other. For example, in the case of the ordinary Ising model, the "field" is what a single spin S_i^z feels due to the interaction with its neighbours. A simple mean-field theory would then be to replace $\sum_{<i,j>} S_i^z S_j^z$ with $\sum_{<i,j>} S_i^z \left\langle S_j^z \right\rangle$, where $\left\langle S_j^z \right\rangle$ is the mean value of S_j^z.

A general mathematical formulation of the mean-field method is the following[11]: We start with the free energy F, we write it in terms of a function S (the "action") containing our field ϕ_i and our external potential H_i and substitute the field with a mean field $\overline{\phi_i}$:

$$Z = e^{-\beta F} = \int \prod_i d\phi_i e^{-\beta S(\phi_i, \vec{H}_i)} \simeq e^{-\beta S(\overline{\phi_i}, \vec{H}_i)} \,, \tag{3.4}$$

where the mean field $\overline{\phi_i}$ satisfies

$$\left. \frac{\partial \mathrm{S}}{\partial \phi_i} \right|_{\overline{\phi}} = 0 \,. \tag{3.5}$$

Furthermore, we can use the Gibbs free energy G, which is simply a Legendre transformation of the (Helmholtz) free energy,

$$G(\vec{m}_i) = F\left(\vec{H}_i(\vec{m}_j)\right) + \sum_i \vec{H}_i(\vec{m}_j) \cdot \vec{m}_i \,. \tag{3.6}$$

Here $\vec{m}_i$ is the order parameter, that satisfies

$$\vec{m}_i(\vec{H}_j) = -\frac{\partial F}{\partial \vec{H}_i} \,, \tag{3.7}$$

and $\vec{H}_i(\vec{m}_j)$ is obtained inverting (3.7). The free energy also satisfies a similar equation:

$$\vec{H}_i = \frac{\partial G}{\partial \vec{m}_i} \,, \tag{3.8}$$

whence we can get for example the zero-field equations by taking the limit $\vec{H}_i \to 0$. Equations (3.5) and (3.8) are the basic equations of the mean field method.

3.3 Putting all this together

We would now like to analyse the Ising model in a transverse field using a Schwinger boson mean-field theory and check if the quantum phase transition at g=1 survives the approximation. Since any mean-field theory suppresses fluctuations (at least partly), it is by no means obvious that we will still find a quantum phase transition after introducing a mean field (Recall that the very existence of a quantum phase transition in the quantum Ising model is due to enhanced fluctuations as $g \to 1$).

We will dedicate this section to develop the Schwinger boson mean field approximation. This process, though, is not unique and, as we will see, different approaches give different results; it is important to compare these results with the exact analytical solution so that we can decide what is the approach that best suits the problem. We will begin with the simplest model, check if it works, and if it does not, then we will go one step further, trying to get a more sophisticated model that fixes the problems, and repeat the process.

3.3.1 Plain Schwinger bosons

Our starting point will be to write the quantum Ising model in terms of Schwinger bosons. Inserting (3.1) into the Hamiltonian (2.1) immediately leads to

$$H_I = -Jg \sum_i \left(a_i^\dagger b_i + b_i^\dagger a_i \right) - J \sum_{<i,j>} \left(a_i^\dagger a_i a_j^\dagger a_j - a_i^\dagger a_i b_j^\dagger b_j - b_i^\dagger b_i a_j^\dagger a_j + b_i^\dagger b_i b_j^\dagger b_j \right). \tag{3.9}$$

Well, the first problem here is evident: we have quadratic terms, that we can deal with easily, and quartic terms, that are harder to treat. Since the mean field approximation has not been used yet, one could think that the first thing to try is to take the mean-field value of two of the four operators appearing in the quartic terms, so that, for example, $a_i^\dagger a_i b_j^\dagger b_j$ would become $a_i^\dagger < a_i b_j^\dagger > b_j$, or $a_i^\dagger a_i < b_j^\dagger b_j >$. The bracketed terms are thus mean values of the operators in the system, so that they are constants and we end up with bilinear terms only.

Unfortunately, this approach fails regardless of what two operators we choose to make constant, because when one tries to diagonalise the Hamil-

tonian, the eigenvalues are complex, so that we do not have physically meaningful energy states. Bearing this in mind, we will now proceed to the next step, where we introduce a new method to deal with biquadratic terms.

3.3.2 The Hubbard-Stratanovich transformation

There exisits an extension of the Gaussian integral into the path integral formalism, called the Hubbard-Stratanovich identity, that will prove useful here. It reads [14, 15]:

$$\exp\left(\frac{J}{n}Z^*Z\epsilon\right) = \int_{-\infty}^{\infty} d^2Q \exp\left[-\left(Z^*Q + ZQ + n\frac{Q^2}{J}\right)\epsilon\right], \tag{3.10}$$

where

$$d^2Q \equiv \frac{\epsilon n}{\pi J}\mathrm{Re}\, Q\, d\mathrm{Im}\, Q\,. \tag{3.11}$$

Here n is the number of Schwinger bosons, Z is a bilinear operator and Q is a complex integration variable that depends on the configuration of sites for our specific problem (see [14]).

If we have a Hamiltonian of the form[1]

$$H = -\frac{J}{N}\sum_{<i,j>} Z_{ij}^* Z_{ij} - \sum_{l,m,m'} j_{lmm'}(\tau) z_{lm}^* z_{lm'}\,, \tag{3.12}$$

where z_{lm} are the single operators in the bilinear terms Z_{ij} (represented by complex numbers), then (3.10) leads to the Lagrangran (see[14]):

$$L = \sum_{i,m} z_{im}^* \partial_\tau z_{im} + \sum_{<i,j>}\left(Z_{ij}^* Q_{ij} + Z_{ij} Q_{ij}^*\right) - \sum_{l,m,m'} (j_{lmm'} + i\lambda_l \delta_{mm'}) z_{lm}^* z_{lm'}\,. \tag{3.13}$$

λ and Q are the saddle point parameters that we choose to be static and uniform when we introduce the mean-field theory:

$$\begin{aligned} Q_{ij} &\to Q\,, \\ \lambda_i &\to -i\lambda\,, \end{aligned} \tag{3.14}$$

[1] The parameter τ entering in the second term in (3.12) plays the role of Euclidian time. It may appear strange that a time variable appears in a Hamiltonian, but in the path integral formalism, equation (3.12) defines what is called an *instantaneous Hamiltonian*, acting at a particular "time slice" of the path being considered. For more details, see [14], [15].

and their actual values are found by minimising the free energy, as discussed in §3.2.

Notice that, if we define

$$\begin{aligned} z_1 &= a \\ z_2 &= ib \end{aligned} \tag{3.15}$$

then the Hamiltonian (3.9) can be written as $H = 2H'$, being

$$H' = -\frac{J}{2} \sum_{<i,j>} Z_{ij}^* Z_{ij} - \frac{Jgi}{2} \sum_i \left(z_{i1}^* z_{i2} + z_{i2}^* z_{i1} \right) \tag{3.16}$$

and

$$Z = \sum_{m=1,2} z_{im}^* z_{jm} \, . \tag{3.17}$$

This has the form of (3.12) and therefore the Hubbard-Stratanovich identity is applicable. We get

$$\begin{aligned} H' = \sum_{im} \lambda z_{im}^* z_{im} - Q \sum_{<i,j>,m} \left(z_{im}^* z_{jm} + z_{jm}^* z_{im} \right) \\ + \tfrac{Jgi}{2} \sum_i \left(z_{i1}^* z_{i2} + z_{i2}^* z_{i1} \right) + nN \tfrac{zQ^2}{2J} - nNS\lambda \, . \end{aligned} \tag{3.18}$$

The last two summands in (3.18) come from the last term in (3.10) and the constraint (3.2) respectively (λ is basically the Lagrange multiplier that ensures that this constraint is fulfilled). Notice also that the "plain" z, without subindices, is not an operator, but simply the number of nearest neighbours in the site ($z = 2$, because we are in 1-D, but it is convenient to write it as z for further purposes). N is the number of sites, as always, and S is the spin. Remember also that n is the number of different Schwinger bosons that we introduce (n=2 in our case).

By going to momentum space, we get

$$H' = \sum_{k,m} \epsilon_k z_{km}^* z_{km} + \frac{Jgi}{2} \sum_k \left(z_{k1}^* z_{k2} + z_{k2}^* z_{k1} \right) \tag{3.19}$$

(We can obviously forget about the constants that appeared in (3.18), since the zero of the energy is not important). Here,

$$\epsilon_k = \lambda - 2Q\gamma_k \, , \tag{3.20}$$

$$\gamma_k = \frac{1}{z} \sum_{\vec{\eta}} e^{i\vec{k}\cdot\vec{\eta}} \, , \tag{3.21}$$

where $\vec{\eta}$ are the nearest neigbour vectors. Again, since we are in 1-D,

$$\gamma_k = \cos ka \,, \tag{3.22}$$

but later on we will need the more general equation (3.21).

From (3.10) we can also get the partition function and hence the free energy F (see [14]):

$$F = n \sum_k \ln \left(1 - e^{-\epsilon_k/T}\right) + nN\frac{zQ^2}{2J} - nNS\lambda \tag{3.23}$$

plus some terms depending neither on λ nor on G; we can omit them since we just need the derivatives of F with respect to λ and G. These are:

$$\frac{1}{N}\sum_k n_k = S \,, \tag{3.24}$$

$$\frac{1}{N}\sum_k n_k\gamma_k = \frac{Q}{J} \,, \tag{3.25}$$

where

$$n_k = \frac{1}{e^{\epsilon_k/T} - 1} \,. \tag{3.26}$$

One can readily find the value for Q from (3.24) and (3.25):

$$Q = JS - \frac{J}{N}\sum_k n_k(1 - \gamma_k) = JS + \mathcal{O}\left(\frac{T}{JS}\right) \,, \tag{3.27}$$

where we have used that the sum over $\mathbf{k}$ is bounded as $\mathbf{k} \to 0$ [14], leading to a power series in T that we can neglect in the limit of low temperature and/or large spin.

Let us now rewrite (3.20) as

$$\epsilon_k = zQ\left(1 - \gamma_k + \frac{1}{4z}\kappa^2\right) \tag{3.28}$$

with

$$\kappa^2 = 4z\left(\frac{\lambda}{zQ} - 1\right) \,. \tag{3.29}$$

To find λ, it is sufficient to recall that our particles are bosons and they will form a condensate at T=0, so that all particles will be sitting in the ground state. Therefore, when we are near T=0, we can approximate:

$$\frac{1}{N}\sum_k n_k = S = \frac{1}{N}n_0 = \frac{4T}{NJS\kappa^2} + O\left(T^2\right) \tag{3.30}$$

so that, for small T, we have

$$\kappa^2 = \frac{4T}{NJS^2}\,, \tag{3.31}$$

which, together with (3.29), implies

$$\lambda = JSz + O\left(\frac{T}{JS}\right)\,. \tag{3.32}$$

This, in turn, means that

$$\epsilon_k = JSz\sin^2 ka\,. \tag{3.33}$$

We can finally go back to (3.19). We see that we have a non-diagonal matrix in m, which is the index for the different Schwinger bosons. Formally, we have

$$H' = \sum_k \begin{pmatrix} \epsilon_k & i\frac{Jg}{2} \\ i\frac{Jg}{2} & \epsilon_k \end{pmatrix}_k\,. \tag{3.34}$$

Therefore, the eigenvalues λ_k of (3.33) are those for which

$$4(\epsilon_k - \lambda_k)^2 - (Jg)^2 = 0\,. \tag{3.35}$$

As $T \to 0$, the momentum of the particles becomes infinitesimally small, so that $k \to 0$ and hence $\epsilon \to 0$. Thus, equation (3.35) becomes

$$4(-\lambda_k)^2 - (Jg)^2 = 0\,, \tag{3.36}$$

which leads to

$$\lambda_k = \pm\frac{Jg}{2}\,. \tag{3.37}$$

On the other hand, to find the quantum phase transition, we must set the energy eigenvalues to zero, as we saw in §2.4. Equating (3.37) to zero, we find $g = 0$, so that the transverse field in (2.1) is killed off, and therefore we end up with a different Hamiltonian, with no transverse field. So, by *reductio ad*

absurdum, we have proven that in fact **the model predicts no quantum phase transition**.

This is actually something that one could intuitively have expected, since around a quantum phase transition point, the energy changes very rapidly, as it is a non-analytical point. The mean field approximation takes an "average" of all values and does not take this change in energy into consideration. Therefore, it is very unlikely that a mean-field theory predicts a quantum phase transition correctly.

3.4 Heisenberg model

After these considerations, one question raises: is it possible at all to find a quantum phase transition using a mean field approximation? To investigate this, we will turn in this section into the Heisenberg model.

The Heisenberg Hamiltonian is a quantum Hamiltonian, because it has non-commuting operators. This is not the case with the Ising Hamiltonian; we need to introduce a transverse field to get a quantum Hamiltonian. This suggests that the Heisenberg Hamiltonian is more likely to present a quantum phase transition in the mean field approximation, because the fact that this is a quantum model indicates that there are bigger fluctuations than for the Ising model. Hopefully, these bigger fluctuations will survive after the mean field approximation and we will get a phase transition at T=0.

Schwinger bosons mean-field theory is developed in [14] for the ferromagnetic Heisenberg model. If one checks the result for this model in that book and compares it with our development for the Ising model in the previous section, one can see that they are essentially identical if we impose 1-D for the Heisenberg model and we set g=0 in the Ising model. This means that, if we develop the mean field approximation for the ferromagnetic Heisenberg model in one dimension, we will get the same energy spectrum as for the Ising Hamiltonian and therefore we will find no phase transition, as we saw in §3.3.2. We therefore have to find another model to study.

It is time to make an observation that will lead us to one of the other possible models to investigate. In the same book by Auerbach, [14], the so-called "Large-n approximations" are presented. These are models that take a large number, n, of Schwinger bosons, instead of only two, which gives in principle better accuracy because many more states are included this way. However, in practice, *it is often easier to work supposing that 2 is a large*

number already, and the theories are often good enough even with only two bosons.

In the book, three different large-n theories are shown for the Heisenberg model. They are basically the same thing; the only difference is that some of the approaches give better results for some particular problems. One model works well for the bosonic ferromagnet; this is the one that is equivalent to the Ising model as discussed in Chapter 2. Another one is for the fermionic ferromagnet, which is out of discussion here because we are trying to get results for the Schwinger *bosons*. Finally, the third one works for the bosonic anti-ferromagnet.

Since the ferromagnetic problem does not show any phase transition, we will consider instead the antiferromagnetic Heisenberg model, and see if it exhiibts a quantum phase transition in the SBMFT approximation.

3.4.1 Antiferromagnetic Heisenberg model

The Heisenberg Hamiltonian for the antiferromagnet is simply

$$H = \frac{J}{n} \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j \,. \tag{3.38}$$

The fact that we divide the first term in (3.38) by n is simply imposed by the large-n approximation; see [14]. This, of course, does not change any essential characteristics of our problem.

We can describe this Hamiltonian in terms of Schwinger bosons if we insert

$$Z = \sum_m z_{im} z_{jm} \tag{3.39}$$

into (3.18). This leads to

$$H = \sum_{i,m} \lambda z^*_{im} z_{im} + Q \sum_{<i,j>,m} \left(z^*_{im} z^*_{jm} + z_{im} z_{jm} \right) + nN \frac{zQ^2}{2J} - nNS\lambda \tag{3.40}$$

or, in momentum space,

$$H = \sum_{\vec{k},m} \left[\lambda z^*_{\vec{k},m} z_{\vec{k},m} + \frac{1}{2} zQ\gamma_{\vec{k}} \left(z^*_{\vec{k},m} z^*_{-\vec{k},m} + z_{\vec{k},m} z_{-\vec{k},m} \right) \right] + nN \frac{zQ^2}{2J} - nNS\lambda \,, \tag{3.41}$$

where $z_{\vec{k},m}$ and $\gamma_{\vec{k},m}$ are simply the analogues of (3.17) and (3.21) in three dimensional momentum and spin vector space, respectively. We can diagonalise (3.41) by means of a Bogoliubov transformation, as in Chapter 2. One could use (2.38) directly, but things are a little easier if we take instead

$$z_{\vec{k},m} = \cosh\theta\alpha_{\vec{k},m} + \sinh\theta\alpha^*_{-\vec{k},m}\,, \tag{3.42}$$

which is also a valid Bogoliubov transformation[2]. Equation (3.41) becomes

$$\begin{aligned} H = \frac{1}{2}\sum_{\vec{k},m}\Big(\lambda\cosh 2\theta + zQ\gamma_{\vec{k}}\sinh 2\theta\Big)\Big(\alpha^*_{\vec{k}m}\alpha_{\vec{k}m} + \alpha_{\vec{k}m}\alpha^*_{\vec{k}m}\Big) \\ + \Big(\lambda\sinh 2\theta + zQ\gamma_{\vec{k}}\cosh 2\theta\Big)\Big(\alpha^*_{\vec{k}m}\alpha^*_{-\vec{k}m} + \alpha_{\vec{k}m}\alpha_{-\vec{k}m}\Big) \\ + nN\frac{zQ^2}{2J} - nN\left(S+\frac{1}{2}\right)\lambda\,. \end{aligned} \tag{3.43}$$

Clearly, we must require

$$\tanh 2\theta = -\frac{zQ\gamma_{\vec{k}}}{\lambda} \tag{3.44}$$

to diagonalise the Hamiltonian, which yields

$$H = \sum_{\vec{k},m}\omega_{\vec{k}}\left(\alpha^*_{\vec{k}m}\alpha_{\vec{k}m} + \frac{1}{2}\right), \tag{3.45}$$

with

$$\omega_{\vec{k}} = \sqrt{\lambda^2 - (zQ\gamma_{\vec{k}})^2}\,. \tag{3.46}$$

The free energy for this model is calculated in [14], as well as the mean field parameter equations. These equations lead to more complicated formulae for the parameters λ and Q, that would require numerical methods to be solved, but since we are dealing with essentially the same Hamiltonian as in §3.3.2, and our goal is to find the parameters at T=0, where we can neglect higher orders in T. It then seems reasonable to use (3.27) and (3.32) as a good approximation to the mean field parameters for this case[3].

[2]Notice that the only requirement when we write a Bogoliubov transformation is that the anticommutation relations be fulfilled.

[3]Remember that the ferromagnetic Heisenberg model is equivalent to (3.16) if we set g=0.

3.4.2 Antiferromagnetic 1-D Heisenberg model with a transverse field

Let us now study the same model as in previous section, but with a transverse field. The Hamiltonian is now

$$H = \frac{J}{n} \sum_{<ij>} \vec{S}_i \vec{S}_j - Jg \sum_i S_i^z \,. \tag{3.47}$$

To take the transverse field into consideration, we do not really have to repeat all the process shown in previous section. It is sufficient to realise, using (3.1) and (3.40), that this term will contribute to the diagonal of the Hamiltonian, so that the change

$$\lambda \to \lambda - JgS \tag{3.48}$$

inserted into the spectrum (3.46) does the trick (the S in (3.48) comes from the S_i^z operator in (3.47)).

Assuming that we are in one dimension, equation (3.46) with the substitutions (3.27) and (3.47) leads to

$$\omega_k = JS\sqrt{4\sin^2 ka + g^2 - 4g} \,. \tag{3.49}$$

Since we are at T=0, the sine vanishes and therefore, if we equate (3.49) to zero, we find that the condition for a quantum phase transition is $g = 4$.

We have then found a quantum phase transition using a mean-field theory. Although we do not know the exact result for the antiferromagnet Heisenberg model to compare with our approximate result, at least we have fulfilled our purpose to show that it is possible to find a quantum phase transition using mean-field theory.

3.5 Discussion and future work

We have seen that the standard SBMFT method does not give a phase transition at all for the Ising and Heisenberg ferromagnets, which is expected as argued above because the concept of mean field washes out all non-analyticities. However, another quantum model, the Heisenberg antiferromagnet, leads to a quantum phase transition when we use the SBMFT approach.

We have thus learnt that some quantum Hamiltonians have strong enough fluctuations, so that a quantum phase transition is found even after using SBMFT. It does not work for all quantum models, though, as it failed for the ferromagnetic Heisenberg model.

Another thing to point out is that these Heisenberg models are "Large-n models", and in our case $n = 2$. This can be a thing to improve, and we could basically repeat the method for a larger number of Schwinger bosons, which in principle should be a way to get a better result. Also, in our derivation, we borrowed the formulae for the mean-field parameters λ and Q from the ferromagnetic Heisenberg model with no external field. This seems reasonable, because we work at low temperature and, since the two models are basically identical, one would expect the parameters to be at least similar to low orders in T. Nevertheless, if we used the exact result for these two parameters, we would improve our approximate theory and find better results, although probably the improvement would not be very big.

It would also be interesting to see what the continuum theory gives in this case. Since the spectrum is not exact, it is obvious that the continuum limit will also give different results from that of the exact model, but this would be a way to gain more knowledge about our approximation.

Finally, one thing that needs to be done if we want to learn more about QPT is, definitely, to study some other models. The Ising model is useful due to its simplicity, as it can be solved fairly easily, and therefore is a good introduction to QPT, but to gain more knowledge, it is worth investigating some different models. In this sense, [1] is a very good source, because further chapters are devoted to other Hamiltonians, such as the quantum rotor, or the Heisenberg model, and non-magnetic phase transitions. There is also a part concerning mean field theories, as an approximate method to describe QPT. One could try to apply the SBMFT to these models, and perhaps this would give a better understanding of the model than that given by (3.49), so that we could improve the method and make it more suitable to different model. This could help us to go deeper into the challenging and beautiful world of quantum phase transitions.

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