Karlsruher Institut für Technologie

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Bachelor thesis

The solution of the 2D Ising model

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Contents

Preface

In an introduction lecture to statistical mechanics you are mostly given a fast "crash course" on some topics. Either you get a very hand-wavy approach to the subject in a mathematical viewpoint - but which nevertheless enhances the physical understanding of it, or the lecturer emphasizes too much the mathematical techniques to the point that it may become too ductile for the students. Although the mathematical approach may be exact and rigorous it may veil the main subject. The aim of this thesis is to discuss a physical issue in a mathematical context, and then collect the mathemati-cal results and re-embed them within the physical frame. As a topic, it is chosen the 2D Ising model to discuss its physical importance using adequate mathematical formalisms.
The Ising model is a very simple model to describe magnetism in solid state bodies. Because of its simplicity it is possible to solve it analytically in 1 and 2 dimensions, for it is not solved yet in 3 or higher dimensions. Although *Lars Onsager* (1903-1976) has solved the 2D Ising model in 1944, some more efforts have been made on that issue in order to provide a solution which comes along in a more natural way. This allows us to apply mathematical formalisms to find an elegant way to solve the problem. Despite its simplicity it teaches us a very important phenomenon, namely that spontaneous symmetry breaking can occur in the thermodynamic limit.
First of all, one shall examine whether the problem is well-defined by considering a canonical ensemble, and by analyzing the appropriate thermodynamic potential, i.e., the free energy in the so-called *thermodynamic limit*. One will carefully investigate under which conditions the thermodynamic limit of the ensembles exists. After that, it will finally be possible to discuss the phase transition in the Ising model, which is established in the specific heat capacity c:

$$c(\beta) \quad := \quad -k_b\beta^2\frac{\partial^2\beta f(\beta)}{\partial\beta^2},$$

where f is the density of the free energy, and $\beta := \frac{1}{k_b T}$ is the inverse temperature.
I want to thank my two advisors: Professor Hundertmark, who helped me find a matching bachelor thesis that could fulfill the requirements of a mathematical and a physical thesis, and find adequate literature for the mathematical frame; Professor Schmalian, who helped me understand the development of the Ising model in condensed matter physics w.r.t. realizability and competing models.

> *It doesn't matter how beautiful your theory is, it doesn't matter how smart you are. If it doesn't agree with experiment, it's wrong.*
> *-R.P. Feynman-*

This is the basic principle under which the (Lenz-)Ising model was refused at the beginning because it did not yield ferromagnetism. Since a physical theory is considered which shall describe nature, the model will be discussed respecting experimental hints for the assumptions and one will later have to justify mathematical steps. Therefore, this thesis is arranged into 3 parts, namely

(i) the physical background for the model,

(ii) the "well-definedness" of the thermodynamic limit,

(iii) the actual calculation of the transition temperature for the 2D Ising model.

In this manner, the physical setting is created first to help understanding how one gets to the idea of the Ising model. After that, the mathematical setting must be defined and both, the physical and the mathematical ones, will give us the chance to understand the 2D Ising model. Nevertheless, at this point one has to already stress that the Ising model represents a certain group of substances; otherwise there would not be any current interest in discussing it. A physical example that realizes the 2D Ising model is hydrogen adsorbed on Fe surface.
In the second chapter it is not intended to historically describe the Ising model in its detail. Instead, the steps towards understanding the Ising model a par with its history shall be emphasized for it was not clear first how it could become a physical model when taking its causal nexus into consideration:

neither some crucial assumptions which imply the Ising model were physically understood, nor its applicability to any experiment. In this sense, the Ising model is a magnificent example for the development of physical theories, but it also draws the line between a mathematical and a physical model.

Importance of an exact solution for a model

0.0.1 Definition (model)**.** *A* physical model *is a set of equations which simplifies by idealizations the scenario it shall describe in order to be solvable, i.e. it provides a well-defined solution, but whose assumptions are based on empirical facts. In addition, it must be compatible with the contemporary established concepts of theoretical physics. A* good physical model *is one that is realized in nature and can provide prognoses to scenarios that are conceptually equivalent the original scenario, but which on the other hand can be defended with the contemporary axiom system.*

In the frame of this thesis this definition will be used to discuss the Ising model. It seems to be a very hard criterion for a physical *attempt*[1] to be a good model but it exhibits both properties, the physical and the mathematical viewpoint. Both are influenced one by the other, so one must always consider both together. A crucial feature demanded in my definition is the *time-dependent* character. Whether an attempt has to be considered a model depends on the mathematical and physical insight one is given, that is why it is important to study physical and mathematical attempts provided in the past. They may not have been adequate descriptions at the time they arose or for the special scenario they were developed for, but they can be applicable in other cases. E.g. many models and theories to describe superconductivity failed in that but some of them could explain phenomena related to that[2]. This does not mean that all physical or mathematical attempts of the past can help us in most recent researches, but some of those are nonetheless useful for these. A famous example for that are the *Navier-Stokes equations*[3]

[1] That is how theories will be called which do not fulfill the above criteria.

[2] I refer to a single lecture Prof. Schmalian gave on that topic.

[3] derived in 1827 and 1845 respectively by *George Gabriel Stokes* (1819-1903) and

and the *Euler equations*[4] which are related to these. At the time they were stated one was far from understanding them. A problem among others was that there were no computers, so one could not even provide a numerical approximation to it, but today the Navier-Stokes equations are discussed very much whenever a fluid is considered. E.g. in game programming their numerical approach have been used to shape water.
The history of science has shown that some physical models had been used by physicists many years before mathematicians could prove that the solution for this problem is well-defined. For instance, the 3d Heisenberg model had been in use for some years when in 1978 mathematicians [FILS78] could prove the existence of a phase transition in that model. A phase transition can just occur in the thermodynamic limit[5]. In a usual introduction course to statistical mechanics one works with the thermodynamic limit (system size$\to \infty$, particle number$\to \infty$) without paying attention whether the thermodynamic potential in the considered ensemble exists. This is not a bad feature of a pure introduction course because one has to learn many physical concepts instead, but it is still crucial in terms of really understanding a model, to take care of its "well-definedness".
With the speed of modern computers today one is able to provide approximate solutions and there are people trying to determine whether there is an exact solution close to the approximate solution, but these methods are very complicated and depend very much on the model. A problem which is related to that is **chaos**. One can consider the magnetic pendulum with 3 sources which is exposed to friction and gravity (cf. figure 1). The "solution", i.e. the endpoint of the motion, depends dramatically on the initial conditions. It is not even given that there is a solution for the initial condition even though there might be given a solution in a neighborhood. In that type of problems one cannot avoid to analyze *stability* of the solution.

One can see, that the specific mathematical issues concerning a (physical) problem are spread widely, whereas a physicist given a model is exposed to "just" 2 problems: 1. providing a solution, 2. agreeing with the experiment. Nonetheless, in order to really understand a model it is unavoidable to care about mathematical points of it as mentioned above. In the 70's and 80's an important step in the physical history was the idea of so-called *renormaliza-*

Claude Louis Marie Henri Navier (1785-1836) respectively

[4] derived in 1755 by *Leonhard Euler* (1707-1783)

[5] This will be precisely discuss in chapter 2.

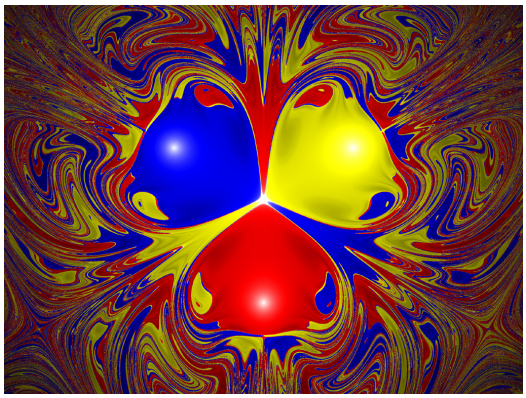

Figure 1: Magnetic Pendulum with 3 sources; the sources are placed in the center of the big areas colored in the particular color. Each pixel is colored in the color of the magnet where the trajectory of the pendulum ends. Source: `http://nylander.wordpress.com/2007/10/27/magnetic-pendulum-strange-attractor/`.

tion. Renormalization gives a certain condition on models to fit into the field which it is ascribed to. It is applied to Feynman integrals which themselves are not well-understood in terms of the present axiom system. However, they can really well describe QED and QCD processes, i.e. one obtains very good agreement with the experiment.
Not an equation is a mathematical object but the solution of it. In that sense, providing an exact solution is the last step in understanding a physical model, it "completes" a physical model.
This thesis aims to describe a certain type of magnetic substances conform with the concept of statistical mechanics. Although it cannot provide high numerical accuracy concerning the transition temperature of those substances one learns how a phase transition can arise in a certain model.

Chapter 1

Historical background of the Ising model

1.1 Weiss's theory of ferromagnetism

According to Martin Niss[1] [Nis05], at the time when *Wilhelm Lenz* (1888-1957) proposed his model of magnetism to his student *Ernst Ising* (1900-1998) in 1920, there were already theories on magnetism which tried to explain it in a classical way. One was given the experimental results by *Pierre Curie* (1859-1906) that there were three types of magnetism, namely diamagnetism, paramagnetism and ferromagnetism, and further he found out that the magnetic susceptibility χ of a paramagnet follows the eponymous law

$$\chi(T) \propto \frac{1}{T} \tag{1.1.1}$$

Paul Langevin (1872-1946), Curie's student, - he believed that macroscopic magnetism arose with molecular microscopic (atomic) magnets which could point in every direction - assumed, according to Niss, that the total magnetic moment "[arose] with the revolution of electrons" in the micro magnets [2] and thus he describes paramagnetism and diamagnetism in 1905 by applying Boltzmann's law to a gas exposed to an external magnetic field. The idea of micro magnets can be seen due to the Maxwell equation $\nabla \cdot B = 0$, i.e., dividing a magnet into two parts creates two new magnets. With the assumption

[1] Roskilde Universitet, Institut for Natur, Systemer og Modeller

[2] [Nis05], p. 273

of free rotatability, neglecting interaction between the micro magnets and assuming

$$E = \mathbf{H} \cdot \mathbf{M}^3 = HM \cos\alpha$$

Langevin derived his famous equation

$$I \quad = \quad MN \left(\coth(\beta MH) - \frac{k_B T}{MH} \right).$$

With Langevin's results *Pierre Weiss* (1865-1940) extended this theory to ferromagnetism in his paper of 1907 [Wei07]. In his attempt to do so he provided the *mean-field hypothesis*[4]

> *Je suppose que chaque molécule éprouve de la part de l'ensemble des molécules environnantes une action égale à celle d'un champ* uniforme *NI proportionnel à l'intensité d'aimantation et de même direction qu'elle.*

i.e., "a molecule experiences, from the collection of molecules surrounding it, an action equal to that of a uniform field proportional to the intensity of magnetization and in the same direction." He then substituted[5] H in the equations above by the total magnetic field H_{tot} under the influence of an external field H_{ext} in order to obtain

$$H_{tot} \quad = \quad NI + H_{ext}.$$

With this equation Weiss argued that below a critical temperature because of spontaneous magnetization a magnetic field was present, even, if the external field was turned off. However, he could not explain how this transition arose in a mathematical viewpoint. Other physicists worked further on improvements of the assumptions and obtained very good agreements with the experiment.

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[3] In this thesis one will not use co- or contravariant vectors if it is not mentioned otherwise, thus, any "$\cdot$" in a product between vectors means the usual Euclidean scalar product, i.e. $A \cdot B := \sum_{i=1}^{3} A_i B_i$.

[4] [Wei07], p. 662

[5] [Wei07], p. 682

1.1.1 Stern's criticism

The German physicist *Otto Stern* (1888-1969) displayed in 1920 [Ste20] that Weiss had applied Langevin's theory to solids neglecting the anisotropy given in a crystal so that the idea of free rotatable micro magnets could not be justified. Further he pointed out that Weiss' theory (as well as the others above mentioned theories) contained some adjustable parameters, namely the magnetic moment and the moment of inertia of the molecules which were fitted by the experiments. One even used the free choice of these constants for their plots of the experimental data. On the other hand, Stern mentions examples for which the moment of inertia was computed using Weiss' and his successors' theory, not anticipating that the free rotatability was not justified anymore in a crystal.
In the following [6] Stern points out an error in Weiss' calculation who had tried in 1913 to circumvent this false assumption by arguing that Curie's law could be deduced considering molecules which had a fixed null position and which were able to vibrate whenever the null positions had no preferred direction as it is the fact in amorphous materials. This implies a much bigger temperature dependence than the assumption actually yielded.

1.2 Lenz's model

Lenz, who knew about Stern's criticism on Weiss' theory - in fact he mentioned Stern's paper in his own paper of 1920 [Len20] - introduced his model by imposing a further restriction on the idea of micro magnets, namely that the directions, that the micro-magnets could have, were "quantized" - he does not mention this term - , i.e., only two directions were allowed ($\rightarrow$ spin up/spin down). He describes this as "turnovers"[7] (*Umklappbewegungen*[8]) and he justifies this turnovers with "position switching among atoms" in "self- and strange diffusion" (*Selbst- und Fremddiffusion*[9]). Prof. Schmalian explained to me that in a current viewpoint this has to be declined as a reason for magnetism since electronic effects dominate and the diffusion processes happen far too slowly.

[6] [Ste20], p. 148-153

[7] I adopted this translation from [Nis05], since *Umklapp processes* mean something different in solid state physics

[8] [Len20], p. 614

[9] [Len20], p. 614

It must be emphasized that at the time when Lenz proposed his model, neither quantum mechanics was developed nor the idea of spin was founded and one was far from understanding the relation between spin and magnetism. For instance, Lenz mentions in his paper a "quantum treatment" (*in quantenmechanischer Betrachtung*[10]) to argue that some angles towards the external magnetic field should be preferred, but Niss explains that this shall be seen as an idea of "space quantization" his advisor A. Sommerfeld had introduced. In this idea, the "directions of the normal vector to the orbit of an electron [...] point only in discrete directions"[11].
The experimental fact Lenz relied on, was that not free rotatability, but anisotropy was given in a crystal lattice[12]. In the following Lenz deduces Curie's law from the assumption, that just flipping of the micro magnets was allowed, by computing the mean magnetic moment in virtue of

$$\bar{\mu} \quad = \quad \mu \frac{\mathrm{e}^{a} - \mathrm{e}^{-a}}{\mathrm{e}^{a} + \mathrm{e}^{-a}} = \mu \tanh a \approx \mu a \propto T^{-1},$$

where $a = \beta\mu H$ is a small parameter for $H \to 0$. This model can only be applied to diamagnetic and paramagnetic substances since in his assumptions Lenz ignores the interaction between the micro magnets. At the end of the paper, Lenz concludes that if "the potential energy of an atom towards its neighbors" is different in the null position than in an angle of π to that - if interaction between the neighbors is allowed - one obtains spontaneous magnetization because of a "natural [...] directedness" (*natürliche* [...] *Gerichtetheit*) in the crystal [13].

1.2.1 Ising's paper

In his own paper [Isi24], Ising imposed further constraints on the model Lenz proposed to him. On one hand, he assumed that the forces acting between the atoms were an electric force that only acts on the nearest neighbors, since they decay very fast. On the other hand, he mentions that the state of minimal energy is obtained if all micro magnets point in the same direction. This last assumption is very important to understand *ferro*magnetism. Ising, however, did not justify his further assumptions in his dissertation[14]. Niss

[10] [Len20], p. 614
[11] [Nis05], p. 278
[12] [Len20] p. 614
[13] [Len20], p. 615
[14] In a modern viewpoint, the fast decay can be seen due to screening effects.

tries to draw parallels to *Walter Schottky*'s (1886-1976) ideas, but he also underlines differences between both models, e.g., the different orientations (Ising demanded spins that are pointing in the plane, Schottky needed spins that are perpendicular to it)[15]. Schottky stated that the spins interacted electro-statically which he justifies by saying that this way he was able to estimate the Curie temperature to the right order. Because it is unclear, according to Niss, if Ising was affected by Schottky's thinking, the motivation behind these assumptions will be left open. The most recent reasons for them were given in quantum mechanics which was developed after Ising had published his dissertation. This will be seen in more detail in the following two sections.

As it is well-known, Ising found no net magnetization in a linear chain of next or next-to-next neighbor coupled micro magnets even when he considered an infinite system (i.e. #micro magnets$\to \infty$). Ising then concludes that either no thermal equilibrium or another reason was given for the Boltzmann distribution not to be applicable[16]. However, as one will see, that is not the crucial point where the attempt breaks down. In his paper of 1925 [Isi25], he tries to add a three-dimensional extension to his linear chain by considering several chains parallel to each other. He does not describe how he wants to arrange these chains to obtain a three-dimensional lattice, but he oversimplifies the coupling by assuming that the single magnetic momenta just add up to a total magnetic momentum, and thus he can apply the one-dimensional result to this "three-dimensional" arrangement. Initially one can understand this result heuristically: Consider a Ising ferromagnetic chain of length N in a single phase and a subchain of length L of the other phase. Such a subchain can be inserted approximately N/L times, thus the entropy changes by approximately

$$\Delta S \quad = \quad k_B \log \frac{N}{L}.$$

With that one obtains a change in the free energy of

$$\Delta F \quad = \quad \Delta U - T\Delta S = \Delta U - k_B T \log \frac{N}{L},$$

which becomes negative for sufficiently large value of N. This heuristic argument can be rigorously established, cf. [SS81], and can be used to justify the

[15] [Nis05], p. 280-281

[16] [Isi24], Ergebnis; I did not find a typewriter version for the dissertation, thus I cannot refer to a certain page number in Ising's thesis.

phase transition in the 2 dimensional Ising model. The crucial assumptions which underly the Ising model are

(i) magnetism arises with micro magnets (this can be replaced by the idea of *spins* in quantum mechanics),

(ii) the crystalline anisotropy yields that only certain orientations are allowed for the micro magnets,

(iii) only nearest neighbors interact electrically,

(iv) in ferromagnets the minimum energy is obtained if all the spins are oriented in the same direction and

(v) a phase transition can only occur if the lattice is taken to be arbitrarily, i.e. infinitely, large.

This last condition requires more mathematical care, since the thermodynamic potentials must stay well-defined for the limit. Though it is essential, since a phase transition of order n represents a discontinuity in the n^{th} derivative of the considered thermodynamic potential in Landau's theory of phase transitions. And because in the case of a finite lattice the density f of the free energy is a finite sum of $\mathcal{C}^\infty(\mathbb{R})$-functions of the temperature and thus it is a $\mathcal{C}^\infty(\mathbb{R})$-function itself, a discontinuity in any derivative of f can only occur in the case of an infinite system. Mathematically one needs further restrictions to obtain a phase transition, but this will be discussed later in the thesis. At first, one further model shall be introduced which was known to Ising and his contemporaries, namely the *Heisenberg model*.
One must pay attention to the fact that under the *dimension* of a spin coupling model it is understood the number of dimensions in which coupling is allowed. The dimension of a spin coupling model is *not* the number of dimensions in which the spins are allowed to point. The *space dimension* of a spin coupling model is defined to be the number of possible orthogonal directions in which the spin can point.

1.3 Heisenberg model

With the birth of quantum mechanics in 1925-1926, *Werner Heisenberg* (1901-1976) derived his own theory of ferromagnetism. Since due to the

Stern-Gerlach experiment given in 1922 *Samuel Goudsmit* (1902-1978) and *George Uhlenbeck* (1900-1988) had already proposed the concept of spin quantization for electrons, Heisenberg wanted to apply it to magnetism. In his paper of 1928 [Hei28] he explains that the interaction between the nearest neighbors could neither be a magnetic force nor the Coulomb force. He uses an exchange integral (*Austauschintegral*[17]) between a pair of electrons which consists of Coulomb terms among the electrons and the core, and he further imposes the Pauli principle according to which he concludes, that the eigenfunction of the corresponding Hamiltonian must be anti-symmetric. He further respects that the electron quanta are indistinguishable, i.e., one has to take into account all the possible permutations to calculate the partition function[18]. Heisenberg demands that only nearest neighbor interactions are non-negligible and the exchange integral is the same for all pairs of electrons. He derives Langevin's equation with Weiss' extension, but he puts further constraints on the calculation. The fact that he could derive this equation lead his contemporaries to accept his theory of ferromagnetism. These however only saw it as a "step in the right direction" and not as a correct explanation, since some constraints Heisenberg imposed were arbitrary[19]. It is important with regard to the understanding of magnetism, that Heisenberg refers to the *Einstein-de Haas effect* to justify that not atomic micro magnets evoke ferromagnetism but the spin (*Eigenmomente*)[20].
One must separate Heisenberg's *theory* of magnetism which was above, described from his *model*

$$H \quad = \quad -2J_E \sum_{i\#j} S_i \cdot S_j. \tag{1.3.1}$$

This Hamiltonian is in a way an extension of the Ising Hamiltonian which only respects the couping $z-$component of the spins and it was first considered to be the correct model to describe ferromagnetism. Due to the simplification of the Heisenberg model, ignoring the coupling of the other two components, and due to the fact that its one-dimensional case did not reveal ferromagnetism, the physical community dismissed the Lenz-Ising model as a realistic representation of ferromagnetism. The actual form of the Hamiltonian in

[17] Heitler and London introduce this exchange integral in [HL27]
[18] [Hei28], p. 624- 627
[19] [Nis05], p. 289
[20] [Hei28], p. 619

eq. (1.3.1) was derived by *Paul Adrien Maurice Dirac* (1902-1984) in a paper in 1929 [Dir29], but he did not explicitly refer to Heisenberg's theory in computing the Hamiltonian, although he mentions Heisenberg's work on the topic. In his own paper Dirac criticizes that Heisenberg used too complicated techniques like group theory, which he did not consider to be adequate to describe a quantum mechanical problem, to explain ferromagnetism[21]:

> *It should therefore be possible to translate the methods and results of group theory into the language of quantum mechanics and so obtain a treatment of the exchange phenomena which do not presuppose any knowledge of groups on the part of the reader.*

In a certain way Dirac anticipates Occam's razor, but Dirac himself drifts to a very combinatorial discussion in deriving the Hamiltonian. However, it will be shown that certain higher mathematical techniques shed another light on the treatment of a physical issue not to veil the physical nature in large non-instructive computations.
One shall understand how Heisenberg's Hamiltonian is the most general form for a Hamiltonian of a 2-fermion-interaction by following some simple steps described in the following subsection.

1.3.1 Derivation of the Heisenberg Hamiltonian

John Hasbrouck Van Vleck (1899-1980) derived in his book[22] in 1932 the form of Heisenberg's Hamiltonian starting with the general non-relativistic Hamiltonian for 2 identical spin-1/2 fermions[23]

$$\begin{aligned} H &:= H_1 + H_2 + V_{12}, \\ H_i &:= \frac{P_i^2}{2m} + V, \end{aligned}$$

imposing the Pauli principle and respecting the spins of the single electrons. V_{12} stands for the coupling between the electrons, whereas V only acts on the single particles. The aim is to transform the Hamiltonian for the case that it is acting on the spin wave function of the electrons instead of the orbital wave function, i.e., one wants to find a corresponding Hamiltonian $H^{(S)}$ s.t.

$$H\psi = E\psi \quad \Leftrightarrow \quad H^{(S)}\chi = E\chi,$$

[21] [Dir29], p. 716
[22] [VV32], p. 316-321
[23] I am here using my own notation to emphasize the crucial steps

where $\psi \in L^2(\mathbb{R}^3)$ and $\chi \in \mathbb{C}^2$. This throws a conceptually completely different light on the problem[24]. With the ansatz[25]

$$\begin{aligned} |\psi_I\rangle &= |\psi_1, \psi_2\rangle \\ |\psi_{II}\rangle &= |\psi_2, \psi_1\rangle , \end{aligned}$$

which respects the indistinguishability of the two particles, the eigenvalue equation becomes

$$\begin{vmatrix} W_0 + K_{12} - E & J_{12} \\ J_{12} & W_0 + K_{12} - E \end{vmatrix} = 0, \tag{1.3.2}$$

where we introduced

$$\begin{aligned} W_0 &:= \langle\psi_I| H_1 + H_2 |\psi_I\rangle = \langle\psi_{II}| H_1 + H_2 |\psi_{II}\rangle \\ K_{12} &:= \langle\psi_I| V_{12} |\psi_I\rangle = \langle\psi_{II}| V_{12} |\psi_{II}\rangle \\ J_{12} &:= \langle\psi_I| V_{12} |\psi_{II}\rangle = \langle\psi_{II}| V_{12} |\psi_I\rangle . \end{aligned}$$

V_{12} is assumed to fulfill the above symmetries, which is, e.g., the case if

$$\langle r_1, r_2| V_{12} |r_1, r_2\rangle = \frac{1}{|r_1 - r_2|},$$

i.e., a Coulomb potential. The eigenvalues with corresponding eigenkets are

$$\begin{aligned} W_1 &= W_0 + K_{12} + J_{12}, \quad |\psi_s\rangle = \frac{\sqrt{2}}{2} \left(|\psi_I\rangle + |\psi_{II}\rangle\right) \\ W_2 &= W_0 + K_{12} - J_{12}, \quad |\psi_a\rangle = \frac{\sqrt{2}}{2} \left(|\psi_I\rangle - |\psi_{II}\rangle\right) . \end{aligned}$$

If one now takes into account that fermions obey the Pauli principle and thus their wave function must be antisymmetric, one concludes that the only possible combinations are that the orbital wave function is antisymmetric and the spin wave function is symmetric and vice versa.

[24] Taking the Dirac equation into consideration one notices that spin arises with the relativistic motion of the electrons. In this sense the spin and the orbital wave function are related.

[25] I use the Dirac notation, Van Vleck himself chose the space representation for the eigenfunctions

Since one is dealing with a non-relativistic discussion, the spin wave function can now be considered separately. The total spin is given by

$$(\mathbf{S_1} + \mathbf{S_2})^2 = \mathbf{S}^{2}{}^{26} = S(S+1),$$

where the total spin quantum number S can attain the eigenvalues 0 and 1 depending on whether the spins are anti-parallel or parallel. The operators $\mathbf{S_i}^2$ themselves have the eigenvalue 3/4. One hence obtains

$$S_1 \cdot S_2 = \frac{1}{2}\left(S^2 - S_1^2 - S_2^2\right) \text{"} = \text{"} \begin{cases} 1/4 & \text{parallel spins} \\ -3/4 & \text{anti-parallel spins} \end{cases} .$$

The last equality shall indicate the possible Eigenvalues of the operator.
The aim is now to derive the interaction potential V_{12} which gives back the above Eigenvalues, starting with the eigenvalue equation (1.3.2). Since a symmetric orbital wave function yields a anti-symmetric spin function and vice versa, one first obtains

$$V_{12} \quad = \begin{cases} K_{12} + J_{12} & \text{spins anti-parallel} \\ K_{12} - J_{12} & \text{spins parallel} \end{cases} .$$

A general ansatz to solve this problem is

$$V_{12} \quad = \quad K_{12} + (x + y(S_1 \cdot S_2))J_{12}.$$

Together with the corresponding eigenvalues of $S_1 \cdot S_2$, one gets a system of linear equations

$$\left| \begin{array}{rcrcr} x & + & \frac{1}{4}y & = & -1 \\ x & - & \frac{3}{4}y & = & 1 \end{array} \right| .$$

With this one obtains

$$V_{12} \quad = \quad K_{12} - \frac{1}{2}J_{12} - 2J_{12}S_1 \cdot S_2.$$

This result gives an even more general form for the Heisenberg Hamiltonian

$$H \quad = \quad -2\sum_{j\#k} J_{jk} S_j \cdot S_k,$$

which in this case only plays the role of an interaction potential.

[26] In here I mean operators by bold letters and the eigenvalue by the normal font.

1.3.2 Approaches to the Heisenberg model

It is now understood, how the Heisenberg model arises naturally. A basic property of the Heisenberg model is that it maintains invariant under rotations. Thus it includes Weiss' imagination of free micro-magnets. Since the Heisenberg model arose out of quantum mechanical considerations, it was viewed a long time to be a candidate for an adequate description of ferromagnetism. In 1931, however, *Hans Bethe* (1906-2005) [Bet31] could solve the one-dimensional periodic, ferromagnetic Quantum Heisenberg model

$$H = -2J \sum_{k=1}^{N} S_k \cdot S_{k+1}, \quad S_{N+1} = S_1, \quad J > 0$$

i.e., he determined the zeroth order eigenfunctions and the first order Eigenvalues for a linear chain of coupled spins with only nearest-neighbor-interaction. The so-called *Bethe ansatz* which he provided in this paper was used many times later to solve a lot of many body problems[27]. One could apply this method to the 1d Ising model, but it required much more effort than the usual transfer matrix method Ising. The computation of the 1d Heisenberg model is not shown in here, but see e.g. [KM98].
In 1966, *Nathaniel David Mermin* (*1935) and *Herbert Wagner* (*1935) [MW66], as well as *Pierre C. Hohenberg* (*1934) [Hoh67], proved that neither the one-dimensional nor the two-dimensional Heisenberg model exhibit spontaneous magnetization.

1.3.1 Theorem (Mermin-Wagner-Hohenberg)**.** *The Heisenberg model*

$$H \quad = \quad -2 \sum_{ij} J_{ij} S_i \cdot S_j - B \cdot \sum_i e^{\mathrm{i}q \cdot R_i} S_i^z$$

with certain J_{ij} does not yield spontaneous magnetization in one or two dimensions, i.e.

$$\lim_{B \to 0} \lim_{N \to \infty} \frac{1}{N} \langle \sum_i e^{\mathrm{i}q \cdot R_i} S_i^z \rangle = 0$$

Proof. Cf. [Roe77] and [MW66]. In [Roe77] a stronger inequality than Bogoliubov's inequality is obtained in order to prove the Mermin-Wagner theorem. □

[27] In the appendix A.1 the Bethe ansatz is described a little.

It is crucial to distinguish between the ferromagnetic/anti-ferromagnetic Quantum/classical Heisenberg model. All four have very different properties and have to be treated mathematically different one from each other. The *classical* d-dimensional Heisenberg model on a finite lattice $\emptyset \neq \Lambda \subseteq \mathbb{Z}^d$, $d \in \mathbb{N}$, with the space dimension $n \in \mathbb{N}$ has the Hamilton function

$$H : (\mathcal{S}_{fin}^{d-1})^{\Lambda 28} \to \mathbb{R}, S \mapsto -\sum_{i,j\in\Lambda, i\neq j} J_i j S_i \cdot S_j + H \cdot \sum_{i\in\Lambda} S_i^{(1)},$$

whereas the Quantum Heisenberg model in that case, but with space dimension $n = 3$, is

$$\mathscr{H} \quad := \quad -\sum_{i,j\in\Lambda, i\neq j} J_{ij} \mathbf{S_i} \cdot \mathbf{S_j} + \boldsymbol{H} \cdot \sum_{i\in\Lambda} \mathbf{S_i^{(1)}}.$$

In here, $\mathbf{S_i} = (\mathbf{S_i^x}, \mathbf{S_i^y}, \mathbf{S_i^z})$ can be represented with the Pauli matrices $\{\tau_i^x, \tau_i^y, \tau_z^i\}$ in virtue of $\mathbf{S_i} = \frac{1}{2}(\tau_i^x, \tau_i^y, \tau_z^i)$. The Heisenberg model is said to be $\{^{ferromagnetic}_{antiferromagnetic}\}$ iff $\exists J \in \{^{\mathbb{R}^+}_{\mathbb{R}^-}\} \forall i, j \in \Lambda : J_{ij} = J$.
Fröhlich, Israel, Lieb and Simon [FILS78] discussed the classical (ferro- and antiferromagnetic) Heisenberg model in any dimension with long range order interaction among other classical models, i.e., they analyzed the existence of a phase transition. In addition, Dyson, Lieb and Simon [DLS78] could treat the n-dimensional, $n \geq 3$, Quantum *anti*-ferromagnetic Heisenberg model. They claimed to have treated the ferromagnetic Heisenberg model, too, but Fröhlich pointed out an error in the proof.

In contrast to the Ising model, there are no exact solutions for the Heisenberg model in higher dimensions than 1. As mentioned in the preface, a model can be considered a model if it provides a solution. The steps I want to emphasize are purely epistemological, namely

- finding an ansatz,
- understanding mathematically why the model actually works,
- computing the model.

As far as the Ising model is concerned, this steps can be attributed to 3 physicists, namely, in the above order, Wilhelm Lenz, *Rudolf Peierls* (1907-

[28] $\mathcal{S}_{fin}^{(n-1)} := \{x \in \mathbb{R}^n | ||x|| = 1\}$ denotes the $(n-1)$-dimensional unit sphere.

1995) and Lars Onsager. Ironically, even though Peierls [Pei36] could show[29] in 1936 that the 2D Ising model exhibits spontaneous magnetization, he did not believe that it could correctly describe ferromagnetism. Peierls' proof shall not be discussed in here because it takes place in the Bachelor thesis of a friend of mine. Considering the Heisenberg model as describing ferromagnetism more adequately to the "more complicate nature than [...] assumed by Ising", Peierls concluded that "the Ising model [was] therefore [then] only of mathematical interest"[30]. In 1944, Onsager [Ons44] then provided the exact computation, but it is not very ostensive. In addition, in contrast to the method discussed below, it cannot exhibit deeper physical insight into the problem.

1.4 Heisenberg model vs. Ising model

In the following, I will discuss Lenz' correct objection towards the idea of rotational invariance of the "micro-magnets" due to the fact, that one is given anisotropy in a crystal lattice, in more detail. Before one can dedicate oneself to that, the symmetries given in the single models shall be demonstrated: The free Heisenberg model - without external field H - has free total spin rotatability, i.e.,

$$[H_{Heis}, \sum_i S_i^2] \quad = \quad 0.$$

Because of

$$[H_{Heis}, \sum_i S_i^{(1)}] \quad = \quad 0$$

the Heisenberg further shares the $\mathbb{Z}_2$ symmetry with the Ising Hamiltonian, i.e., flipping every single spin $S_i \to -S_i$ leaves the Hamiltonian invariant. Due to the $\mathbb{Z}_2$ symmetry of the bare Hamiltonians, the magnetization vanishes for both models in the finite case. There are different types of magnetization (cf. [GUW11], p. 193-194):

- The *thermodynamic magnetization* m_{th} is defined by

$$\forall \beta \in \mathbb{R}^+ : \quad m_{th}(\beta) \quad := \quad - \lim_{h \to 0^+} \frac{f(\beta, h) - f(\beta, 0)}{h}.$$

[29] As Griffith [Gri64] says himself in his own paper, *N.G. van Kampen* and *M.E. Fisher* pointed to him, that Peierls actually had an error in his calculation. However, in that paper Griffith could correct the first attempt of the proof.

[30] [Pei36], p. 477

This limit exists since f is concave. $f(\beta, h)$ denotes the van Hove-limit of the free energy with non-vanishing external magnetic field h (cf. chapter 2).

- The *residual magnetization* m_{res} is defined by

$$\forall \beta \in \mathbb{R}^+ : \quad m_{res}(\beta) \quad := \quad \lim_{h \to 0^+} \lim_{|\Lambda| \to \infty \text{ v.H.}} \frac{1}{|\Lambda|} \langle M_\Lambda(\beta, h) \rangle.$$

In here $\lim_{|\Lambda| \to \infty \text{ v.H.}}$ stands for the van Hove limit (cf. again 2) and the mean value operator $\langle \cdot \rangle$ depends on whether one is dealing with boundary conditions or not.

- The *spontaneous magnetization* is defined by

$$\forall \beta \in \mathbb{R}^+ : \quad m_{sp}(\beta) \quad := \quad \liminf_{|\Lambda| \to \infty \text{ v.H.}} \frac{1}{|\Lambda|} \langle |M_\Lambda(\beta, 0)| \rangle.$$

Because it is easier to calculate, one works with

$$\forall \beta \in \mathbb{R}^+ : \quad \tilde{m}^2_{sp}(\beta) \quad := \quad \liminf_{|\Lambda| \to \infty \text{ v.H.}} \frac{1}{|\Lambda|} \langle M_\Lambda(\beta, 0)^2 \rangle.$$

At this point, it is unclear if these types of magnetization even exist. They are mentioned to stress the fact, that there are different mathematical definitions of the macroscopic observable, the magnetization.

If one respects the possible anisotropy Lenz already mentioned (cf. section 1.2), one concludes that physically the Heisenberg model is not the more general case for the Ising model, although it is mathematically (by reducing the space dimension to 1). So, if one wants to analyze (anti-)ferromagnetic properties of a material, one has to start considering the Hamiltonian

$$H \quad = \quad -2 \sum_{i \neq j} J_{ij} \left(\alpha_{xy} (S^x_i S^x_j + S^y_i S^y_j) + \alpha_z S^z_i S^z_j \right).$$

Three special cases which are realized in nature are

(i) $\alpha_{xy} = \alpha_z \neq 0$: the Heisenberg model,

(ii) $\alpha_{xy} = 0, \alpha_z \neq 0$: the Ising model,

(iii) $\alpha_{xy} \neq 0, \alpha_z = 0$: the xy-model.

In order to determine the domains in which either the Heisenberg model or the Ising model is an adequate description, one must discuss microscopic reasons for possible anisotropy in a crystal, so-called *magnetocrystalline anisotropy*[31].

Dipole-dipole interaction

If the multipole expansion of the magnetic field B is taken into consideration, one obtains dipole-dipole interaction for the ions as a small effect additional to the exchange effect discussed before. Although the correction might be small, it behaves like $|r_i - r_j|^{-3}$ and can, thus, cause anisotropy in the electronic structure of the crystal. Defining

$$e_{ij} \quad := \quad \frac{r_i - r_j}{|r_i - r_j|} \quad i \neq j$$

one can write the corresponding Hamiltonian for the dipole-dipole interaction as follows:

$$H_{dip} \quad := \quad \sum_{i \neq j} \frac{D_{ij}}{|r_i - r_j|^3} \left(S_i \cdot S_j - 3(S_i \cdot e_{ij})(S_j \cdot e_{ij}) \right).$$

In here, one identifies the magnetic moment μ_i of an ion with the spin S_i in virtue of

$$\mu_i \quad = \quad g\mu_B S_i.$$

Here μ_B and g are the Bohr magneton and the corresponding Landé-factor for the electrons.

Spin-orbit interaction

A further reason for anisotropy within a crystal is the spin-orbit interaction, that arises, if one analyzes the Dirac equation

$$\left(\not{\mathcal{P}} - m - \gamma^0 V \right) \psi \quad = \quad 0$$

with $\mathcal{P}$ being the corresponding 4-vector to the 3-momentum P. The equivalent Hamiltonian to describe this problem is

$$\begin{aligned} H \quad &= \quad \alpha \cdot P + \beta m + V \\ \beta \quad &= \quad \gamma^0, \quad \alpha^i \quad = \quad \gamma^0 \gamma^i \end{aligned}$$

[31] For this I consulted [Say10]

with the Dirac matrices γ^μ. By applying the *Foldy-Wouthuysen transformation*, which decouples particles and antiparticles, one obtains, besides the relativistic correction and the Zeemann term, a spin-orbit coupling term

$$H_{SO} \quad = \quad \sum_i \underbrace{\frac{\hbar^2}{2m^2c^2}\frac{1}{r_i}\left(\frac{\partial \Phi}{\partial r}\right)_i}_{=:\lambda_i} S_i \cdot L_i.$$

In here, m is the electron mass. Depending on the coupling λ_i in the given crystal, the Hamiltonian including this coupling is not invariant towards spin rotation anymore.

Chapter 2

Existence of the thermodynamic limit

Before one dedicates oneself to the thermodynamic limit for spin systems, spin interactions must first be discussed. In this chapter, I refer basically to [KS04]. In the following let $d \in \mathbb{N}$.

2.1 Spin systems

As mentioned above, one is given the fact that the spin is quantized in *up* (denoted as 1) and *down* (denoted as 0) spin. It seems paradox to talk about *classical* spin, since the spin is a Quantum feature. A *classical* consideration means the description using the Hamilton *function*. In this way, one can rigorously quantize the system by identifying the Hamilton function with the Hamilton *operator*. In chapter 1 it is explained how a spin coupling arises, but in order to provide a thermodynamic limit - which has not been defined, yet - one must take care whether the series, one is dealing with, is converging. If one were not able to obtain a converging series, the term "model" for the above mentioned theories could not be justified and these stayed *attempts*.

2.1.1 Topological and stochastical intermezzo

2.1.1 Definition (Topological space)**.** *A* topological space *is a pair* $(T, \mathcal{O})$ *where* T *is a set and* $\mathcal{O}$*, the* topology *on* T *respectively the set of so-called*

open sets, *fulfills the following:*

(i) $\emptyset, T \in \mathcal{O}$,

(ii) $\forall O_1, O_2 \in \mathcal{O}$: $O_1 \cap O_2 \in \mathcal{O}$,

(iii) $\forall O_1, O_2, \ldots \in \mathcal{O}$: $\bigcup_{i=1}^{\infty} O_i \in \mathcal{O}$.

If it is clear which topology T is equipped with one says:"T is a topological space".

2.1.2 Definition (Continuous map)**.** *For two topological spaces $(X, \mathcal{O}_X)$ and $(Y, \mathcal{O}_Y)$ a map $f : X \to Y$ is called* continuous *iff*

$$\forall O \in \mathcal{O}_Y : \quad f^{-1}(O) \in \mathcal{O}_X.$$

2.1.3 Definition (Product topology)**.** [1] *Let I be an index set and $\{(X_i, \mathcal{O}_{X_i}) | i \in I\}$ be a family of topological spaces. Define*

$$\begin{aligned} \underset{i\in I}{\times} X_i \quad &:= \quad \{(x_i)_{i\in I} | \forall i \in I : x_i \in X_i\}, \\ \forall i \in I : \pi_j : \underset{i\in I}{\times} X_i &\to X_j, (x_i)_{i\in I} \mapsto x_j \text{[2]}. \end{aligned}$$

The product topology *is the smallest (or coarsest[3]) topology with respect to $\subseteq$ as partial order on which all π_i, $i \in I$ are continuous.*

2.1.4 Definition (σ-algebra)**.** *Let M be a set. A* σ-algebra *on M is a set $\mathcal{M} \subseteq \mathcal{P}(M)$ of sets s.t.*

(i) $M \in \mathcal{M}$,

(ii) $\forall A \in \mathcal{M}$: $A^c \in \mathcal{M}$,

(iii) $\forall A_1, A_2, \ldots \in \mathcal{M}$: $\bigcup_{i=1}^{\infty} A_i \in \mathcal{M}$.

2.1.5 Definition. *Let Ω be a set and $\mathcal{A}$ be a σ-algebra on Ω. Let $\mathbb{P} : \mathcal{A} \to \mathbb{R}$ be a map s.t.*

---

[1] cf. [Jän08], chapter 6

[2] $\forall j \in I$ π_j is called the *canonical projection.*

[3] Let X be a set and $\mathcal{O}_1$ and $\mathcal{O}_2$ be two topologies on X. $\mathcal{O}_1$ is said to be $\{^{\text{coarser}}_{\text{finer}}\}$ than $\mathcal{O}_2$ iff $\mathcal{O}_1 \{\subseteq\} \mathcal{O}_2$.

(i) $\mathbb{P}(\Omega) = 1$,

(ii) $\forall A \in \mathcal{A}$: $\mathbb{P}(A^c) = 1 - \mathbb{P}(A)$,

(iii) $\forall A_1, A_2, \ldots \in \mathcal{A}, \forall i \neq j : A_i \cap A_j = \emptyset$: $\mathbb{P}(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} \mathbb{P}(A_i)$.

$\mathbb{P}$ *is called a* probability measure *on* Ω *and* $(\Omega, \mathcal{A}, \mathbb{P})$ *a* probability space.

In order to discuss a general setup, the following definition for a classical spin is adopted from [KS04].

2.1.6 Definition (Classical spin)**.** [4] *A* classical spin *is a measure space* $(E, \mathcal{E}, \mu)$ *with the so-called* a-priori measure μ.

2.1.2 Classical systems

Finite spin systems

Define the set of spin orientation for a single spin

$$E \quad := \quad \{-1; 1\}.^{5}$$

2.1.7 Definition. *Let* $\Lambda \subseteq \mathbb{Z}^d$ *and*

$$\Omega_\Lambda \quad := \quad E^\Lambda.$$

$\omega \in \Omega_\Lambda$ *is called a* spin configuration *on* Λ[6].

A *finite lattice* is a subset $\Lambda \subseteq \mathbb{Z}^d$ with $0 < |\Lambda| < \infty$[7]. In order to define a probability measure, one may just use the power set $\mathcal{P}(\Lambda)$ of Λ. Before it is possible to find a probability measure which maximizes the entropy under the constraint of given internal energy, i.e., if one considers a canonical ensemble, we shall discuss the most general form of an interaction Hamiltonian for the system Λ.

---

[4] cf. [KS04], p. 44

[5] In the set of this chapter it is more convenient to deal with this notation for up and down spin. One finds a bijective map, $\{-1; 1\} \to \{0; 1\}, s \to \frac{s+1}{2}$, to identify both notations.

[6] Recall, that $\omega \in \Omega_\Lambda$ is a map which maps each vertex $i \in \Lambda$ to a spin orientation (up/down).

[7] In here, one uses the counter measure in order to determine the volume of a finite subset of $\mathbb{Z}^d$.

2.1.8 Definition (Finite Ising model)**.** *Let* $\Lambda \subseteq \mathbb{Z}^d$, $0 < |\Lambda| < \infty$ *and*

$$J : \mathcal{P}(\Lambda) \to \mathbb{R}.$$

The Hamilton function for the classical Ising model *on* Λ *is*

$$H_\Lambda : \Omega_\Lambda \to \mathbb{R}, (\sigma_1, \sigma_2, \ldots, \sigma_{|\Lambda|}) \mapsto -\sum_{L \subseteq \Lambda} J(L) \prod_{i \in L} {\sigma_i}^8. \tag{2.1.1}$$

2.1.9 Remark.

- *Note that one is dealing in here with a finite summation, thus,* H_Λ *attains finite values if it is applied to a* $\sigma \in \Omega_\Lambda$.
- *In the case of a finite lattice* $\Lambda \subseteq \mathbb{Z}^d$*, a map* $J : \mathcal{P}(\Lambda) \to \mathbb{R}$ *is called an interaction potential.*

In a finite lattice Λ, the probability measure for a particle being in a certain state is defined by maximizing the entropy S_Λ under the constraints of given observables. In the case of a *canonical ensemble*, i.e., under the constraint of fixed internal energy, one obtains as a probability measure

$$P_\Lambda : \Omega_\Lambda \to [0,1], \sigma \mapsto \frac{\mathrm{e}^{-\beta H_\Lambda(\sigma)}}{\sum\limits_{\sigma' \in \Omega_\Lambda} \mathrm{e}^{-\beta H_\Lambda(\sigma')}}$$

This result will not be shown, since it is given in any textbook[9].

Infinite spin systems

If one wants to proceed to the case of an infinite lattice $\Lambda \subseteq \mathbb{Z}^d$, $|\Lambda| = \infty$, one has to face several problems:

- The expression for the (classical) Hamilton function does not converge for every spin configuration $\sigma \in \Omega_\Lambda$.

[8] For $L \in \mathcal{S}_{fin}(d)$ and $(\sigma_i)_{i \in L} \in \Omega_L$ one will denote $\sigma_L := \prod\limits_{i \in L} \sigma_i$.

[9] Again, it is recommended [KS04]. It is explained how the density matrix belonging to the maximal entropy can be obtained in the quantum mechanical case(chapter 4). The classical case for a *finite* lattice can be obtained through introducing Lagrange multipliers for the constraints.

- A probability measure cannot be defined because there is not even a system of measurable[10] sets on which it is possible to define it. Note that $\mathcal{P}(\Lambda)$ is not a suitable σ-algebra to define a (probability) measure on it!

- One cannot ensure that there is an asymptotic measure.

This problem can be circumvented if a topology on $\Omega := E^{\mathbb{Z}^d}$ is introduced, so that there is a concept of open sets on Ω, in order to define *observables* which are defined to be continuous maps. For a start, one chooses the discrete topology $\mathcal{P}(E)$ on E and then one defines $\mathcal{O}$ to be the *product topology* on Ω. One finally obtains a suitable σ-algebra for the spin configurations

$$\mathcal{A} \quad := \quad \sigma(\mathcal{O}).^{11}$$

2.1.10 Remark. *Starting with*

$$\mathcal{S}_{fin}(d) \quad := \quad \{\Lambda \subseteq \mathbb{Z}^d | 0 < |\Lambda| < \infty\},$$

the set of all finite subsets of $\mathbb{Z}^d$, the canonical projection π_Λ for $\Lambda \subseteq \mathbb{Z}^d$ is defined in virtue of

$$\pi_\Lambda : \Omega \to \Omega_\Lambda, \sigma \mapsto \sigma\big|_\Lambda = (\sigma_l)_{l\in\Lambda}{}^{12}.$$

For the given purpose it is sufficient to define a measure on $\mathcal{I}$,

$$\mathcal{I} \quad := \quad \{\pi_\Lambda^{-1}(\sigma) | \Lambda \in \mathcal{S}_{fin}(d), \sigma \in \Omega_\Lambda\},$$

which consists of finite lattices. In general, a phase transition, which in the case of this thesis is established in the heat capacity, appears whenever the corresponding Gibbs measure stops being unique. A discussion can be found in [KS04].

---

[10] Note: The σ-algebra defines the measurable sets. In order to provide a well-defined measure, one looks for a generating system on which one can define a measure.

[11] For a system of sets $\mathcal{E}$ $\sigma(\mathcal{E}) := \bigcap_{\mathcal{M}\supseteq\mathcal{E}\ \sigma\text{-algebra}} \mathcal{M}$ means the smallest σ-algebra which contains $\mathcal{E}$, i.e. $\forall$ σ-algebras $\mathcal{M}$ containing $\mathcal{E}$ one has $\sigma(\mathcal{E}) \subseteq \mathcal{M}$.

[12] Note, that $\forall\sigma \in \Omega \forall i \in \mathbb{Z}^d : \quad \sigma_i := \sigma\big|_i$.

2.1.11 Definition (Microscopic observable). [13] *A continuous map*

$$f : \Omega \to \mathbb{R} \tag{2.1.2}$$

is called a (microscopic) classical observable.

2.1.12 Definition. *An* Ising (interaction) potential (without boundary conditions) *on* $\mathbb{Z}^d$ *is a map* $J : \mathcal{S}_{fin}(d) \to \mathbb{R}$ *with*

$$||J||_d^{(I)} := \sup_{i \in \mathbb{Z}^d} \sum_{i \in \Lambda \in \mathcal{S}_{fin}(d)} \frac{|J(\Lambda)|}{|\Lambda|} < \infty. \tag{2.1.3}$$

$$\mathcal{R}(J) := \sup_{\Lambda \in \mathcal{S}_{fin}(d), J(\Lambda) \neq 0} (\mathrm{diam}(\Lambda)) \tag{2.1.4}$$

is called the range *of* J *where for* $\Lambda \in \mathcal{S}_{fin}(d)$

$$\mathrm{diam}(\Lambda) := \max_{i,j \in \Lambda} (||i - j||_1)^{14}$$

is the diameter *of* Λ.

2.1.13 Remark.

- *One can easily verify that eq.* (2.1.3) *defines a norm on* $\{J : \mathcal{S}_{fin}(d) \to \mathbb{R}\}$.
- *One could think of other possible norms on* $\{J : \mathcal{S}_{fin}(d) \to \mathbb{R}\}$, *e.g.*

$$||J|| := \sup_{\Lambda \in \mathcal{S}_{fin}(d)} \frac{|J(\Lambda)|}{|\Lambda|}.$$

  Though in order to provide a well-defined free energy, it is sufficient to look at $||\cdot||_d^{(I)}$ *as it will be seen below. In addition,* $||\cdot||$ *does not include all interactions on a single spin of the lattice whereas* $||\cdot||_d^{(I)}$ *does.*

- *From the definition of* $||\cdot||_d^{(I)}$ *one can see that* $J : \mathcal{S}_{fin}(d) \to \mathbb{R}$ *must decay sufficiently fast in order to be an Ising potential. This feature renders the physical nature of the exchange integral discussed above.*

---

[13] cf. [KS04], p.57

[14] $\forall x, y \in \mathbb{R}^d : ||x - y||_1 := \sum_{i=1}^{d} |x_i - y_i|$

2.1.14 Definition. *Let $J : \mathcal{S}_{fin}(d) \to \mathbb{R}$ be an Ising potential. J is said to be*

- *a* next-neighbor potential *iff* $\mathcal{R}(J) \leq 1$,
- translational invariant *iff* $\forall \Lambda \in \mathcal{S}_{fin}(d) \forall a \in \mathbb{Z}^d : J(\Lambda + a) = J(\Lambda)$[15],
- ferromagnetic *iff* $J \geq 0$.[16]

2.1.15 Remark. *In the transition to an infinite system, one starts by considering a finite system on which the spin configuration is fixed, but the information about the surrounding spins on the lattice is left vacant. Nonetheless, in the set of the general interaction that was treated now, it is unavoidable to discuss the interaction on the surface, that means the interaction between the spins in the considered finite system with the environment. The aim will be to pick a sequence of finite systems, so that the interaction with the environment becomes irrelevant for the limit. Using this approach, one can ensure that any boundary conditions can be imposed and the limit stays the same.*

2.1.16 Definition. $J : \mathcal{S}_{fin}(d) \to \mathbb{R}$ *is defined to be an* Ising potential with boundary condition *iff*

$$\forall \Lambda \in \mathcal{S}_{fin}(d) : \sum_{L \in \mathcal{S}_{fin}(d), L \cap \Lambda \neq \emptyset} |J(L)| < \infty$$

Remark. *It is*

$$\begin{aligned} \emptyset &\neq \{J : \mathcal{S}_{fin}(d) \to \mathbb{R} | \mathcal{R}(J) < \infty\} \\ &\subseteq \left\{ J : \mathcal{S}_{fin}(d) \to \mathbb{R} | \forall \Lambda \in \mathcal{S}_{fin}(d) \sum_{L \in \mathcal{S}_{fin}(d), L \cap \Lambda \neq \emptyset} |J(L)| < \infty \right\}. \end{aligned}$$

It is now possible to allow boundary conditions on a $\Lambda \in \mathcal{S}_{fin}(d)$.

2.1.17 Definition. *Let $\Lambda \in \mathcal{S}_{fin}(d)$, $\tau \in \Omega_{\Lambda^c}$. For an Ising potential with boundary condition $J : \mathcal{S}_{fin}(d) \to \mathbb{R}$ one defines the Hamilton function for the classical Ising model* with boundary condition τ *to be*

$$H_\Lambda^\tau : \Omega_\Lambda \to \mathbb{R}, \sigma \mapsto - \sum_{L \in \mathcal{S}_{fin}(d), L \cap \Lambda \neq \emptyset} J(L) \sigma_{L \cap \Lambda} \tau_{L \cap \Lambda^c}. \tag{2.1.5}$$

[15] $\forall \Lambda \subseteq \mathbb{R}^d a \in \mathbb{R}^d : \Lambda + a := \{l + a | l \in \Lambda\}$

[16] Note that this definition depends on the definition of the Hamiltonian J is ascribed to!

2.1.18 Remark. *For the given purposes, it is sufficient to consider Ising potentials with boundary conditions with finite range. Chapter 3 deals with next-neighbor potentials.*

2.1.19 Lemma. *Let $\Lambda \in \mathcal{S}_{fin}(d)$, $J : \mathcal{S}_{fin}(d) \to \mathbb{R}$ be an Ising potential and $H_\Lambda : \Omega_\Lambda \to \mathbb{R}$ be the in eq. (2.1.1) defined corresponding Ising Hamilton function. One obtains*

$$||H_\Lambda||_\infty \quad \leq \quad |\Lambda| \cdot ||J||_d^{(I)},$$

where $||\cdot||_\infty$ means the usual supreme norm on $\{\Omega_\Lambda \to \mathbb{R}\}$. So the energy density is bounded for Ising potentials.

Proof. One has

$$||H_\Lambda||_\infty = \max_{\sigma\in\Omega_\Lambda} \left| \sum_{L\subseteq\Lambda} J(L)\sigma_L \right| \leq \sum_{L\subseteq\Lambda} |J(L)| = \sum_{L\subseteq\Lambda} \underbrace{\sum_{i\in L}}_{=\sum_{i\in\Lambda} \mathbb{1}_L(i)} \frac{|J(L)|}{|L|}$$

$$= \sum_{i\in\Lambda} \sum_{i\in L\subseteq\Lambda} \frac{|J(L)|}{|L|} \leq \sum_{i\in\Lambda} \underbrace{\sum_{i\in L\in\mathcal{S}_{fin}(d)} \frac{|J(L)|}{|L|}}_{\leq ||J||_d^{(I)}} \leq |\Lambda| \cdot ||J||_d^{(I)}$$

□

2.1.3 Quantum spin systems

The Hilbert space $\mathcal{H}^{(1)}$ of a single 1/2-spin can be described as

$$\mathcal{H}^{(1)} \quad := \quad \mathbb{C}^2$$

and thus the Hilbert space for an n 1/2-spin system, $n \in \mathbb{N}$, becomes

$$\mathcal{H}^{(n)} \quad := \quad \bigotimes_{i=1}^{n} \mathbb{C}^2.$$

In order to find the corresponding Hamilton operator $\mathcal{H}$ to the Hamilton function $H : \Omega_\Lambda \to \mathbb{R}$ in eq. (2.1.1), one identifies

$$\forall i \in \Lambda : E \to B(\mathcal{H}), \sigma_i \mapsto \mathrm{Id} \otimes \ldots \otimes \mathrm{Id} \otimes \underbrace{\sigma^z}_{i^{th} \text{ position}} \otimes \mathrm{Id} \otimes \ldots \otimes \mathrm{Id}. \quad (2.1.6)$$

Here, σ^z is the Pauli matrix

$$\sigma^z \quad := \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

represented in the canonical basis of a single up $\binom{1}{0}$ and down $\binom{0}{1}$ spin. In this thesis the fact that one can map a classical problem to a Quantum mechanical problem will be used in order to solve it.

2.1.20 Definition (Quantum mechanical observable)**.** *A* Quantum mechanical observable *on a Hilbert space $\mathcal{H}$ is a self-adjoint operator $O : \mathcal{H} \to \mathcal{H}$.*

2.1.21 Remark. *Let $n \in \mathbb{N}$. If one wants to map a classical spin system to a Quantum spin system, one extends*

$$\phi : E \to \mathcal{H}^{(1)}, \begin{cases} 1 \mapsto \binom{1}{0} \\ -1 \mapsto \binom{0}{1} \end{cases}$$

to a map on E^n in virtue of

$$\phi_n : E^n \to \mathcal{H}^{(n)}, (\sigma_1, \sigma_2, \ldots, \sigma_n) \mapsto \bigotimes_{i=1}^{n} \phi(\sigma_i).$$

Define[17]

$$\psi_n : \mathcal{C}(E^n, \mathbb{R}) \to B(\mathcal{H})$$

by

$$\forall O \in \mathcal{C}(E^n, \mathbb{R}) \quad \forall \sigma \in E^n : \quad \psi_n(O)\phi_n(\sigma) = O(\sigma)\phi_n(\sigma).$$

So, $\psi_n(O)$ is diagonal on $\{\phi_n(\sigma) | \sigma \in E^n\}$, which itself defines a basis of $\mathcal{H}^{(n)}$. An example was given in eq. (2.1.6)*.*

2.2 Thermodynamic limit in a classical spin system

We now want to consider the limit of a certain sequence of finite lattices before to define the limit for the density of the free energy. In the classical

[17] In here one denote for two topological spaces A, B $\mathcal{C}(A, B) := \{f : A \to B | f \text{ continuous}\}$

case the free energy is defined by

$$\forall \Lambda \in \mathcal{S}_{fin}(d): \quad f_\Lambda : \mathbb{R}^+ \to \mathbb{R}, \beta \mapsto -\frac{1}{\beta|\Lambda|} \log \left(\sum_{\sigma \in \Omega_\Lambda} \mathrm{e}^{-\beta H_\Lambda(\sigma)} \right). \tag{2.2.1}$$

Again a notation for the case that one is dealing with boundary conditions on H shall be introduced. I.e., for $\Lambda \in \mathcal{S}_{fin}(d)$, $\tau \in \Omega_{\Lambda^c}$, one defines

$$f_\Lambda^\tau : \mathbb{R}^+ \to \mathbb{R}, \beta \mapsto -\frac{1}{\beta|\Lambda|} \log \left(\sum_{\sigma \in \Omega_\Lambda} \mathrm{e}^{-\beta H_\Lambda^\tau(\sigma)} \right) \tag{2.2.2}$$

in the case of an Ising potential with boundary condition τ.

2.2.1 Definition (van Hove sequence)**.** *A sequence* $(\Lambda_n)_{n\in\mathbb{N}} \in \left(\mathbb{Z}^d\right)^{\mathbb{N}}$ *of subsets* $\Lambda_n \subseteq \mathbb{Z}^d$ *is called a* van Hove sequence *iff*

$$\lim_{n\to\infty} |\Lambda_n| = \infty \quad \textit{and} \quad \forall h \in \mathbb{N}: \lim_{n\to\infty} \frac{V_h(\Lambda_n)}{|\Lambda_n|} = 0,$$

where

$$\begin{aligned} \forall M \in \mathcal{S}_{fin}(d) \quad \forall h \in \mathbb{N}: \quad & V_h(M) := |\{i \in M | d(i, M^c) \leq h\}| \\ \forall i \in \mathbb{Z}^d \quad \forall M \subseteq \mathbb{Z}^d: \quad & d(i, M) := \min_{j\in M} ||i - j||_1. \end{aligned}$$

$(\Lambda_n)_{n\in\mathbb{N}}$ *is said to* diverge in the sense of van Hove *or to* exhaust $\mathbb{Z}^d$ in the sense of van Hove.

2.2.2 Remark. *The crucial feature of a van Hove sequence is that the volume of the boundary becomes sufficiently small, so that it becomes irrelevant in the limit. In this way, it is possible to ensure that boundary conditions do not affect the thermodynamic limit of the free energy.*

Before one can study the general case of van Hove sequences a special van Hove sequence shall be analyzed, namely a sequence of cubes with increasing edge length.

2.2.3 Example. *Setting*

$$\begin{aligned} \forall n \in \mathbb{N}: \quad \Lambda^d(n) \quad &:= \quad \{0; 1; \ldots; n-1\}^d \\ \forall t \in \mathbb{Z}^d \forall n \in \mathbb{N}: \quad \Lambda_t^d(n) \quad &:= \quad \{nt + l | l \in \Lambda^d(n)\}, \end{aligned}$$

one obtains

$$\begin{aligned}\forall h, n \in \mathbb{N}: \quad V_h(\Lambda^d(n)) &= |\Lambda^d(n) \setminus \Lambda^d(n-2h-2)| \\ &= n^d - (n-2h-2)^d \\ &= 2(h+1)\sum_{k=0}^{d-1} n^k \underbrace{(n-2h-2)}_{\leq n}{}^{d-1-k} \\ &\leq 3d(h+1)\frac{|\Lambda^d(n)|}{n},\end{aligned}$$

and thus

$$\forall h \in \mathbb{N}: \quad \lim_{n\to\infty} \frac{V_h(\Lambda^d(n))}{|\Lambda^d(n)|} = 0.$$

Hence, $(\Lambda^d(n))_{n\in\mathbb{N}}$ is an example for a van Hove sequence which justifies the last comment in the last remark.

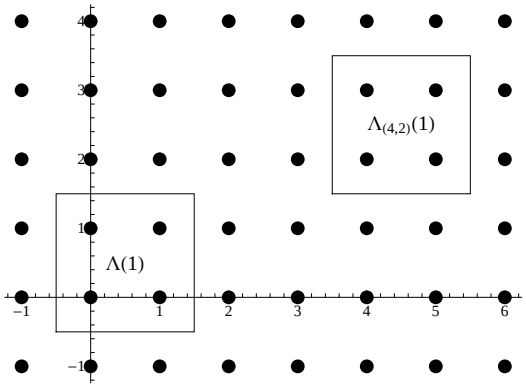


Figure 2.1: The enclosed vertices belong to the considered translates of the unit square.

2.2.4 Remark. *The fact that for $\Lambda \subseteq \mathbb{Z}^d$ the maximal number of neighbors*

for $l \in \Lambda$ in Λ^c is $2d$ yields an upper bound on $V_h(\Lambda)$,

$$\begin{aligned} V_h(\Lambda) &= |\bigcup_{i=1}^{h} \underbrace{\{l \in \Lambda | d(l, \Lambda^c) = i\}}_{=\{l \in \Lambda | d(l, \partial\Lambda) = i-1\}}| \\ &\leq \left(1 + 2d + (2d)^2 + \ldots + (2d)^h\right) \underbrace{|\partial\Lambda|}_{=V_1(\Lambda)} \\ &= \frac{1-(2d)^{h+1}}{1-2d} V_1(\Lambda) \end{aligned}$$

This inequality is not sharp, but it is sufficient to prove the statement below. So, in general it is sufficient to demand

$$\lim_{n\to\infty} \frac{V_1(\Lambda_n)}{|\Lambda_n|} = 0$$

for a sequence $(\Lambda_n)_{n\in\mathbb{N}} \in (\mathcal{S}_{fin}(d))^{\mathbb{N}}$ to be a van Hove sequence.

2.2.5 Lemma. *Let $J : \mathcal{S}_{fin}(d) \to \mathbb{R}$ be a translational invariant Ising potential with finite range $\mathcal{R}(J) < \infty$. One has*

$$\begin{aligned} &\exists n_0 \in \mathbb{N} \forall n_1, n_2 \geq n_0 \quad \forall \beta \in \mathbb{R}^+ : \\ &\qquad |f_{\Lambda^d(n_1)}(\beta) - f_{\Lambda^d(n_2)}(\beta)| \leq 2d\mathcal{R}(J)||J||_d^{(I)} \left(\frac{1}{n_1} + \frac{1}{n_2}\right), \end{aligned}$$

so $(f_{\Lambda^d(n)}(\beta)_{n\in\mathbb{N}}$ is a Cauchy sequence uniformly in $\beta \in \mathbb{R}^+$. In particular,

$$\forall \Lambda^d \in \mathcal{S}_{fin}(d) \forall \beta \in \mathbb{R}^+ : \quad f_{\Lambda^d}(\beta) := \lim_{n\to\infty} f_{\Lambda^d(n)}(\beta)$$

is well-defined.

Proof. Let $\beta > 0$. We will show that

$$|\Delta| \leq 2d\mathcal{R}(J)\frac{1}{n_1} \tag{2.2.3}$$

holds for sufficiently large n_1 and n_2 where

$$\Delta := f_{\Lambda^d(n_1 n_2)}(\beta) - f_{\Lambda^d(n_1)}(\beta).$$

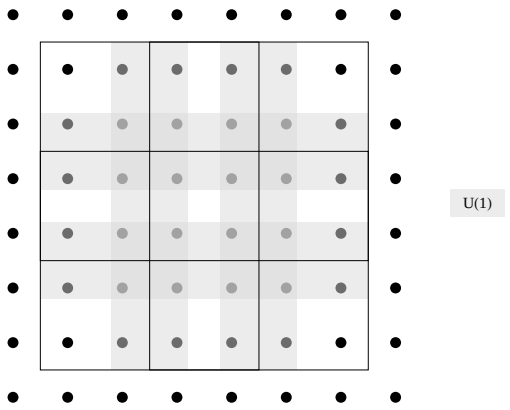


Figure 2.2: $\Lambda^2(3 \cdot 3)$ with embedded translates of $\Lambda^2(3)$. It is further shown the catchment of $U(1)$, i.e., the maximal area of interaction between the translates for $\mathcal{R}(J) \leq 1$. The darker shaded areas illustrate the sets in which the sites experience more boundary interaction because they interact with 2 sites of 2 adjacent cubes.

The triangle inequality then implies the statement of the lemma,

$$\begin{aligned} |f_{\Lambda^d(n_1)}(\beta) - f_{\Lambda^d(n_2)}(\beta)| &\leq |f_{\Lambda^d(n_1 n_2)}(\beta) - f_{\Lambda^d(n_1)}(\beta)| \\ &\quad + |f_{\Lambda^d(n_1 n_2)}(\beta) - f_{\Lambda^d(n_2)}(\beta)| \\ &\leq 2d\mathcal{R}(J)||J||_d^{(I)} \left(\frac{1}{n_1} + \frac{1}{n_2}\right). \end{aligned}$$

Now let $n_1, n_2 > 2\mathcal{R}(J)$. The trick is to subdivide

$$H_{\Lambda^d(n_1 n_2)} = \underbrace{\sum_{i \in \Lambda^d(n_2)} H_{\Lambda_i^d(n_1)}}_{=: H^{(I)}_{\Lambda^d(n_1 n_2)}} + \underbrace{(H_{\Lambda^d(n_1 n_2)} - H^{(I)}_{\Lambda^d(n_1 n_2)})}_{=: H^{(II)}_{\Lambda^d(n_1 n_2)}} \tag{2.2.4}$$

in order to reduce the problem to the interaction within the n_2^d translates of $\Lambda^d(n_1)$ which fill $\Lambda^d(n_1 n_2)$ and the interaction between the translates of $\Lambda^d(n_1)$.

Since

$$\left(\sum_{\sigma\in\Omega_{\Lambda^d(n_1)}} \mathrm{e}^{-\beta H_{\Lambda^d(n_1)}}\right)^{|\Lambda^d(n_2)|} = \underbrace{\sum_{\sigma\in\Omega_{\Lambda^d(n_1)}} \cdots \sum_{\sigma\in\Omega_{\Lambda^d(n_1)}}}_{|\Lambda^d(n_2)|=\sum_{i\in\Lambda^d(n_2)} 1 = n_2^d \text{ times}} \exp\left[-\beta \sum_{i\in\Lambda^d(n_2)} \underbrace{H_{\Lambda^d(n_1)}}_{J \overset{\text{transl.-inv.}}{=} H_{\Lambda_i^d(n_1)}}\right]$$

$$= \sum_{\sigma\in\Omega_{\Lambda^d(n_1 n_2)}} \mathrm{e}^{-\beta H^{(I)}_{\Lambda^d(n_1 n_2)}} \tag{2.2.5}$$

one finds

$$\begin{aligned}\Delta &= \frac{1}{\beta|\Lambda^d(n_1 n_2)|} \log\left(\sum_{\sigma\in\Omega_{\Lambda^d(n_1 n_2)}} \mathrm{e}^{-\beta H_{\Lambda^d(n_1 n_2)}(\sigma)}\right) \\ &\quad - \frac{1}{\beta|\Lambda^d(n_1)|} \log\left(\sum_{\sigma\in\Omega_{\Lambda^d(n_1)}} \mathrm{e}^{-\beta H_{\Lambda^d(n_1)}(\sigma)}\right) \\ &= \frac{1}{\beta\Lambda^d(n_1 n_2)} \log\left[\frac{\sum_{\sigma\in\Omega_{\Lambda^d(n_1 n_2)}} \exp\left(-\beta H_{\Lambda^d(n_1 n_2)}(\sigma)\right)}{\sum_{\sigma\in\Omega_{\Lambda^d(n_1 n_2)}} \exp\left(-\beta H^{(I)}_{\Lambda^d(n_1 n_2)}(\sigma)\right)}\right]\end{aligned}$$

For the next step the following claim is needed:
Claim: Let $n \in \mathbb{N}$, $a_1, a_2, \ldots a_n, b_1, b_2, \ldots, b_n \in \mathbb{R}^+$. Then

$$\frac{\sum_{i=1}^n a_i}{\sum_{i=1}^n b_i} \leq \max_{i=1}^n \frac{a_i}{b_i}. \tag{2.2.6}$$

Proof of the claim: One has

$$\frac{\sum_{i=1}^n a_i}{\sum_{i=1}^n b_i} = \frac{\sum_{i=1}^n \frac{a_i}{b_i} b_i}{\sum_{i=1}^n b_i} \leq \max_{i=1}^n \frac{a_i}{b_i}.$$

With that one can estimate Δ:

$$\begin{aligned}\beta|\Lambda^d(n_1n_2)||\Delta| &\overset{\log}{\underset{\text{increasing}}{\leq}} \log\left[\max(\{\max_{\sigma\in\Omega_{\Lambda^d(n_1n_2)}} \mathrm{e}^{\mp\beta(H_{\Lambda^d(n_1n_2)}(\sigma)-H^{(I)}_{\Lambda^d(n_1n_2)}(\sigma))}\})\right]\\ &\overset{\exp}{\underset{\text{increasing}}{=}} \log\left[\exp\left(\max_{\sigma\in\Omega_{\Lambda^d(n_1n_2)}} \mp H^{(II)}_{\Lambda^d(n_1n_2)}(\sigma)\right)\right]\\ &= ||H^{(II)}_{\Lambda^d(n_1n_2)}||_\infty \end{aligned} \tag{2.2.7}$$

We can represent $H^{(II)}$ by a sum in virtue of

$$\forall\sigma\in\Omega_{\Lambda^d(n_1n_2)}: \quad H^{(II)}_{\Lambda^d(n_1n_2)}(\sigma) \quad =: \quad -\sum_{L\in\mathcal{B}} J(L)\sigma_L$$

for some $\mathcal{B}\subseteq\mathcal{P}(\Lambda^d(n_1n_2))$ and we define

$$\begin{aligned} I &:= \bigcup_{L\in\mathcal{B}} L \subseteq U(\mathcal{R}(\mathcal{J})),\\ U(R) &:= \bigcup_{k=1}^{n_2-1}\bigcup_{i=1}^{d}\{l\in\Lambda^d(n_1n_2)\big||l_i-kn_1+\frac{1}{2}|<R\}. \end{aligned}$$

Hence, one has

$$\begin{aligned}|U(R)| &\overset{\text{sub-additivity of the}}{\underset{\text{counter measure}}{\leq}} \sum_{k=1}^{n_2-1}\sum_{i=1}^{d} \underbrace{|\{b\in\mathbb{Z}^d|b_i-kn_1+\frac{1}{2}|<R\}|}_{\overset{\text{transl.-inv. of the}}{\underset{\text{counter measure}}{=}}|\{b\in\mathbb{Z}^d|b_i|<R\}|=2R(n_1n_2)^{d-1}}\\ &= 2d(n_2-1)R(n_1n_2)^{d-1}\\ &\leq 2dR|\Lambda^d(n_1n_2)|\frac{1}{n_1}. \end{aligned}$$

Lemma 2.1.19 now yields

$$||H^{(II)}_{\Lambda^d(n_1n_2)}||_\infty \overset{2.1.19}{\leq} \underbrace{|I|}_{\leq|U(\mathcal{R}(J)|}\cdot||J||^{(I)}_d \leq 2d\mathcal{R}(J)||J||^{(I)}_d|\Lambda^d(n_1n_2)|\frac{1}{n_1}$$

The inequality eq. (2.2.7) finally gives

$$|\Delta| \overset{(2.2.7)}{\leq} 2d\mathcal{R}(J)||J||^{(I)}_d\frac{1}{n_1}$$

as stated in eq. (2.2.3). □

2.2.6 Remark. *If boundary conditions are taken into consideration, one only has to consider the boundary interaction with the surrounding spins. For $n_1, n_2 \in \mathbb{N}$ one subdivides the Hamilton function with boundary condition $\tau_{n_1,n_2} \in \Omega_{\Lambda(n_1n_2)^c}$ exactly as in eq. (2.2.4). One obtains for $\sigma \in \Omega_{\Lambda(n_1n_2)}$*

$$H^{(II),\tau_{n_1,n_2}}_{\Lambda(n_1n_2)}(\sigma) \quad =: \quad -\sum_{L\in\mathcal{B}} J(L)\sigma_{L\cap\Lambda}\tau_{L\cap\Lambda^c}$$

with

$$I := \bigcup_{L\in\mathcal{B}} L \subseteq U(\mathcal{R}(J)) \cup \left(\Lambda(n_1n_2 + 2\mathcal{R}(J)) - \mathcal{R}(J)\sum_{i=1}^{d}\hat{e}_i\right) \setminus \left(\Lambda(n_1n_2 - 2\mathcal{R}(J) - 2) + (\mathcal{R}(J)+1)\sum_{i=1}^{d}\hat{e}_i\right).$$

Thus, one has

$$\begin{aligned} ||H^{(II),\tau_{n_1,n_2}}_{\Lambda(n_1n_2)}|| &\overset{2.1.19}{\leq} |I|\cdot||J||^{(I)}_d \leq \left(2d\mathcal{R}(J)|\Lambda^d(n_1n_2)|/n_1 + (n_1n_2+2\mathcal{R}(J))^d\right. \\ &\quad \left. -(n_1n_2 - 2\mathcal{R}(J) - 2)^d\right)||J||^{(I)}_d \\ &\overset{\substack{cf.\ algebra \\ in\ ex.\ 2.2.3}}{\leq} 2d\left(\underbrace{(2\mathcal{R}(J)+1)/n_2}_{\leq 2\mathcal{R}(J)+1} + \mathcal{R}(J)\right)||J||^{(I)}_d \frac{|\Lambda^d(n_1n_2)|}{n_1} \\ &\leq 2d(3\mathcal{R}(J)+1)||J||^{(I)}_d \frac{|\Lambda^d(n_1n_2)|}{n_1}, \end{aligned}$$

which is equivalent to the result of Lemma 2.2.5.

A more general framework for the thermodynamic limit of van Hove sequences shall now be considered, since one will deal with boundary conditions on the Hamiltonian. In addition, one will allow infinitely ranged Ising potentials. This requires the following lemma.

2.2.7 Lemma. *Let $\Lambda \in \mathcal{S}_{fin}(d)$ and $J_1 : \mathcal{S}_{fin}(d) \to \mathbb{R}$ and $J_2 : \mathcal{S}_{fin}(d) \to \mathbb{R}$ be two Ising potentials and let $f^{(J_1)}_\Lambda : \mathbb{R}^+ \to \mathbb{R}$ resp. $f^{(J_2)}_\Lambda : \mathbb{R}+ \to \mathbb{R}$ be the corresponding free energies. Then*

$$|f^{(J_1)}_\Lambda(\beta) - f^{(J_2)}_\Lambda(\beta)| \leq ||J_1 - J_2||^{(I)}_d. \tag{2.2.8}$$

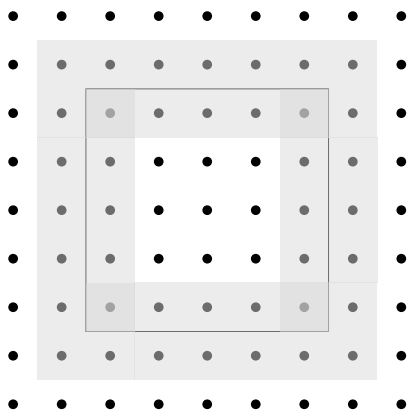


Figure 2.3: Maximal zone of boundary interaction for $\Lambda^2(5)$ for $\mathcal{R}(J) = 1$.

In particular, for any $\beta \in \mathbb{R}^+$

$$f_{\Lambda,\beta} : \{J : \mathcal{S}_{fin}(d) \to \mathbb{R} | J \text{ Ising potential}\} \to \mathbb{R}, J \to f_\Lambda^{(J)}(\beta)$$

is a Lipschitz continuous functional on $\{J : \mathcal{S}_{fin}(d) \to \mathbb{R} | J \text{ Ising potential}\}$.

Remark. *The inequality* (2.2.8) *holds uniformly in* $\beta \in \mathbb{R}^+$ *and* $\Lambda \in \mathcal{S}_{fin}(d)$.

Proof of Lemma 2.2.7. Let

$$\forall 1 \leq i \leq 2 : \quad H_\Lambda^{(J_i)} : \Omega_\Lambda \to \mathbb{R}, \sigma \mapsto - \sum_{L \in \mathcal{S}_{fin}(d), L \cap \Lambda \neq \emptyset} J_i(L) \sigma_{L \cap \Lambda}.$$

Clearly

$$H_\Lambda^{(J+J')} \quad = \quad H_\Lambda^{(J)} + H_\Lambda^{(J')}. \tag{2.2.9}$$

One finds

$$\begin{aligned} f_\Lambda^{(J_2)}(\beta) - f_\Lambda^{(J_1)}(\beta) \quad &= \quad \frac{1}{\beta|\Lambda|} \log \left(\frac{\sum\limits_{\sigma \in \Omega_\Lambda} \mathrm{e}^{-\beta H_\Lambda^{(J_1)}}}{\sum\limits_{\sigma \in \Omega_\Lambda} \mathrm{e}^{-\beta H_\Lambda^{(J_2)}}} \right) \\ &\overset{(2.2.6)}{\leq} \log \left[\max_{\sigma \in \Omega_\Lambda} \left(\exp(\beta \underbrace{(H_\Lambda^{(J_2)} - H_\Lambda^{(J_1)})}_{\overset{(2.2.9)}{=} H_\Lambda^{(J_2 - J_1)}}) \right) \right] \\ &\leq \quad \frac{1}{|\Lambda|} ||H_\Lambda^{(J_2 - J_1)}||_\infty \overset{2.1.19}{\leq} ||J_2 - J_1||_d^{(I)}. \end{aligned}$$

Switching J_1 and J_2 yields the claim. □

2.2.8 Theorem (Thermodynamic limit of the free energy in classical spin systems)**.** *Let $(\Lambda_n)_{n\in\mathbb{N}} \in (\mathcal{S}_{fin}(d))^{\mathbb{N}}$ be a van Hove sequence and let further $J : \mathcal{S}_{fin}(d) \to \mathbb{R}$ be a translational invariant Ising potential. Then*

(i)

$$f : \mathbb{R}^+ \to \mathbb{R}, \beta \mapsto \lim_{n\to\infty} f_{\Lambda_n}(\beta)$$

is a well-defined function, i.e., for another van Hove sequence $(\Lambda'_n)_{n\in\mathbb{N}} \in (\mathcal{S}_{fin}(d))^{\mathbb{N}}$ one finds the same limit,

$$\forall \beta \in \mathbb{R}^+ : \quad \lim_{n\to\infty} f_{\Lambda'_n}(\beta) = \lim_{n\to\infty} f_{\Lambda_n}(\beta).$$

(ii) if J further has finite range and $(\tau_n)_{n\in\mathbb{N}}$, $\forall n \in \mathbb{N} : \tau_n \in \Omega_{\Lambda_n^c}$, is a sequence of boundary conditions corresponding to $(\Lambda_n)_{n\in\mathbb{N}}$, one has

$$\forall \beta \in \mathbb{R}^+ : \quad \lim_{n\to\infty} f^{\tau_n}_{\Lambda_n}(\beta) = \lim_{n\to\infty} f_{\Lambda_n}(\beta) = f(\beta).$$

Moreover $\mathbb{R}^+ \to \mathbb{R}, \beta \mapsto \beta f(\beta)$ is a concave function.

Proof. Define

$$F : \mathbb{R}^+ \to \mathbb{R}, \beta \mapsto \lim_{n\to\infty} f_{\Lambda^d(n)}(\beta).$$

The basic idea is to deduce the thermodynamic limit of the free energy for a van Hove sequence to the thermodynamic limit for a sequence of cubes, so one wants to show f=F.
Case 1: One starts by considering J having finite range $\mathcal{R}(J) < \infty$ and one ignores boundary conditions. The aim is to deduce the case of a general van Hove sequence to the case of a sequence of unions of cubes and treating the boundary separately. Let $(a_n) \in \mathbb{N}^{\mathbb{N}}$ with $a_n \to \infty$ $(n \to \infty)$ and

$$\lim_{n\in\mathbb{N}} \underbrace{\frac{V_1(\Lambda_n)}{|\Lambda_n|}}_{=:\frac{1}{b_n}} \frac{1-(2d)^{a_n}}{1-2d} = 0.$$

E.g., pick

$$\forall n \in \mathbb{N} : \quad a_n \quad := \quad \lfloor \frac{\log[(2d-1)\sqrt{b_n}+1]}{\log(2d)} \rfloor$$

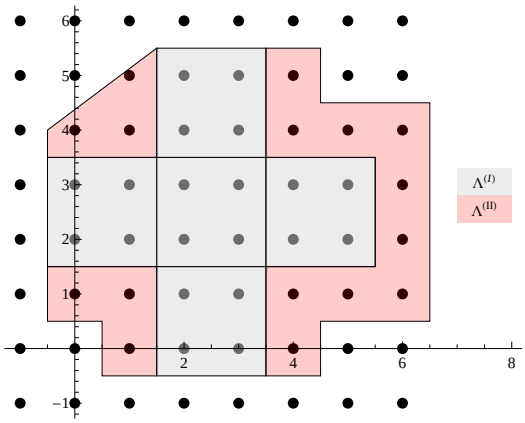


Figure 2.4: Partition of a set $\Lambda := \Lambda^{(I)} \dot{\cup} \Lambda^{(II)}$

and use the fact that $(\Lambda_n)_{n\in\mathbb{N}}$ is a van Hove sequence, in particular

$$\lim_{n\to\infty} \frac{V_1(\Lambda_n)}{|\Lambda_n|} \quad = \quad 0$$

One defines

$$\forall n \in \mathbb{N}: \quad T_n \quad := \quad \{t \in \mathbb{Z}^d | \Lambda_t^d(a) \subseteq \Lambda_n\}.$$

Let $n \in \mathbb{N}$ and set

$$\Lambda_n^{(I)} := \bigcup_{t\in T_n} \Lambda_t^d(a_n) \qquad \Lambda_n^{(II)} := \Lambda_n \setminus \Lambda_n^{(I)}.$$

In the same manner, the Hamilton function is divided in virtue of

$$H_{\Lambda_n} \quad = \quad \underbrace{H_{\Lambda_n^{(I)}}}_{=:H_{\Lambda_n}^{(I)}} + \underbrace{(H_{\Lambda_n} - H_{\Lambda_n^{(I)}})}_{=:H_{\Lambda_n}^{(II)}}.$$

Setting

$$\forall \beta \in \mathbb{R}^+: \quad f_{\Lambda_n}^{(I)}(\beta) \quad := \quad -\frac{1}{\beta|\Lambda_n|} \log\left(\sum_{\sigma\in\Omega_{\Lambda_n}} \mathrm{e}^{-\beta H_{\Lambda_n}^{(I)}}\right)$$

and one estimates

$$\begin{aligned} |f_{\Lambda_n}(\beta) - F(\beta)| \quad &\leq \quad |\underbrace{f_{\Lambda_n}(\beta) - f^{(I)}_{\Lambda_n}(\beta)}_{=:\Delta_1}| + |\underbrace{f^{(I)}_{\Lambda_n}(\beta) - f_{\Lambda^d(a_n)}(\beta)}_{=:\Delta_2}| \\ &\quad + |\underbrace{f_{\Lambda^d(a_n)}(\beta) - F(\beta)}_{=:\Delta_3}|. \end{aligned}$$

Analogously to the proof of 2.2.5, one obtains with the inequality given in (2.2.6)

$$|\Delta_1| \quad \leq \quad \frac{||H^{(II)}_{\Lambda_n}||_\infty}{|\Lambda_n|}.$$

Again, one can write

$$\forall \sigma \in \Omega_{\Lambda_n}: \quad H^{(II)}_{\Lambda_n}(\sigma) \quad =: \quad -\sum_{L \in \mathcal{B}} J(L)\sigma_L$$

with

$$\begin{aligned} I \quad &:= \quad \bigcup_{L \in \mathcal{B}} L \subseteq U_{a_n}(\mathcal{R}(J)) \\ \forall a, R \in \mathbb{N}: \quad U_a(R) \quad &:= \quad \Lambda^{(II)}_n \cup \underbrace{\bigcup_{i=1}^{d} \bigcup_{t \in \mathbb{Z}} \{l \in \Lambda_n | |l_i - at + \frac{1}{2}| < R\}}_{=:\mathcal{U}_a(R)}. \end{aligned}$$

It is $\forall a \in \mathbb{N}: \operatorname{diam}(\Lambda(a)) = d(a-1)$ and hence

$$\Lambda^{(II)}_n \subseteq \{l \in \Lambda_n | d(l, \Lambda^c_n) \leq d(a_n - 1)\}$$

which yields

$$|\Lambda^{(II)}_n| \leq V_{(a_n-1)d}(\Lambda_n).$$

So,

$$\begin{aligned} 0 \leq \lim_{k\to\infty} \frac{|\Lambda^{(II)}_k|}{|\Lambda_k|} \leq \lim_{k\to\infty} \frac{V_{(a_n-1)d}(\Lambda_k)}{|\Lambda_k|} \overset{2.2.4}{\leq} \lim_{n\in\mathbb{N}} \frac{V_1(\Lambda_n)}{|\Lambda_n|} \frac{1-(2d)^{a_n}}{1-2d} = 0 \\ \Rightarrow \lim_{k\to\infty} \frac{|\Lambda^{(II)}_k|}{|\Lambda_k|} = 0. \end{aligned}$$

Taking a look at the density of interactions in $\mathcal{U}_a(R)$ with respect to Λ_n gives

$$\frac{|\mathcal{U}_a(R)|}{|\Lambda_n|} \leq \frac{a^d - (a-2R-2)^d}{a^d}.$$

This is the highest ratio of boundary interactions with range $\mathcal{R}(J)$. With that one can estimate

$$\frac{|U_{a_n}(\mathcal{R}(J))|}{|\Lambda_n|} \leq \frac{|\Lambda_n^{(II)}|}{|\Lambda_n|} + \frac{a_n^d - (a_n - 2\mathcal{R}(J) - 2)^d}{a_n^d} \to 0 \quad (n \to \infty).$$

Hence holds

$$|\Delta_1| \quad \leq \quad \frac{||H_{\Lambda_n}^{(II)}||_\infty}{|\Lambda_n|} \overset{2.1.19}{\leq} \frac{|U_{a_n}(\mathcal{R}(J))}{|\Lambda_n|} ||J||_d^{(I)} \to 0 \quad (n \to \infty).$$

One has

$$H_{\Lambda_n}^{(I)} \quad = \quad -\sum_{t \in T_n} \sum_{L \subseteq \Lambda_t^d(a_n)} J(L)\sigma_L \overset{J \text{ transl.-inv.}}{=} -|T_n| \sum_{L \subseteq \Lambda^d(a_n)} J(L)\sigma_L \qquad (2.2.10)$$

and hence

$$\sum_{\sigma \in \Omega_{\Lambda_n}} \mathrm{e}^{-\beta H_{\Lambda_n}^{(I)}(\sigma)} \overset{\text{cf. (2.2.5)}}{=} \underbrace{2^{|\Lambda_n^{(II)}|}}_{=\text{total \# spin configurations in } \Lambda_n \setminus \Lambda_n^{(I)} = \Lambda_n^{(II)}} \left(\sum_{\sigma \in \Omega_{\Lambda^d(a_n)}} \mathrm{e}^{-\beta H_{\Lambda^d(a_n)}(\sigma)} \right)^{|T_n|}$$

As in the proof of Lemma 2.2.5 one obtains

$$\begin{aligned}
\beta\Delta_2 &= -\frac{1}{|\Lambda_n|} \log \left(\sum_{\sigma \in \Omega_{\Lambda_n}} \mathrm{e}^{-\beta H_{\Lambda_n}^{(I)}(\sigma)} \right) + \frac{1}{|\Lambda^d(a_n)|} \log \left(\sum_{\sigma \in \Omega_{\Lambda^d(a_n)}} \mathrm{e}^{-\beta H_{\Lambda^d(a_n)}(\sigma)} \right) \\
&\overset{|T_n| = \frac{|\Lambda_n^{(I)}|}{|\Lambda^d(a_n)|}}{=} -\frac{|\Lambda_n^{(II)}|}{|\Lambda_n|} + \beta f_{\Lambda(a_n)}(\beta) \left(1 - \frac{|\Lambda_n^{(I)}|}{|\Lambda_n} \right) \\
&= \frac{|\Lambda_n^{(II)}|}{|\Lambda_n|} \left(\beta \underbrace{f_{\Lambda(a_n)(\beta)}}_{\to F(\beta)(n \to \infty)} - \log(2) \right) \to 0 \quad (n \to \infty)
\end{aligned}$$

By definition it is

$$\Delta_3 \to 0 \quad (n \to \infty)$$

and thus

$$|f_{\Lambda_n}(\beta) - F(\beta)| \leq \sum_{i=1}^{3} |\Delta_i| \to 0 \quad (n \to \infty).$$

Case 2: J has infinite range. Define the truncated potential $J_R : \mathcal{S}_{fin}(d) \to \mathbb{R}$ for $R \in \mathbb{N}$ to be

$$J_R : \mathcal{S}_{fin}(d) \to \mathbb{R}, \Lambda \mapsto \begin{cases} J(\Lambda) & \text{diam}(\Lambda) \leq R \\ 0 & \text{diam}(\Lambda) > R \end{cases}.$$

With the notation of Lemma 2.2.7 one finds

$$\begin{aligned} |f^J_{\Lambda_n}(\beta) - F(\beta)| &\leq |f^J_{\Lambda_n}(\beta) - f^{J_R}_{\Lambda_n}(\beta)| + |f^{J_R}_{\Lambda_n}(\beta) - F(\beta)| \\ &\overset{(2.2.8)}{\leq} ||J - J_R||^{(I)}_d + |f^{J_R}_{\Lambda_n}(\beta) - F(\beta)| \to 0 \quad (n, R \to \infty). \end{aligned}$$

Case 3: Now let J have finite range again and $(\tau_n)_{n\in\mathbb{N}}$, $\forall n \in \mathbb{N} : \tau_n \in \Omega_{\Lambda_n^c}$, be a sequence of boundary conditions. The only difference to the previous case occurs in Δ_1. One more time, one rewrites $H^{\tau_n}_{\Lambda_n}$ as

$$H^{\tau_n}_{\Lambda_n} = H^{(I)}_{\Lambda_n} + \underbrace{H^{\tau_n}_{\Lambda_n} - H^{(I)}_{\Lambda_n}}_{=:H^{(II),\tau_n}_{\Lambda_n}}$$

with

$$\forall \sigma \in \Omega_{\Lambda_n:} \quad H^{(II),\tau_n}_{\Lambda_n}(\sigma) =: -\sum_{L\in\tilde{\mathcal{B}}} J(L)\sigma_{L\cap\Lambda_n}(\tau_n)_{L\cap\Lambda_n^c}.$$

It is

$$\begin{aligned} \tilde{I} &:= \bigcup_{L\in\tilde{\mathcal{B}}} L \subseteq W_{a_n}(\mathcal{R}(J)) \\ W_a(R) &:= U_a(R) \cup \{l \in \Lambda_n^c | d(l, \Lambda_n) \leq R\} \end{aligned}$$

Similar to remark 2.2.4, one has the following estimation

$$\begin{aligned} |W_a(R)| &\leq |U_a(R)| + V_1(\Lambda_n)\left(2d + (2d)^2 + \ldots + (2d)^R\right) \\ &= |U_a(R)| + 2d\frac{(2d)^R - 1}{2d - 1} V_1(\Lambda_n). \end{aligned}$$

Setting

$$\begin{aligned} \forall \beta \in \mathbb{R}^+ : \quad f_{\Lambda_n}^{\tau_n}(\beta) &:= -\frac{1}{\beta|\Lambda_n|} \log \left(\sum_{\sigma \in \Omega_{\Lambda_n}} \mathrm{e}^{-\beta H_{\Lambda_n}^{\tau_n}} \right), \\ \Delta_1^{\tau_n} &:= f_{\Lambda_n}(\beta) - f_{\Lambda_n}^{(I)}(\beta) \end{aligned}$$

there is an upper bound on $|\Delta_1^{\tau_n}|$ analogously to case 1

$$\begin{aligned} |\Delta_1^{\tau_n}| &\leq \frac{||H_{\Lambda_n}^{(II),\tau_n}||_\infty}{|\Lambda_n|} \\ &\overset{2.1.19}{\leq} \left(\frac{|U_{a_n}(\mathcal{R}(J))|}{|\Lambda_n|} + 2d \frac{(2d)^R - 1}{2d-1} \underbrace{\frac{V_1(\Lambda_n)}{|\Lambda_n|}}_{\substack{(\Lambda_n)_{n\in\mathbb{N}} \\ \xrightarrow[\text{van Hove}]{} 0 (n\to\infty)}} \right) ||J||_d^{(I)} \to 0 (n \to \infty). \end{aligned}$$

This yields

$$\forall \beta \in \mathbb{R}^+ : \quad |f_{\Lambda_n}^{\tau_n}(\beta) - F(\beta)| \leq |\Delta_1^{\tau_n}| + |\Delta_2| + |\Delta_3| \to 0 \quad (n \to \infty).$$

So, one could provide that for any van Hove sequence the limit of the density of the free energy with or without boundary conditions is equal to the limit of the density of the free energy for a sequence of cubes with growing edge length. In particular, the thermodynamic limit for the free energy is well-defined in the case of van Hove sequences. □

2.2.9 Remark. *Before proceeding to the actual calculation, the result of this powerful theorem shall be analyzed. In the proof $\Lambda_n^{(I)} \cup U_{a_n}(\mathcal{R}(J))$ contains all possible interactions among spins in the sequence element Λ_n, i.e., one can impose periodic boundary conditions on Λ_n. Periodic boundary conditions are equivalent to the projection $\mathbb{Z}^d \to \mathbb{Z}^{d-k} \times \overset{k}{\underset{l=1}{\times}} \mathbb{Z}/(i_{n_l}\mathbb{Z})$. For the thermodynamic limit one considers the limit of $n_1, n_2, \ldots, n_k \to \infty$. This feature later will turn out to be useful for the actual computation of the free energy.*

If one only considers Ising potentials with finite range, finitely many structural defects (or sufficiently few s.t. the van Hove feature is not violated) such as point defects and torsion become irrelevant for the free energy of large systems. This property is crucial if one wants to deal with a real crystal which can be described by the 2-dimensional Ising model.

Chapter 3

Calculation of the critical temperature

The discussion in this section is followed the paper by Lieb, Mattis and Schultz [LMS64]. Instead of a graph theoretical approach to the Ising model, a so-called *fermionization* will be used instead. Since one needs some further calculations to comprehend the chain of thought and since some results in the paper above turned out to be wrong, the calculation shall be displayed in more detail at this point. Because we want to calculate the temperature of the phase transition in the 2D classical Ising model explicitly, some more technical steps will be taken. However, important steps are motivated by the physics underlying the computation and thus they naturally arise.
Remark 2.1.21 allows to map the classical 2D Ising model to a Quantum model by the given identification. Under these identifications, one has

$$\forall n \in \mathbb{N} \quad \forall O \in \mathcal{C}(E^n): \quad \mathrm{Tr}_{\{\psi_n(\sigma)|\sigma\in E^n\}}\psi_n(O) \quad = \quad \sum_{\sigma\in E^n} O(\sigma)^1$$

Let $n \in \mathbb{N}$, $O \in \mathcal{C}(E^n)$. With the *continuous functional calculus* one can even provide for a real valued function $f \in \mathcal{C}(\underbrace{[\min_{\sigma\in E^n} O(\sigma), \max_{\sigma\in E^n} O(\sigma)]}_{=:I_n}, \mathbb{R})$

$$\mathrm{Tr}_{\{\psi_n(\sigma)|\sigma\in E^n\}}\Phi_{\psi_n(O)}(f) \quad = \quad \sum_{\sigma\in E^n} (f\circ O)(\sigma),$$

[1] Notation as in remark 2.1.21

where

$$\Phi_{\psi_n(O)} : \mathcal{C}(I_n, \mathbb{R})^2 \to B(E^n)$$

is the functional calculus for $\psi_n(O)$ defined by

$$\forall g \in \mathcal{C}(I_n, \mathbb{R}) \forall \sigma \in E^n : \quad \Phi_{\psi_n(O)}(g)\phi_n(\sigma) = g(O(\sigma))\phi_n(\sigma).$$

Thus one can solve the classical 2D Ising model by solving its Quantum mechanical image. We will work with

$$\mathcal{H} \quad := \quad (E^M)^N \tilde{=} E^{MN}$$

for some $M, N \in \mathbb{N}$.

3.1 The general setup

The general Hamiltonian for the Ising model exposed to an external field H is

$$\begin{aligned}
\mathscr{H} \quad &:= \quad \sum_{n=1}^{N} (\mathcal{H}_n + \mathcal{K}_{1,n} + \mathcal{K}_{2,n}) && (3.1.1)\\
\mathcal{H}_n \quad &:= \quad H \sum_{m=1}^{M} \sigma^x_{n,m} \quad : \text{coupling to external field}\\
\mathcal{K}_{1,n} \quad &:= \quad K_1 \sum_{m=1}^{M} \sigma^x_{n-1,m}\sigma^x_{n,m} \quad : \text{row interaction}\\
\mathcal{K}_{2,n} \quad &:= \quad K_2 \sum_{m=1}^{M} \sigma^x_{n,m}\sigma^x_{n,m+1} \quad : \text{column interaction}
\end{aligned}$$

Here one denotes $H := \beta h$, $K_1 := \beta J_1$ and $K_2 := \beta J_2$ where h is the external magnetic field and J_1 (resp. J_2) is the coupling constant among spins in a row (resp. in a column). Once chooses

$$\sigma^x \quad = \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

[2]Usually one defines the functional calculus on $\mathcal{C}_b(\mathbb{R}, \mathbb{R})$ but since it is always possible to extend a continuous function on a closed interval to a function in $\mathcal{C}_b(\mathbb{R}, \mathbb{R})$ it is sufficient to only consider functions on $\mathcal{C}(I_n, \mathbb{R})$. Note: For two normed spaces $(A, ||\cdot||_A), (B, ||\cdot||_B)$ one denotes $\mathcal{C}_b(A, B) := \{g \in \mathcal{C}(A, B) | \sup_{x \in A} ||g(x)||_B < \infty\}$.

to be the the spin matrix in this problem in order to simplify the computations below.
Before one can calculate the partition function, it is easy to derive a recursion relation for the density matrix of a distribution of configurations in a lattice of $N+1$ rows depending on that of N rows, i.e., the marginal distribution or *reduced density matrix*. Instead of imposing cyclicity on the *columns*, one will demand cyclic (resp. anti-cyclic) conditions in a *row*, in particular

$$\forall 1 \leq n \leq N : \sigma^x_{n,M+1} \quad = \quad \sigma^x_{n,1}.$$

By the discussion above (cf. remark 2.2.9), one has that the free energy stays the same for the "Quantum" case in the thermodynamic limit. The density operator for $N+1$ rows is[3]

$$\begin{aligned} \rho_N(\Sigma_0, \Sigma_1, \ldots, \Sigma_N) &:= \exp[\sum_{n=1}^{N}(\mathcal{H}_n + \mathcal{K}_{1,n} + \mathcal{K}_{2,n})]\rho_0(\Sigma_0), \\ \Sigma_n &:= (\sigma^x_{n,1}, \ldots, \sigma^x_{n,M}), \\ \sigma^x_{i,j} &:= \mathrm{Id} \otimes \ldots \otimes \mathrm{Id} \otimes \underbrace{\sigma^x}_{\text{position } (i,j)} \otimes \mathrm{Id} \otimes \ldots \otimes \mathrm{Id}. \end{aligned}$$

$(i,j) \in \{1;2;\ldots;M\} \times \{1;2;\ldots;N\}$ is identified with its canonical image in $\{1;2;\ldots;MN\}$. In here, $\rho_0(\Sigma_0)$ indicates the density operator of a boundary condition in the first row. Note that we have already seen that these are irrelevant in the thermodynamic limit.

As usual, the reduced density operator is defined as

$$\rho^{red}_N(\Sigma_N) \quad := \quad \mathrm{Tr}_{\Sigma_0,\Sigma_1,\ldots\Sigma_{N-1}}[\rho_N(\Sigma_0, \Sigma_1, \ldots \Sigma_N)].$$

It is possible to derive a recursion relation for the reduced density operator. This will be the aim of the following proposition.

3.1.1 Proposition. *It is possible to rewrite* $\rho^{red}_N(\Sigma_N)$ *as*

$$\rho^{red}_N(\Sigma_N) \quad = \quad \exp(\mathcal{H}_N + \mathcal{K}_{2,N})\mathcal{O}[\rho^{red}_{N-1}(\Sigma_N)]$$

for some operator $\mathcal{O} \in B(\mathcal{H})$.

[3]Small remark to the notation: This notation reflects that one is dealing with a *classical* problem. So, the original partition function is obtained if one identifies $\sigma^x_{i,j}$ with its eigenvalues and takes the trace. Note: $\rho_N : B(\mathcal{H})^{N+1} \to B(\mathcal{H})$ and $\rho^{red}_n : B(\mathcal{H}) \to B(\mathcal{H})$ are maps, not operators on $\mathcal{H}$.

Proof. One has

$$\rho_N^{red}(\Sigma_N) \quad = \quad \exp(\mathcal{H}_N + \mathcal{K}_{2,N}) \mathrm{Tr}_{\Sigma_{N-1}}[\exp(\mathcal{K}_{1,N}) \rho_{N-1}^{red}(\Sigma_{N-1})]. \quad (3.1.2)$$

Since $\sigma^2 = 1$ for any Pauli matrix σ and $[\sigma^x_{i_1,j_1}, \sigma^x_{i_2,j_2}] = 0 \quad \forall i_1, i_2, j_1, j_2$, one obtains by expanding $\rho_N^{red}(\Sigma_n)$ in the canonical form:

$$\begin{aligned} \rho_{N-1}^{red}(\Sigma_{N-1}) \quad =: \quad & r^{(0)} + \sum_{m_1} r^{(1)}_{m_1} \sigma^x_{m_1}{}' + \sum_{m_1 \neq m_2} r^{(2)}_{m_1,m_2} \sigma^x_{m_1}{}' \sigma^x_{m_2}{}' + \dots \\ & + r^{(M)} \sigma^{x\prime}_1 \sigma^{x\prime}_2 \cdots \sigma^x_M{}' \end{aligned} \quad (3.1.3)$$

Here we put

$$\forall m \in \{1; 2; \dots; M\} : \quad \sigma^x_m{}' \quad := \quad \sigma^x_{N-1,m}.$$

The $\binom{M}{0} + \binom{M}{1} + \dots + \binom{M}{M} = 2^M$ coefficients in eq. (3.1.3) correspond to the 2^M spin configurations in the $(N-1)^{st}$ row. This guarantees that all possible spin configurations are respected. With (3.1.3) one has to calculate in eq. (3.1.2) terms of the form

$$\mathrm{Tr}_{\Sigma_{N-1}}[\exp(\mathcal{K}_{1,N}) \sigma^x_{m_1}{}' \cdots \sigma^x_{m_r}{}'] \quad \stackrel{def.}{=} \quad \mathrm{Tr}_{\Sigma_{N-1}}[\prod_{m=1}^{M} \exp(K_1 \sigma^x_m \sigma^x_m{}') \sigma^x_{m_1}{}' \cdots \sigma^x_{m_r}{}'], \quad (3.1.4)$$

$$\forall m \in \{1; 2; \dots; M\} : \quad \sigma^x_m \quad := \quad \sigma^x_{N,m}.$$

One applies the trace step by step by considering terms like the following

$$\begin{aligned} \mathrm{Tr}_{\sigma^x_m{}'}[\exp(K_1 \sigma^x_m{}' \sigma^x_m)] \quad &= \quad 2\cosh(K_1 \sigma^x_m) = 2\cosh K_1 \\ \mathrm{Tr}_{\sigma^x_m{}'}[\exp(K_1 \sigma^x_m{}' \sigma^x_m) \sigma^x_m{}'] \quad &= \quad 2\sinh(K_1 \sigma^x_m) = 2\sigma^x_m \sinh K_1. \end{aligned}$$

Eq. (3.1.4) yields

$$\mathrm{Tr}_{\Sigma_{N-1}}[\exp(\mathcal{K}_{1,N}) \sigma^x_{m_1}{}' \cdots \sigma^x_{m_r}{}'] \quad = \quad (2\cosh K_1)^M (\tanh K_1)^r \sigma^x_{m_1} \cdots \sigma^x_{m_r}$$

and thus

$$\begin{aligned} \mathrm{Tr}_{\Sigma_{N-1}}[\exp(\mathcal{K}_{1,N}) \rho_{N-1}(\Sigma_{N-1})] \quad &\stackrel{(3.1.3)}{=} \quad (2\cosh K_1)^M \rho_{N-1}(\tanh K_1 \Sigma_N) \\ &=: \quad \mathcal{O}[\rho_{N-1}(\Sigma_N)] \end{aligned}$$

Here one introduced an operator $\mathcal{O}$ which still has to be determined. With $\mathcal{O}$ (3.1.2) simply becomes

$$\rho_N(\Sigma_N) \quad = \quad \exp(\mathcal{H}_N + \mathcal{K}_{2,N}) \mathcal{O}[\rho_{N-1}(\Sigma_N)]$$

□

3.1.2 Remark. *It is not possible to write $\mathcal{O}$ in the form $(2\cosh K_1)^M(\tanh K_1)^{\mathcal{M}}$ in virtue of an operator identity because all but the zeroth order term in eq.* (3.1.3) *would match this identity if $\mathcal{M}$ counts the σ^x's in every single term of the expansion* (3.1.3)*. The zeroth order term required $\mathcal{M}\cdot \mathrm{Id} = 0$ which implies $\mathcal{M} = 0$, a contradiction to the requirements for the other terms in the expansion. Since the partition function is the trace of the density operator introduced above, it is sufficient if $\mathcal{M}$ is implicitly determined in virtue of its action on a state. It will turn out that it is convenient to consider the action on the vacuum $|0\rangle$ in the N^{th} row defined to have all spins are down. The corresponding raising and lowering operators for the spins are as usual*

$$\begin{aligned} \sigma_m^{\mp}|i\rangle \quad &:= \sigma_{N,m}^{\mp}|i\rangle \quad := \delta_{i_{N,m},\{1\}_0}\,|i_{1,1},\ldots,i_{N,m-1},\{{}^0_1\},i_{N,m+1},\ldots,i_{N,M}\rangle\,, \\ \sigma_m^+ + \sigma_m^- \quad &= \quad \sigma_m^x, \end{aligned}$$

where $|i\rangle$ is written as

$$\begin{aligned} |i\rangle \quad &:= \quad |i_{1,1},\ldots,i_{1,M},i_{2,1},\ldots,i_{2,M},\ldots,i_{N,M}\rangle \\ &:= \quad |i_{1,1}\rangle\otimes\ldots\otimes|i_{N,M}\rangle \end{aligned}$$

for $i = (i_{1,1},\ldots,i_{N,M}) \in E^{MN}$. In here, one choses

$$|1\rangle \quad = \quad \begin{pmatrix}1\\0\end{pmatrix}, \qquad |0\rangle \quad = \quad \begin{pmatrix}0\\1\end{pmatrix}.$$

In the following, the notation "$|0\rangle$" will be overloaded in order to define it the vacuum state for the N^{th} row, the state with all spins down ($\binom{0}{1}$) in the N^{th} row. With regard to counting the number of σ^x's in $\rho_N(\Sigma_N)$ whenever that operators is applied to the vacuum, one has to set

$$\mathcal{M} \quad := \quad \sum_{m=1}^{M}\sigma_m^+\sigma_m^-. \tag{3.1.5}$$

In order to simplify the algebra in the following, define K_1^* in virtue of

$$\tanh K_1 \quad =: \quad \exp(-2K_1^*) \tag{3.1.6}$$

assuming that a ferromagnetic *($J_1, J_2 \geq 0$) Ising lattice is treated with respect to simplifying some considerations. This is* not *a restriction: the antiferromagnetic case would only imply further case analyses. The obtained*

recursion relation is

$$\begin{aligned}\rho_N(\Sigma_N)\,|0\rangle &= (2\cosh K_1)^M \exp(\mathcal{H}_N + \mathcal{K}_{2,N}) \\ &\quad \times \exp(-2K_1^* \sum_{m=1}^{M} \sigma_m^+\sigma_m^-)\rho_{N-1}(\Sigma_N)\,|0\rangle \\ &= (2\cosh K_1)^{MN} \left(\mathrm{e}^{\mathcal{K}_{2,N}} \mathrm{e}^{\mathcal{H}_N} \mathrm{e}^{-2K_1^* \sum\limits_{m=1}^{M} \sigma_m^+\sigma_m^-} \right)^N \rho_0(\Sigma_N)\,|0\rangle\,.\end{aligned}$$

As an transformation invariant functional, one may consider the trace in the basis of spins in the z-direction (cf. $|1\rangle, |0\rangle$ *above). In the representation of this basis,* σ^x *has no diagonal elements such that only the zeroth order term in the canonical expansion* (3.1.3) *contributes to the trace. This fact justifies the initial choice of* σ^x *as spin operators and it allows to consider only the vacuum state if the calculation of the trace is taken into account and if its contribution is counted* 2^M *times. This number corresponds the number of possible spin configurations in the* N^{th} *row. It is*

$$Z := \mathrm{Tr}_{\Sigma_N}[\rho_N(\Sigma_N)] = 2^M \langle 0|\, \rho_N(\Sigma_N)\,|0\rangle \tag{3.1.7}$$

The aim of the next chapter will be to calculate (3.1.7) *before determining the transition temperature* T_c *Onsager once obtained. In the following, the external field* H *will not be taken into account anymore since it causes yet unsolved problems in the computation. Nonetheless, in the thermodynamic limit the density of the free energy will be non-analytic and will hence represent a phase transition.*

3.2 Diagonalization of $\rho_N^{red}(\Sigma_N)$

Preliminaries: Z can be rewritten as follows

$$\begin{aligned} Z &= \mathrm{Tr}(V^N) \\ V &:= V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}} \\ V_1 &;= (2\cosh K_1)^M \exp(-2K_1^* \sum \sigma_m^+\sigma_m^-) \\ &\overset{(3.2.3)}{=} (2\sinh(2K_1))^{\frac{M}{2}} \exp[-2K_1^* \sum(\sigma_m^+\sigma_m^- - \frac{1}{2})] \qquad (3.2.1) \\ V_2 &:= \exp(K_2 \sum \sigma_m^x \sigma_{m+1}^x) \qquad (3.2.2)\end{aligned}$$

where the boundary conditions set by $\rho_0(\Sigma_N)$ are dropped and replaced by the normalization

$$\rho_0(\Sigma_N) \quad := \quad 2^{-M}.$$

In addition, one used the following trigonometrical identity

$$\begin{aligned} & 2\sinh x \cosh x = \sinh(2x) \\ \Rightarrow \quad & 2\cosh K_1 \exp(-K_1^*) \overset{(3.1.6)}{=} 2\cosh K_1 \sqrt{\tanh K_1} = \sqrt{2\sinh(2K_1)}. \end{aligned} \tag{3.2.3}$$

One can diagonalize V using the so-called *fermionization*.

3.2.1 Definition. *Let $\mathcal{F} := \{f_1; f_2; \ldots; f_1^+; f_2^+; \ldots\}$ be a set of operators. $\mathcal{F}$ is said to be a set of* fermion operators *if the elements obey the following algebra:*

$$\begin{array}{rccl} \forall m,n: & \{f_m^+, f_n^+\} & = & \{f_m, f_n\} = 0, \\ & \{f_m^+, f_n\} & = & \delta_{mn}. \end{array}$$

By $\{\cdot,\cdot\} : \mathcal{F}^2 \to \mathbb{R}$ we denote the anti-commutator. This fermion operators are also called Grassmann numbers *because of their algebra.*

3.2.2 Remark. *It can already be seen that $f \in \mathcal{F}$ represents a fermion. f, namely, obeys the* Pauli principle*:*

$$f^2 = \frac{1}{2}\{f, f\} = 0$$

If a state is defined by $\prod_{j\in J} f_j^+ |0\rangle$ for $|0\rangle$ being the vacuum defined by

$$\forall j: \quad f_j |0\rangle = 0,$$

one has to fix the order of the f_j^+ in the product $\prod_{j\in J} f_j^+$, as to not have an ambiguity in this expression. The sign will be specified in the particular cases.

The algebra for the spin creation and annihilation operators is given by

$$\forall m \neq n: \quad \left([\sigma_m^\pm.\sigma_n^\pm] = 0 \wedge \{\sigma_m^+, \sigma_m^-\} = 1 \wedge (\sigma_m^+)^2 = (\sigma_m^-)^2 = 0\right)$$

In here, bosonic as well as fermionic features appear. So, it is necessary to find a transformation which turns spin operators into fermions with regard to reflecting the physical properties of the considered particles.

Jordan-Wigner-transformation

The annihilation and creation operators for the new set of fermions are given by the following transformation

$$\begin{aligned} c_m &:= \exp(\pi \mathrm{i} \sum_{j=1}^{m-1} \sigma_j^+ \sigma_j^-)\sigma_m^- \\ c_m^+ &:= \exp(\pi \mathrm{i} \sum_{j=1}^{m-1} \sigma_j^+ \sigma_j^-)\sigma_m^+ \end{aligned} \tag{3.2.4}$$

This transformation was introduced by *Pascual Jordan* (1902-1980) and *Eugene Wigner* (1902-1995) [JW28] in 1928. Before proceeding, we shall show that these annihilation and creation operators indeed are fermionic operators.

3.2.3 Lemma. *The c_m/c_m^+ are fermion operators.*

Proof. Let $m, n \in \{1, 2, \ldots, M\}$, $m > n$. First of all, one obtains

$$\begin{aligned} \{c_m, c_m\} &= 2\mathrm{e}^{\pi \mathrm{i} \sum_{j=1}^{m-1} \sigma_j^+ \sigma_j^-} \sigma_m^- \mathrm{e}^{\pi \mathrm{i} \sum_{j=1}^{m-1} \sigma_j^+ \sigma_j^-} \sigma_m^- \\ &= 2\sigma_m^- \underbrace{\mathrm{e}^{2\pi \mathrm{i} \sum_{j=1}^{m-1} \sigma_j^+ \sigma_j^-}}_{=1} \sigma_m^- = 2(\sigma_m^-)^2 = 0 \end{aligned}$$

by using the *Baker-Campbell-Hausdorff formula*

$$\mathrm{e}^A \mathrm{e}^B = \mathrm{e}^{A+B} \mathrm{e}^{-[A,B]/2}$$

which holds for operators $A, B : H \to H$ on an arbitrary Hilbertspace H if $[A, [A, B]] = [B, [A, B]] = 0$, where $[\cdot, \cdot] : B(H)^2 \to B(H)$ is the commutator. We also took into account that $\sigma_m^\pm$ and $\sigma_j^+ \sigma_j^-$, $1 \leq j \leq m-1$, act on different spaces, so in particular,

$$[\sigma_m^\pm, \mathrm{e}^{\pi \mathrm{i} \sum_{j=1}^{m-1} \sigma_j^+ \sigma_j^-}] = 0.$$

Furthermore, one has

$$\begin{aligned} \{c_m, c_n\} &= \mathrm{e}^{\pi \mathrm{i} \sum_{j=1}^{m-1} \sigma_j^+ \sigma_j^-} \sigma_m^- \mathrm{e}^{\pi \mathrm{i} \sum_{j=1}^{n-1} \sigma_j^+ \sigma_j^-} \sigma_n^- + \text{Term with } m \leftrightarrow n \\ &\overset{[\sigma_m^-, \sigma_n^-]=0}{=} \mathrm{e}^{\pi \mathrm{i} \sum_{j=n}^{m-1} \sigma_j^+ \sigma_j^-} \sigma_n^- \sigma_m^- + \sigma_n^- \mathrm{e}^{\pi \mathrm{i} \sum_{j=n}^{m-1} \sigma_j^+ \sigma_j^-} \sigma_m^-. \end{aligned}$$

Now let *for the moment* $|0\rangle$ be any state with the n^{th} spin down and $|1\rangle$ conversely be a state with the n^{th} spin up. Then

$$\begin{aligned}\{c_m, c_n\}\,|0\rangle &= 0+0=0\\ \{c_m, c_n\}\,|1\rangle &= \mathrm{e}^{\pi\mathrm{i}\sum_{j=n+1}^{m-1}\sigma_j^+\sigma_j^-}\sigma_m^+\,|0\rangle + \sigma_n^-\mathrm{e}^{\pi\mathrm{i}}\mathrm{e}^{\pi\mathrm{i}\sum_{j=n+1}^{m-1}\sigma_j^+\sigma_j^-}\sigma_m^+\,|1\rangle \overset{[\sigma_n^-,e^{\cdots}]}{=} 0\end{aligned}$$

In here, 0 means 0 in the considered Hilbert space. So again, the demanded operator identity shall be obtained due to applying the operator to a state, in this case to any state. Hence, in this space holds the operator identity demanded in the claim. With analogous steps one obtains $\{c_m^+, c_n^+\} = 0$. Then

$$\{c_m^+, c_m\} \overset{\text{cf. above}}{=} \{\sigma_m^+, \sigma_m^-\} = 1$$

Finally, the two last anti-commutators $\{c_m^+, c_n\}$ and $\{c_n^+, c_m\}$ can be treated by following the same arguments as above. □

3.2.4 Remark. *Since*

$$c_m^+ c_m = \sigma_m^+\sigma_m^-, \tag{3.2.5}$$

implicated by (3.2.4)*, one can easily invert* (3.2.4) *to see that*

$$\begin{aligned}\sigma_m^- &= \exp(\pi\mathrm{i}\sum_{j=1}^{m-1} c_j^+ c_j)c_m\\ \sigma_m^+ &= \exp(\pi\mathrm{i}\sum_{j=1}^{m-1} c_j^+ c_j)c_m^+.\end{aligned}$$

Eq. (3.2.5) *means that the occupation number operator for the c- and the σ-fermions remains the same. By eq.* (3.2.1)*, V_1 stays diagonal in this representation*

$$V_1 = (2\sinh(2K_1))^{M/2}\exp[-2K_1^*\sum_m(c_m^+c_m - \frac{1}{2})]. \tag{3.2.6}$$

With respect to calculating V_2, $\sigma_m^x\sigma_{m+1}^x$ will be transformed in the next lemma. We will not prove the lemma since it is easy to obtain the results by applying the techniques of the proof above.

3.2.5 Lemma. *For the operators defined in* (3.2.4) *and in the case cyclic boundary conditions are imposed, the following relation to the* $\sigma_m^{\pm}$ *hold:*

$$\forall m < M : \begin{cases} \sigma_m^+\sigma_{m+1}^- &= c_m^+c_{m+1} \\ \sigma_m^+\sigma_{m+1}^+ &= c_m^+c_{m+1}^+ \\ \sigma_m^-\sigma_{m+1}^+ &= -c_mc_{m+1}^+ \\ \sigma_m^-\sigma_{m+1}^- &= -c_mc_{m+1} \end{cases}$$

Furthermore,

$$\begin{aligned} \sigma_M^+\sigma_1^- &= -\exp(\pi\mathrm{i}\mathcal{M})c_M^+c_1 \\ \sigma_M^+\sigma_1^+ &= -\exp(\pi\mathrm{i}\mathcal{M})c_M^+c_1^+ \\ \sigma_M^-\sigma_1^+ &= \exp(\pi\mathrm{i}\mathcal{M})c_Mc_1^+ \\ \sigma_M^-\sigma_1^- &= \exp(\pi\mathrm{i}\mathcal{M})c_Mc_1. \end{aligned}$$

With this lemma one can rewrite V_2 as

$$\begin{aligned} V_2 \overset{(3.2.2)}{=} & \exp[K_2\sum_{m=1}^{M}(\sigma_m^+ + \sigma_m^-)(\sigma_{m+1}^+ + \sigma_{m+1}^-)] \\ = & \exp[K_2\sum_{m=1}^{M}(c_m^+c_{m+1}^+ + c_m^+c_{m+1} - c_mc_{m+1}^+ - c_mc_{m+1}) \\ & - \mathrm{e}^{\pi\mathrm{i}\mathcal{M}}(c_M^+c_1^+ + c_M^+c_1 - c_Mc_1^+ - c_Mc_1)] \\ = & \exp[K_2\sum_{m=1}^{M}(c_m^+ - c_m)(c_{m+1}^+ + c_{m+1}) - \mathrm{e}^{\pi\mathrm{i}\mathcal{M}}(c_M^+ - c_M)(c_1^+ + c_1)] \end{aligned}$$

Since it is

$$\{\mathrm{e}^{\pi\mathrm{i}\mathcal{M}}, c_m\} = \{\mathrm{e}^{\pi\mathrm{i}\mathcal{M}}, c_m^+\} = 0$$

and since the exponents in V_1 and V_2, respectively, only contain the product of exactly two c_m/c_m^+-operators, one gets using

$$[\exp(\pi\mathrm{i}\mathcal{M}), V_1] = [\exp(\pi\mathrm{i}\mathcal{M}), V_2] = 0,$$

that the parity of $\mathcal{M}$ is conserved. So in the following one may consider the single subspaces, with odd and even particle number respectively, in order to simplify the calculation. This allows to rewrite V_2 as

$$V_2^{\pm} = \exp[K_2\sum_{m=1}^{M}(c_m^+ - c_m)(c_{m+1}^+ + c_{m+1})] \tag{3.2.7}$$

with

$$\begin{array}{llll} c_{M+1} & := -c_1 & c^+_{m+1} & = -c^+_1 \quad \text{if acting on an odd \#fermions} \\ c_{M+1} & := c_1 & c^+_{m+1} & = c^+_1 \quad \text{if acting on an even \#fermions} \end{array} \tag{3.2.8}$$

In the case of an odd number of fermions, we will speak of *cyclic* boundary conditions and otherwise we will speak of *anti-cyclic* boundary conditions. V_2^+ is defined to act on an even number of particles, V_2^- on an odd number of states respectively. The challenge we now face is to diagonalize V_1, V_2 and V_3 simultaneously. The aim of the next paragraph will be to write V in the simple form

$$V = \exp(-\sum_q \epsilon_q a_q^+ a_q + E_0)$$

It will be seen that this is possible with a simple linear transformation as

$$a_q = \sum_m (a_{qm} c_m + b_{qm} c_m^+), ^4$$

a so-called *Bogoliubov transformation* This transformation will be obtained in two steps.

Bogoliubov-Valatin transformation

The *translation invariance* due to periodic boundary conditions yields operators η_q by

$$c_m \quad =: \quad M^{-\frac{1}{2}} e^{-\mathrm{i}\pi/4} \sum_q e^{\mathrm{i}qm} \eta_q = M^{-\frac{1}{2}} e^{-\mathrm{i}\pi/4} \big(\sum_{q>0} \big(e^{\mathrm{i}qm} \eta_q + e^{-\mathrm{i}qm} \eta_{-q} \big) + \eta_0 \big) \tag{3.2.9}$$

There are two problems one has to be aware of: The first problem one faces is the range of the sum in eq. (3.2.9), the second is to invert eq. (3.2.9). To phrase this: One is looking for the discrete inverse Fourier transform. The first problem will be treated with the following lemma.

3.2.6 Lemma. *For any even $k \in \{0, 1, \ldots, 2M\}$, one has*

$$\frac{1}{M} \sum_m e^{\mathrm{i}\frac{km}{M}\pi} \quad = \quad \delta_{k,0} + \delta_{k,2M}$$

.

[4] If it is not mentioned otherwise the summation on m will run from 1 to M in this chapter.

Proof. Let $k \notin \{0, 2M\}$ be even. Then

$$\begin{aligned} \sum_m e^{\mathrm{i}\frac{km}{M}\pi} &= \sum_m (e^{\mathrm{i}\frac{k}{M}\pi})^m = \frac{1 - e^{\mathrm{i}\frac{k(M+1)}{M}\pi}}{1 - e^{\mathrm{i}\frac{k}{M}\pi}} - 1 = \\ &= \frac{e^{\mathrm{i}\frac{k}{M}\pi}(1 - e^{\mathrm{i}k\pi})}{1 - e^{\mathrm{i}\frac{k}{M}\pi}} = 0 \end{aligned}$$

The formula for the geometric sum is used in here. On the other hand, one has for $k \in \{0, 2M\}$:

$$\frac{1}{M} \sum_m \underbrace{e^{\mathrm{i}\frac{km}{M}\pi}}_{=1} = 1$$

□

Lemma 3.2.6 is an orthonormal relation for e^{iqm}. With its help, eq. (3.2.9) can be inverted,

$$\eta_q = e^{\mathrm{i}\pi/4} \sum_m e^{-\mathrm{i}qm} c_m$$

This yields that the operators η_q themselves are fermionic operators. So, they also obey the anti-commutation relations that are given for the c_m. Equation (3.2.8) implies

$$0 = c_{M+1} + c_1 = M^{-\frac{1}{2}} \mathrm{e}^{-\mathrm{i}\pi/4} \sum_q \mathrm{e}^{\mathrm{i}q} \eta_q (\mathrm{e}^{\mathrm{i}qM} + 1)$$

Since the η_q-operators are linear independent for different q, this can only be the case if $q = (2k+1)\pi/M$ for $k \in \mathbb{Z}$. One is free to choose M to be *even*. Because of $e^{\mathrm{i}((2k+1)+2M)\pi/M} = e^{\mathrm{i}(2k+1)\pi/M}$, one can further impose w.l.o.g. the condition

$$q \in O := \{\pm\pi/M; \pm 3\pi/M; \ldots; \pm(M-1)\pi/M\}.$$

Analogously, one obtains from

$$0 = c_{M+1} - c_1 = M^{-\frac{1}{2}} e^{-\mathrm{i}\pi/4} \sum_q e^{\mathrm{i}q} \eta_q (e^{\mathrm{i}qM} - 1)$$

the following range for q for the case of an even number of states,

$$q \in E := \{0; \pm 2\pi/M; \ldots; \pm(M-2)\pi/M; \pi\}.$$

In the case of "even states" one must be careful with $q \in \{0; \pi\}$. Both values only appear with only one sign; that causes some subtleties in the calculations below.
In both cases, even or odd number of η-fermions, the summation includes the *first Brillouin zone*. It is

$$|O| = |E| = M,$$

which guarantees that one does not miss out a state[5]. The number of η-particles equals the number of c-particles, in particular

$$\mathcal{M} = \sum_m c_m^+ c_m = \frac{1}{M} \sum_{m,q_1,q_2} \mathrm{e}^{\mathrm{i}(q_2-q_1)m} \eta_{q_1}^+ \eta_{q_2} \overset{3.2.6}{=} \sum_q \eta_q^+ \eta_q \qquad (3.2.10)$$

From now on a summation/product on q runs on $q \in X \in \{E; O\}$ depending on whether one is dealing with cyclic respectively anti-cyclic boundary conditions. It will be clear which summation/product shall be used in the particular case. $V^{\pm}$ will be expressed in terms of the new fermion set in the next lemma.

3.2.7 Lemma. *V can be written in the form*

$$V^{\pm} = (2\sinh(2K_1))^{M/2} (V_1 V_\pi)^{\frac{1\pm1}{2}} \prod_{0<q<\pi} V_q \qquad (3.2.11)$$

where

$$\forall 0 < q < \pi : \quad \begin{cases} V_q &= V_{2q}^{\frac{1}{2}} V_{1q} V_{2q}^{\frac{1}{2}} \\ V_{1q} &= \exp[-2K_1^*(\eta_q^+\eta_q + \eta_{-q}^+\eta_{-q} - 1)] \\ V_{2q} &= \exp\big[2K_2[\cos q(\eta_q^+\eta_q + \eta_{-q}^+\eta_{-q} - 1)^6 \\ & \quad + \sin q(\eta_q\eta_{-q} + \eta_{-q}^+\eta_q^+)]\big] \end{cases}$$

and

$$V_0 = \exp[-2(K_1^* - K_2)(\eta_0^+\eta_0 - \frac{1}{2})]$$
$$V_\pi = \exp[-2(K_1^* + K_2)(\eta_\pi^+\eta_\pi - \frac{1}{2})]$$

[5]Small remark to the terminology: The term *state* will be used for $\omega \in E^{MN}$ and an eigenstate of f^+f for a fermion operator f will be called an *$f-$particle/fermion*.

[6]In [LMS64] Lieb, Mattis and Schultz had a flaw in here: Instead of $(\eta_q^+\eta_q + \eta_{-q}^+\eta_{-q} - 1)$, they obtained $(\eta_q^+\eta_q + \eta_{-q}^+\eta_{-q})$. Mattis corrects this in [Mat03], but this solution was independently obtained.

Proof. For the exponent of V_1 (cf. eq. (3.2.6)) one obtains

$$\begin{aligned}\sum_m (c_m^+ c_m - \frac{1}{2}) &= \frac{1}{M}\sum_{m q_1 q_2} e^{\mathrm{i}(q_2-q_1)m}\eta_{q_1}^+\eta_{q_2} - \frac{M}{2} \\ &\overset{3.2.6}{=} \sum_{0<q<\pi}(\eta_q^+\eta_q + \eta_{-q}^+\eta_{-q} - 1) + [(\eta_0^+\eta_0 - \frac{1}{2}) \\ &\quad + (\eta_\pi^+\eta_\pi - \frac{1}{2})]\mathbb{1}_{\{\mathrm{even}\}}.\end{aligned}$$

$\mathbb{1}_{\mathrm{even}}$ means that one should only take care of this term with regard to cyclic boundary conditions. Since all the terms are occupation number operators and these commute one with each other, it is possible to factorize V_1 in virtue of

$$\begin{aligned}V_1 &= (2\sinh(2K_1))^{M/2}\left(\mathrm{e}^{-2K_1^*(\eta_0^+\eta_0-\frac{1}{2})}\mathrm{e}^{-2K_1^*(\eta_\pi^+\eta_\pi-\frac{1}{2})}\right)^{1-\mathbb{1}_{\{even\}}}\prod_{0<q<\pi} V_{1q}, \\ \forall 0<q<\pi: \quad V_{1q} &:= \mathrm{e}^{-2K_1^*(\eta_q^+\eta_q+\eta_{-q}^+\eta_{-q}-1)}.\end{aligned}$$

With

$$\begin{aligned}\sum_m \mathrm{e}^{-\mathrm{i}(q_2+q_1)m} &\overset{3.2.6}{=} \delta_{q_1,-q_2} + \delta_{q_1,q_2}\delta_{q_1,\pi} \\ \sum_m \mathrm{e}^{\mathrm{i}(q_2-q_1)m} &\overset{3.2.6}{=} \delta_{q_1,q_2}\end{aligned}$$

one obtains for the exponent of V_2 (cf. eq. (3.2.7))

$$\begin{aligned}
\sum_m (c_m^+ - c_m)(c_{m+1}^+ + c_{m+1}) &= \frac{1}{M}\sum_{mq_1q_2}\left(\mathrm{e}^{-\mathrm{i}\pi/4}\mathrm{e}^{-\mathrm{i}q_1 m}\eta_{q_1}^+ - \mathrm{e}^{\mathrm{i}\pi/4}\mathrm{e}^{\mathrm{i}q_1 m}\eta_{q_1}\right)\\
&\quad\cdot\left(\mathrm{e}^{-\mathrm{i}\pi/4}\mathrm{e}^{-\mathrm{i}q_2(m+1)}\eta_{q_2}^+ + \mathrm{e}^{\mathrm{i}\pi/4}\mathrm{e}^{\mathrm{i}q_2(m+1)}\eta_{q_2}\right)\\
&= \frac{1}{M}\sum_{mq_1q_2}\left(\mathrm{e}^{-\mathrm{i}\pi/2}\mathrm{e}^{-\mathrm{i}(q_2+q_1)m}\mathrm{e}^{-\mathrm{i}q_2}\eta_{q_1}^+\eta_{q_2}^+\right.\\
&\quad+\ \mathrm{e}^{\mathrm{i}(q_2-q_1)m}\mathrm{e}^{\mathrm{i}q_2}\eta_{q_1}^+\eta_{q_2} - \mathrm{e}^{\mathrm{i}(q_1-q_2)m}\mathrm{e}^{-\mathrm{i}q_2}\eta_{q_1}\eta_{q_2}^+\\
&\quad-\ \left.\mathrm{e}^{\mathrm{i}\pi/2}\mathrm{e}^{\mathrm{i}(q_1+q_2)m}\mathrm{e}^{\mathrm{i}q_2}\eta_{q_1}\eta_{q_2}\right)\\
&\overset{3.2.6}{=} [2(\eta_0^+\eta_0 - \frac{1}{2}) - 2(\eta_\pi^+\eta_\pi - \frac{1}{2})]\mathbb{1}_{\{\text{even}\}}\\
&\quad+2\sum_q[\sin q(\underbrace{-\eta_q^+\eta_{-q}^+}_{=\eta_{-q}^+\eta_q^+} + \eta_q\eta_{-q})\\
&\quad+\cos q(\eta_q^+\eta_q + \eta_{-q}^+\eta_{-q} - 1)].
\end{aligned}$$

Here again, the result means that one should only take care of the η_0 and the η_π terms if cyclic boundary conditions are imposed. Using the property that $\eta_0^+\eta_0$ and $\eta_\pi^+\eta_\pi$ commute with all the other operators since they act on other states, one obtains

$$\begin{aligned}
V_2 &= \left(\mathrm{e}^{2K_2\left(\eta_0^+\eta_0-\frac{1}{2}\right)}\mathrm{e}^{-2K_2\left(\eta_\pi^+\eta_\pi-\frac{1}{2}\right)}\right)^{\mathbb{1}_{\{even\}}}\prod_{0<q<\pi}V_{2q},\\
\forall 0<q<\pi:\quad V_{2q} &:= \mathrm{e}^{2K_2\left(\sin q(\eta_{-q}^+\eta_q^+ + \eta_q\eta_{-q}) + \cos q(\eta_q^+\eta_q + \eta_{-q}^+\eta_{-q} - 1)\right)}.
\end{aligned}$$

Gathering the $\eta_0^+\eta_0$- and $\eta_\pi^+\eta_\pi$-terms from V_1 and V_2 gives

$$\begin{aligned}
V_0 &:= \mathrm{e}^{-2(K_1^*-K_2)(\eta_0^+\eta_0-\frac{1}{2})},\\
V_\pi &:= \mathrm{e}^{-2(K_1^*+K_2)(\eta_\pi^+\eta_\pi-\frac{1}{2})}.
\end{aligned}$$

Rearranging the factors in $V^\pm = V_2^{\frac{1}{2}}V_1V_2^{\frac{1}{2}}$ by using that

$$\forall q_1\neq q_2:\quad [V_{2q_1}^{\frac{1}{2}}, V_{2q_2}^{\frac{1}{2}}] = 0$$

yields the claim. □

An important feature of the representation of $V^{\pm}$ given in the last lemma is that all V_q, $q \in X \in \{E;O\}$, commute one with each other. Hence, they can be independently diagonalized. Starting with the usual definition the η-vacuum Φ_0 in virtue of

$$\forall q \in X \in \{E;O\}: \quad \eta_q \Phi_0 \quad = \quad 0$$

one sets

$$\forall q \in X \in \{E;O\}: \quad \begin{cases} \Phi_q & := & \eta_q^+ \Phi_0 \\ \Phi_{-q} & := & \eta_{-q}^+ \Phi_0 \\ \Phi_{-q,q} & := & \eta_{-q}^+ \eta_q^+ \Phi_0. \end{cases}$$

Note that these are the only 4 possible particle number configurations belonging to one $q \in X \in \{E;O\}$ because of the Pauli principl. V_0 and V_π are diagonal in the occupation number representation. Let $q \in X \setminus \{0\}$, $X \in \{E;O\}$.

	Φ_0	$\Phi_{-q,q}$	Φ_q	Φ_{-q}
$\eta_q \eta_{-q}$	0	Φ_0	0	0
$\eta_{-q}^+ \eta_q^+$	$\Phi_{-q,q}$	0	0	0
$\eta_q^+ \eta_q + \eta_{-q}^+ \eta_{-q}$	0	$2\Phi_{-q,q}$	Φ_q	Φ_{-q}

Table 3.1: Effect of the operators appearing in V_q on the Φ, $0 < q < \pi$

Considering table 3.1, V_q is already diagonal in $\{\Phi_q, \Phi_{-q}\}$,

$$V_q \Phi_{\pm q} \quad = \quad \Phi_{\pm q},$$

and V_{1q} is diagonal in $\{\Phi_0, \Phi_{-q,q}\}$,

$$V_{1q} \quad = \quad \begin{pmatrix} \mathrm{e}^{2K_1^*} & 0 \\ 0 & \mathrm{e}^{-2K_1^*} \end{pmatrix}^{7},$$

whereas in that basis, V_{2q} has the representation

$$V_{2q} \quad = \quad \mathrm{e}^{2K_2(-\cos q\tau_3 + \sin q\tau_1)},$$

[7] The standard notation is used in here. The "="-sign should not be interpreted as an identity, but as an identification.

where $\{\tau_1;\tau_2;\tau_3\}$ are the Pauli matrices. From now on, one will stay in the representation of $\{\Phi_0, \Phi_{-q,q}\}$. Let $\tau := (\tau_1, \tau_2, \tau_3)$ and define

$$n_q \quad := \quad (\sin q, 0, -\cos q)^T.$$

With the identity

$$\forall \phi \in \mathbb{R}^3 \setminus \{0\}: \quad \mathrm{e}^{\phi\cdot\tau} \quad = \quad I_2 \cosh|\phi| + \left(\frac{\phi}{|\phi|}\cdot\tau\right)\sinh|\phi|^8, \qquad (3.2.12)$$

one gets

$$\begin{aligned} V_{2q}^{\frac{1}{2}} \quad &= \quad \mathrm{e}^{K_2 n_q\cdot\tau} = I_2\cosh K_2 + (n_q\cdot\tau)\sinh K_2 \\ &= \quad \begin{pmatrix} \cosh K_2 - \cos q \sinh K_2 & \sin q \sinh K_2 \\ \sin q \sinh(2K_2) & \cosh K_2 + \cos q \sinh K_2 \end{pmatrix}. \end{aligned}$$

Hence it is

$$V_q \quad = \quad V_{2q}^{\frac{1}{2}} V_{1q} V_{2q}^{\frac{1}{2}} = \begin{pmatrix} A_q & B_q \\ B_q & C_q \end{pmatrix}$$

with

$$\begin{aligned} A_q \quad &:= \quad (\cosh K_2 - \cos q \sinh K_2)^2 \mathrm{e}^{2K_1^*} + (\sin q \sinh K_2)^2 \mathrm{e}^{-2K_1^*}, \\ B_q \quad &:= \quad (\cosh K_2 - \cos q \sinh K_2)(\sin q \sinh K_2)\mathrm{e}^{2K_1^*} \\ &\quad\; +(\sin q \sinh K_2)(\cosh K_2 + \cos q \sinh K_2)\mathrm{e}^{-2K_1^*} \\ &= \quad 2\sin q \sinh K_2 \left(\cosh K_2 \cosh(2K_1^*) - \cos q \sinh K_2 \sinh(2K_1^*)\right), \\ C_q \quad &:= \quad (\sin q \sinh K_2)^2 \mathrm{e}^{2K_1^*} + (\cosh K_2 + \cos q \sinh K_2)^2 \mathrm{e}^{-2K_1^*}. \end{aligned}$$

The eigenvalues of V_q are[9]

$$\mathrm{e}^{\pm\epsilon_q} \quad := \quad \frac{1}{2}(A_q + C_q) \pm \sqrt{\frac{1}{4}(A_q + C_q)^2 + B_q^2},$$

[8] For the proof see the appendix. I_n means the identity matrix in n dimensions

[9] From here on the calculation coincides with that of [LMS64].

where[10]

$$\begin{aligned}\epsilon_q &= \operatorname{arcosh}\,[\frac{1}{2}(\mathrm{e}^{\epsilon_q}+\mathrm{e}^{-\epsilon_q})] = \operatorname{arcosh}\,[\frac{1}{2}(A_q+C_q)] \\ &= \operatorname{arcosh}\,[(\sin^2 q \sinh^2 K_2 + \cosh^2 K_2 + \cos^2 q \sinh^2 K_2)\cosh(2K_1^*) \\ &\quad - 2\cos q \sinh_{K_2} \cosh K_2 \sinh(2K_1^*)] \\ &= \operatorname{arcosh}\,[\cosh(2K_2)\cosh(2K_1^*) - \cos q \sinh(2K_2)\sinh(2K_1^*)].\end{aligned} \tag{3.2.13}$$

Note

$$\epsilon_q = \epsilon_{-q}. \tag{3.2.14}$$

Orthonormalized eigenvectors belonging to these eigenvalues are

$$\begin{array}{rclcrcl} \Psi_0 &:=& \cos\alpha_q\Phi_0 + \sin\alpha_q\Phi_{-q,q}, & & V_q\Psi_0 &=& \mathrm{e}^{\epsilon_q}\Psi_0 \\ \Psi_{-q,q} &:=& -\sin\alpha_q\Phi_0 + \cos\alpha_q\Phi_{-q,q}, & & V_q\Psi_{-q,q} &=& \mathrm{e}^{-\epsilon_q}\Psi_{-q,q} \end{array} \tag{3.2.15}$$

where inserting these linear combinations into the eigenvalue equation yields

$$\tan\alpha_q = \frac{B_q}{\mathrm{e}^{\epsilon_q} - C_q}.$$

This gives

$$\begin{aligned}\tan(2\alpha_q) &= \frac{2\tan\alpha_q}{1-\tan^2\alpha_q} = \frac{2B_q(\mathrm{e}^{\epsilon_q}-C_q)}{(\mathrm{e}^{\epsilon_q}-C_q)^2 - B_q^2} \\ &\overset{\mathrm{e}^{\epsilon_q}\ \mathrm{EV}}{=}_{\text{of } V_q} \frac{2B_q(\mathrm{e}^{\epsilon_q}-C_q)}{(A_q-C_q)\mathrm{e}^{\epsilon_q} + C_q(C_q-A_q)} = \frac{2B_q}{A_q-C_q},\end{aligned}$$

which defines α_q up to a multiple of $\pi/2$. Now one introduces the Bogoliubov-Valatin transformation[11] in order to rewrite the eigenvectors. Let

$$\begin{array}{rcl} \xi_q &:=& \cos\alpha_q\eta_q + \sin\alpha_q\eta_{-q}^+ \\ \xi_{-q} &:=& \cos\alpha_q\eta_{-q} - \sin\alpha_q\eta_q^+ \end{array} \tag{3.2.16}$$

and define

$$\begin{array}{rcl} \Psi_q &:=& \xi_q^+\Psi_0 = (\cos\alpha_q\eta_q^+ + \sin\alpha_q\eta_{-q})(\cos\alpha_q + \sin\alpha_q\eta_{-q}^+\eta_q^+)\Phi_0 = \Phi_q \\ \Psi_{-q} &:=& \xi_{-q}^+\Psi_0 = \ldots = \Phi_{-q}. \end{array}$$

[10] In here, the notation "arcosh a" which is not very common in the Anglo-Saxon region is used for the positive root of $\cosh x = a$. Analogously arsinh a, artanh a and so on are defined.

[11] cf. [LMS64], p. 863

Then

$$\begin{array}{rcccl} & & \xi_q\Psi_0 & = & \xi_{-q}\Psi_0 = 0 \\ \xi^+_{-q} & \underbrace{\xi^+_q\Psi_0}_{=\Phi_q=\eta^+_q\Phi_0} & = & & (\cos\alpha_q\eta^+_{-q} - \sin\alpha_q\eta_q)\eta^+_q\Phi_0 = \Psi_{-q,q}. \end{array}$$

These relations justify the notations in (3.2.15). Thus $\Psi_0, \Psi_q, \Psi_{-q}$ and $\Psi_{-q,q}$ are the four possible eigenvectors of V_q modulo the defined ground state Φ_0[12]. With these, one can rewrite V_q in virtue of

$$V_q = \mathrm{e}^{\epsilon_q(\xi^+_q\xi_q + \xi^+_{-q}\xi_{-q}-1)}.$$

Defining

$$\begin{array}{llll} \alpha_0 := 0, & \epsilon_0 := 2(K_1^* - K_2), \\ \alpha_\pi := 0, & \epsilon_\pi := 2(K_1^* + K_2), \end{array}$$ [13]

one finds

$$V^{\pm} = (2\sinh(2K_1))^{M/2}\mathrm{e}^{-\sum_q \epsilon_q(\xi^+_q\xi_q - \frac{1}{2})}. \tag{3.2.17}$$

Before continuing, (3.2.16) shall be inverted. One has

$$\forall q: \quad \begin{pmatrix} \xi_q \\ \xi^+_q \\ \xi_{-q} \\ \xi^+_{-q} \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\alpha_q & & & \sin\alpha_q \\ & \cos\alpha_q & \sin\alpha_q & \\ & -\sin\alpha_q & \cos\alpha_q & \\ -\sin\alpha_q & & & \cos\alpha_q \end{pmatrix}}_{=:\mathcal{D}(\alpha_q)} \cdot \begin{pmatrix} \eta_q \\ \eta^+_q \\ \eta_{-q} \\ \eta^+_{-q} \end{pmatrix}$$

with $\mathcal{D}(\alpha_q)^{-1} = \mathcal{D}(\alpha_q)^+ = \mathcal{D}(-\alpha_q)$. In order to determine the eigenvectors belonging to V, one picks up the above discussion on the parity of the particle number. It holds

$$\begin{array}{rcl} \mathcal{M} & \overset{(3.2.10)}{=} & \sum_q \eta^+_q\eta_q = \sum_{0<q<\pi}(\eta^+_q\eta_q + \eta^+_{-q}\eta_{-q}) + (\eta^+_0\eta_0 + \eta^+_\pi\eta_\pi)\mathbb{1}_{\{even\}} \\ & = & \sum_q (\mathcal{D}(-\alpha_q)\xi_q)^+\mathcal{D}(-\alpha_q)\xi_q = \sum_q \xi^+_q\xi_q, \end{array}$$

[12] E.g. there is a $U(1)$-symmetry of the ground state.

[13] Note, that these pure definitions obey $\epsilon_0 = \pm\lim_{q\to 0}\epsilon_q$ for $T\{^{>T_c}_{<T_c}\}$ because ϵ_q is defined to be positive for $0 < q < \pi$, $\epsilon_\pi = \lim_{q\to\pi}\epsilon_q$ respectively. T_c is defined in virtue of $K_1^* = K_2 \Leftrightarrow \sinh(2J_1\beta_c))\sinh(2J_2\beta_c) = 1$.

i.e., the total number of η-particles equals the number of ξ-particles. With this observation, one may just consider the eigenvectors with an even number of particles in the case of V^+ and for V^- these with an odd number of particles. Now the largest eigenvalue for both cases has to be determined because the other eigenvalues will be suppressed in the thermodynamic limit as we will below in more detail. The largest eigenvalue for V^+ is

$$\begin{aligned} \Lambda^+ &:= (2\sinh(2K_1))^{M/2} \mathrm{e}^{\frac{1}{2}\sum_q \epsilon_q}, \\ V^+\Psi_0 &= \Lambda^+\Psi_0, \end{aligned}$$

since the vacuum contains an even number of particles (namely 0). For V^- the eigenvector with the largest eigenvalue must contain at least one particle. Using the fact that

$$\forall q > 0: \quad \epsilon_q \overset{(3.2.13)}{=} \operatorname{arcosh}\left[\cosh(2K_2)\cosh(2K_1^*) - \underbrace{\cos q}_{\leq 1}\sinh(2K_2)\sinh(2K_1^*)\right]$$

$$\underset{increasing}{\overset{\operatorname{arcosh}}{\geq}} \operatorname{arcosh}\left[\cosh[2(K_2 - K_1^*)]\right] = |2(K_2 - K_1^*)| \geq \epsilon_0,$$

one obtains the largest eigenvalue Λ^- of V^- for one particle with "momentum" $q = 0$, i.e.,

$$\begin{aligned} \Lambda^- &:= (2\sinh(2K_1))^{M/2} \mathrm{e}^{-\epsilon_0/2 + \frac{1}{2}\sum_{q\neq 0}\epsilon_q} \\ V^-\xi_0^+\Psi_0 &= \Lambda^-\xi_0^+\Psi_0. \end{aligned}$$

As noted above in a footnote, ϵ_0 is related to ϵ_q, $q \neq 0$, in virtue of

$$\epsilon_0 = 2(K_1^* - K_2) = \begin{cases} \lim_{q\to 0}\epsilon_q & T \geq T_c \\ -\lim_{q\to 0}\epsilon_q & T < T_c \end{cases}, \tag{3.2.18}$$

where T_c is defined by

$$\sinh(\frac{J_1}{k_b T_c})\sinh(\frac{J_2}{k_b T_c}) = 1. \tag{3.2.19}$$

(3.2.18) can easily verified using figure 3.1.

For both cases, Λ^+ and Λ^-, one can rewrite the exponent for $T < T_c$ as follows

$$\frac{1}{2}\sum_q |\epsilon_q| = \frac{M}{4\pi}\sum_q \frac{2\pi}{M}|\epsilon_q|,$$

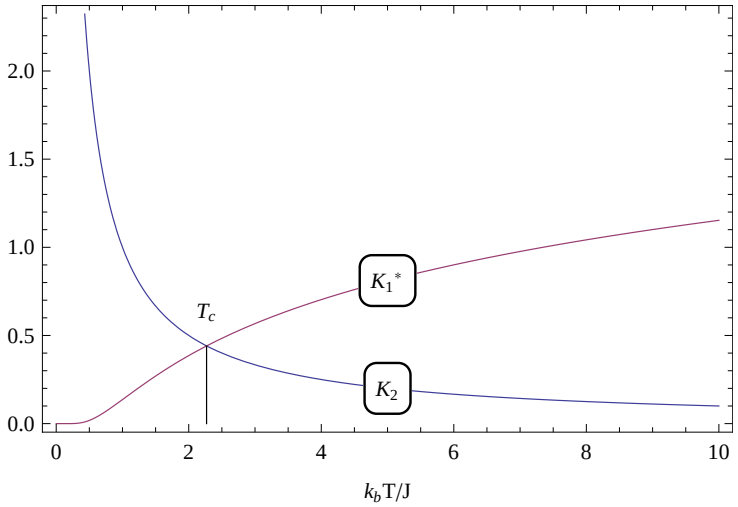


Figure 3.1: Graphs for $K_2(k_bT/J) = \frac{J}{k_BT}$, $K_1^*(k_bT/J) = -\frac{1}{2}\log[\tanh(\frac{J}{k_BT})]$, the isotropic case.

This can be identified with a Riemann sum. One finally obtains

$$\begin{aligned}
f_{\{1;2;\ldots;M\}\times\{1;2;\ldots;N\}}(T) &:= -\frac{k_bT}{MN}\log Z^{\pm} = -\frac{k_bT}{MN}\log\left[\mathrm{Tr}_{\Sigma_N}((V^{\pm})^N)\right] \\
&= -k_bT\left[\frac{1}{MN}\log\left[\left(\Lambda^{\pm}\right)^N\right] + \frac{1}{MN}\log\left(\sum_{\lambda\in\sigma(V^{\pm})}\frac{\lambda^N}{(\Lambda^{\pm})^N}\right)\right] \\
&= -k_bT\left[\frac{1}{2}\log\left(2\sinh\left(2K_1\right)\right) + \frac{1}{4\pi}\sum_q\frac{2\pi}{M}|\epsilon_q|\right. \\
&\quad \left. -\frac{|\epsilon_0|+\epsilon_0}{2M}\mathbb{1}_{\{even\}} + \frac{1}{MN}\log\left(\sum_{\lambda\in\sigma(V^{\pm})}\frac{\lambda^N}{(\Lambda^{\pm})^N}\right)\right] \\
&\underset{M,N\to\infty}{\to} -\frac{k_bT}{2}\left(\log\left(2\sinh\left(2K_1\right)\right) + \frac{1}{2\pi}\int_{-\pi}^{\pi}|\epsilon_q|\,\mathrm{d}q\right),
\end{aligned}$$

where we used that $\lambda^N \in \sigma((V^{\pm})^N) \Leftrightarrow \lambda \in \sigma(V^{\pm})$ and

$$1 \quad \leq \quad \sum_{\lambda\in\sigma(V^{\pm})}\frac{\lambda^N}{(\Lambda^{\pm})^N} \quad \leq \quad 2^M,$$

since $\sigma(V^{\pm}) \ni \lambda > 0$ by eq. (3.2.17) and the configuration space of Σ_N with respect to which the trace is taken, is 2^M-dimensional. Ao the degeneracy of $\Lambda^{\pm}$ does not affect the result. One sets

$$\forall \beta \in \mathbb{R}^+ : \quad f(\beta) \quad := \quad \lim_{M,N\to\infty} f_{\{1;2;\ldots;M\}\times\{1;2;\ldots;N\}}(\frac{k_b}{\beta}).$$

3.3 Critical phenomena

The free energy per volume f shall now be analyzed with regard to assuring that f exhibits a phase transition. One could also look at the *spontaneous magnetization* (resp. its the second momentum) defined by

$$m_{sp} \quad := \quad \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \langle \sum_{i\in\Lambda_n} \sigma_i \rangle = \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \frac{\sum\limits_{\sigma\in\Omega_{\Lambda_n}} \sum\limits_{i\in\Lambda_n} \sigma_i \mathrm{e}^{-\beta H_{\Lambda_n}(\sigma)}}{\sum\limits_{\sigma\in\Omega_{\Lambda_N}} \mathrm{e}^{-\beta H_{\Lambda_n}(\sigma)}}$$

for $\beta \in \mathbb{R}^+$. One usually considers the correlation of spins, the distance of which grows to infinity. The expectation value of the correlation is positive below T_c and 0 above[14]. Nonetheless, neither the existence of the limit in the definition of m_{sp}, nor the existence of n-point spin-correlation functions, $n \geq 2$, can be established easily. In contrast to the free energy, the limit of the correlation function depends very much on the boundary conditions[15]. Nevertheless, a spontaneous symmetry breaking is reflected in the specific heat capacity. Initially, the integral appearing in f shall be transformed in order to make it treatable[16]. With the identity given by Onsager

$$\forall z \in \mathbb{R} : |z| \quad = \quad \frac{1}{\pi} \int_0^{\pi} \log[2(\cosh z - \cos t)] \mathrm{d}t \tag{3.3.1}$$

and assuming $K_1 = K_2 =: K$, $K^* := K_1^*$, the integral becomes

$$\frac{1}{\pi^2} \int_0^{\pi} \mathrm{d}q \int_0^{\pi} \mathrm{d}k \log[2(\underbrace{\cosh(2K)\coth(2K)}_{=:Q} \underbrace{-\cos k - \cos q}_{=-2\cos\frac{q+k}{2}\cos\frac{q-k}{2}})], \tag{3.3.2}$$

[14] Cf. [LMS64], p. 864-871; [Bax89] recommends [MW73].
[15] Cf. [KS04], p.106
[16] For this section cf. [Hua87].

In here, one already used that $\epsilon_{-q} = \epsilon_q \geq 0 \forall q \neq 0$ and $\epsilon_0 := \lim_{q\to 0} \epsilon_q$ was redefined in order to have the continuous extension to $[-\pi, \pi]\setminus\{0\} \to \mathbb{R}, q \mapsto \epsilon_q$. In addition, the identities

$$\begin{aligned}
\cosh(2K^*) &\overset{(3.1.6)}{=} \frac{1}{2}(\coth K + \tanh K) = \frac{1}{2}\frac{\cosh^2 K - \sinh^2 K}{\sinh K \cosh K} \\
&= \coth(2K), \\
\sinh(2K_1^*) &\overset{(3.1.6)}{=} \frac{1}{2}(\coth K - \tanh K) = \frac{1}{\sinh(2K)}
\end{aligned}$$ [17]

were used. With regard to applying the transformation rule, one must assure that $G : \mathbb{R}^2 \to \mathbb{R}, (q,k) \mapsto \log[2(\cosh(2K)\coth(2K) - \cos k - \cos q)]\mathbb{1}_{[0,\pi]}(q)\mathbb{1}_{[0,\pi]}(k)$ is a integrable function. Clearly, G is measurable. For $K \neq K^*$ one has

$$\begin{aligned}
\forall q, k \in [0,\pi]: \quad -\infty &< \log[\cosh(2(K^* - K)) - 1] \\
&\leq \log[\cosh(2K^*)\cosh(2K) - \cos q - \cos k] \\
&\leq \log[\cosh(2(K^* + K)) + 1] < \infty,
\end{aligned}$$

where trigonometrical identities and the fact that $\sinh(2K^*)\sinh(2K) = 1$ are used. Thus, G is integrable. By the *transformation rule*, one may now transform

$$\phi : \mathbb{R}^2 \to \mathbb{R}^2, \begin{pmatrix} q \\ k \end{pmatrix} \mapsto \begin{pmatrix} \frac{1}{2}(q+k) \\ \frac{1}{2}(q-k) \end{pmatrix}.$$

Since $|\det(\phi)| = \frac{1}{2} \neq 0$ and the characteristic functions in G transform as

$$\forall q, k \in \mathbb{R}^2: \quad \mathbb{1}_{[0,\pi]}(q)\mathbb{1}_{[0,\pi]}(k) = \mathbb{1}_{[0,\pi]}(\phi_1(q,k))\mathbb{1}_{[-\pi/2,\pi/2]}(\phi_2(q,k)),$$

[17] One does not use the transformation $\sinh 2K^* = \sqrt{1 + \cosh 2K^*}$ since it requires case analyses.

one obtains

$$\begin{aligned} I :=& \frac{1}{\pi^2}\int_0^\pi \mathrm{d}q \int_0^\pi \mathrm{d}k \ \log[2(Q-2\cos\frac{q+k}{2}\cos\frac{q-k}{2})] \\ =& \quad \frac{1}{\pi^2}\int_0^\pi \mathrm{d}x \int_0^{\pi/2} \mathrm{d}y \ \log[2(Q-2\cos x\cos y)] \\ =& \quad \frac{1}{\pi^2}\int_0^\pi \mathrm{d}x \int_0^{\pi/2} \mathrm{d}y \ \log\left(\frac{Q}{\cos y}-2\cos x\right) \\ & + \frac{1}{\pi^2}\int_0^\pi \mathrm{d}x \int_0^{\pi/2} \mathrm{d}y \ \log(2\cos y) \\ \overset{(3.3.1)}{=}& \quad \frac{1}{\pi}\int_0^{\pi/2} \mathrm{d}y \ \log(2\cos y) + \frac{1}{\pi}\int_0^{\pi/2} \mathrm{d}y \ \mathrm{arcosh}\ \left(\frac{Q}{2\cos y}\right). \end{aligned}$$

Short trigonometrical excursus: Let $x \in [1,\infty) = \mathrm{Ran}(\mathrm{arcosh}\ )$.

$$\begin{aligned} y \quad :=& \quad \mathrm{arcosh}\ x \geq 0 \quad \Rightarrow \quad x = \cosh y = \frac{1}{2}\left(\mathrm{e}^y + \mathrm{e}^{-y}\right) \\ \Leftrightarrow& \quad \mathrm{e}^{2y} - 2x\mathrm{e}^y + 1 = 0 \\ \Leftrightarrow& \quad \mathrm{e}^y \in \left\{x \pm \sqrt{x^2-1}\right\} \\ \overset{\mathrm{e}^y \geq 1}{\Rightarrow}& \quad y \quad = \quad \log(x+\sqrt{x^2-1}). \end{aligned}$$

With that one obtains

$$\begin{aligned} I \quad =& \quad \frac{1}{\pi}\int_0^{\pi/2} \mathrm{d}y \ \log[D(1+\sqrt{1-(2/D)^2\cos^2 y})] \\ \overset{y\to\frac{\pi}{2}-y}{=}& \quad \frac{1}{\pi}\int_0^{\pi/2} \mathrm{d}y \ \log[D(1+\sqrt{1-(2/D)^2\sin^2 y})]. \end{aligned}$$

One then has for $\beta \in \mathbb{R}^+$:

$$\begin{aligned}\beta f(\beta) &= -\frac{1}{2}[\log(2\sinh(2K)) + I] \\ &= -\log(2\cosh(2K)) - \frac{1}{\pi}\int_0^{\pi/2} \mathrm{d}\phi \ \log\left[\frac{1}{2}\left(1+\sqrt{1-k^2\sin^2\phi}\right)\right],\end{aligned}$$

where we defined

$$k := \frac{2}{D} = \frac{2\sinh(2K)}{\cosh^2(2K)}.$$

It is now possible to determine the density of the internal energy[18] by denoting $\Sigma := \sqrt{1-k^2\sin^2\phi}$

$$\begin{aligned}u(\beta) &= \frac{\partial \beta f(\beta)}{\partial \beta} = -2J\tanh(2K) + \frac{k}{\pi}\frac{\partial k}{\partial \beta}\int_0^{\pi/2}\mathrm{d}\phi\ \frac{\sin^2\phi}{\Sigma(1+\Sigma)} \\ &\overset{\substack{k^2\sin^2\phi = \\ (1-\Sigma)(1+\Sigma)}}{=} -2J\tanh(2K) + \frac{k}{\pi}\frac{\partial k}{\partial \beta}\left(-\frac{\pi}{2k^2} + \frac{1}{k^2}\int_0^{\pi/2}\mathrm{d}\phi\ \frac{1}{\Sigma}\right).\end{aligned}$$

It is

$$\begin{aligned}\frac{1}{k}\frac{\partial k}{\partial \beta} &= \frac{\partial \log k}{\partial \beta} = 2J\left(\coth(2K) - 2\tanh(2K)\right) \\ &= 2J\coth(2K)\underbrace{\left(1-2\tanh^2(2K)\right)}_{=:l}\end{aligned}$$

and so

$$u(\beta) = -J\coth(2K)\left(1-\frac{2l}{\pi}K_1(k)\right),$$

where

$$K_1(k) := \int_0^{\pi/2}\frac{\mathrm{d}\phi}{\sqrt{1-k^2\sin^2\phi}}$$

[18] Again, in here one has to be cautious in switching the order of integration and derivation, but that issue shall not be discussed in here because the theory of elliptic integrals requires more care.

is the *complete elliptic integral of the first kind*. In order to prevent more not-instructive analysis, only the solution for the specific heat shall be presented as stated in [Hua87]

$$\begin{aligned} c(\beta) &= -k_b\beta^2\frac{\partial u}{\partial \beta}(\beta) \\ &= \frac{2k_b}{\pi}(\beta J \coth 2K)^2\left[2K_1(k) - 2E_1(k) - (1-l)\left(\frac{\pi}{2} + lK_1(k)\right)\right]. \end{aligned}$$

$E_1(k)$ is the *complete elliptic integral of the second kind*,

$$E_1(k) := \int_0^{\pi/2} \mathrm{d}\phi\ \sqrt{1-k^2\sin^2\phi}.$$

The complete elliptic integrals shall be approximated near $k = 1$ since

$$\begin{aligned} &\sinh(2K_c) = 1 \quad \cosh(2K_c) = \sqrt{1+\sinh^2(2K)} = \sqrt{2} \\ &\Rightarrow \lim_{T\to T_c} k = 1, \quad K_c^{-1} = \frac{2}{\operatorname{arcosh}\sqrt{2}} = \frac{2}{\log[\sqrt{2}+1]} \approx 2.269 \end{aligned}$$

One can approximate

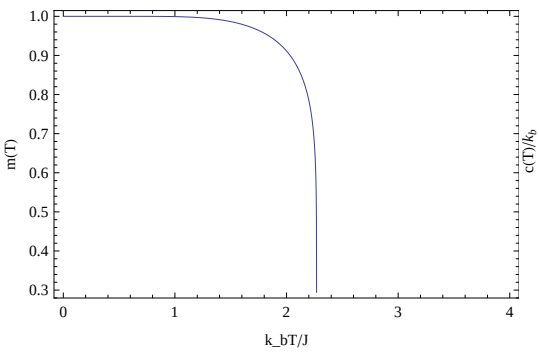
$$\begin{aligned} K_1(k) &\approx \log 4l, \quad \frac{\partial K_1}{\partial k}(k) \approx \frac{\pi}{2}, \\ E_1(k) &\approx 1 \end{aligned}$$

and thus

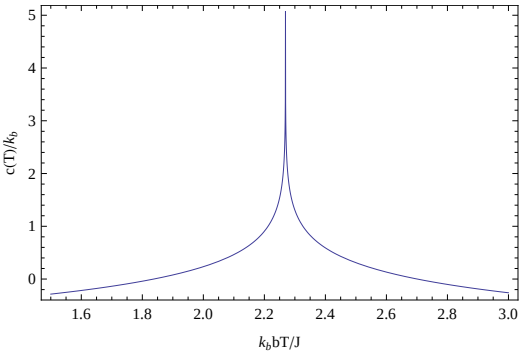
$$c(\beta) \approx \frac{2k_b}{\pi}\left(\frac{2J}{k_bT_c}\right)^2\left[-\log\left|1-\frac{T}{T_c}\right| + \log\left(\frac{k_bT_c}{2J}\right) - (1+\frac{\pi}{4})\right]$$

In fig. 3.2a it is shown the graph for the spontaneous magnetization *Chen Ning Yang* (*1922) [Yan52] obtained[19].

[19] cf. [Hua87], p. 391



(a) Spontaneous magnetization calculated by Yang



(b) Specific heat capacity

Chapter 4

Conclusio

As seen, the concept of spontaneous symmetry breaking can be rigorously established. Although the Lenz-Ising model might not explain ferromagnetism in general materials, one learned how to give a complete discussion of a physical model. Taking into consideration that the Lenz-Ising model is a very crude description based on many assumptions which were *neither* physically explicable *nor* mathematically understood, it gives hope that contemporary physical attempts may become well-understood models. It was tried to carve out the importance of the correlation between mathematics and physics, although other factors (e.g. the economical factor) may play a big role in contemporary research. Though physicists argue with the fact that one is only given *finite* lattices in nature, it is now clear that the spontaneous symmetry breaking can only occur if one deals with *infinite* systems. Moreover, the finite systems appearing in nature are still huge compared to the micro-structure.
Still, the Ising model is investigated with regard to a solution in d dimensions. There are different generalizations to the Ising model as the *Potts model* and different vertex models, and there is also the Heisenberg model, seen in the first chapter. These were not discuss in here in order to present a closed treatment which is not possible for the other models. Also the historical aspect of the Ising model should be stressed, in particular, that Lenz needed a certain physical *feeling* to provide his model. It was quite disillusioning to Lenz when his PhD student Ising could not provide spontaneous magnetization in the linear chain and it might have been even more disillusioning when Heisenberg derived his model of ferromagnetism out of Quantum mechanical considerations. However, the fact that the 2D Ising model displays magneti-

zation in the thermodynamic sheds a better light on the Ising model. It was seen that the concept of spontaneously broken symmetries was unavoidable in here and it also plays a big role in most recent research, as well in solid state as in particle physics.

Appendix A

Further comments

A.1 Bethe ansatz

Since it is a powerful tool which can be applied in variations to modern problems, the idea of the Bethe ansatz mentioned in section 1.3.2 shall be displayed on the 1D spin-1/2 Heisenberg Hamiltonian[1]:
First of all, one rewrites the Hamiltonian in terms of Spin creation and annihilation operators

$$S_k^{\pm} \quad := \quad S_k^x \pm \mathrm{i} S_k^y$$

in order to obtain

$$H \quad = \quad -J \sum_{k=1}^{N} \left(S_k^+ S_{k+1}^- + S_k^- S_{k+1}^+ + 2 S_k^z S_{k+1}^z \right).$$

[1] [KM98] was consulted to understand the basic ideas

The emerging operators S_i^+, S_j^- and S_k^z $(i,j,k \in \{1;2;\ldots;N\})$ fulfill the following algebra[2]

$$\begin{aligned}[S_i^+, S_j^-] &= 2S_i^z\delta_{ij} \\ [S_i^z, S_j^\pm] &= \pm\delta_{ij}S^\pm\delta_{ij}.\end{aligned}$$

With these relations, one obtains that the total momentum in the $z-$direction is conserved,

$$S^z := \sum_{k=1}^{N} S_k^z,$$

and the complete ordered state

$$|1\rangle := |\underbrace{1,1,\ldots,1}_{N \text{ spins}}\rangle$$

is an eigenvector with eigenvalue $E^{(0)} := -JN/4$. In order to determine all the eigenvectors, one can fix the total z-spin, i.e., one considers the problem

$$\begin{vmatrix} H|\psi^{(r)}\rangle &= & E^{(r)} & |\psi^{(r)}\rangle \\ S^z|\psi^{(r)}\rangle &= & (N/2-r) & |\psi^{(r)}\rangle \end{vmatrix}.$$

This problem divides the union of eigenspaces to H into orthogonal subspaces with fixed total z-spin component. With respect to understanding the concept of the Bethe ansatz, one will only perform the case $r = 1$ and then look at the general case.
For $r = 1$ define

$$|n\rangle := S_n^-|1\rangle \quad \forall n \in \{1;2;\ldots;N\}$$

and make the ansatz

$$|\psi^{(1)}\rangle = \sum_{n=1}^{N} a(n)|n\rangle.$$

---

[2]In here, one is dealing with spin-1/2 operators, so

$$\begin{aligned} S_i^z|\ldots \underbrace{\{{}^1_0\}}_{i^{th} \text{ position}} \ldots\rangle &= (2\cdot\{{}^1_0\}-1)\frac{1}{2}|\ldots\{{}^1_0\}\ldots\rangle, \\ S_i^\pm|\ldots 1\ldots\rangle &= \{{}^0_1\}\cdot|\ldots 0\ldots\rangle \\ S_i^\pm|\ldots 0\ldots\rangle &= \{{}^1_0\}\cdot|\ldots 1\ldots\rangle \end{aligned}$$

.

Since for $n \in \{1; 2; \ldots; N\}$

$$\begin{aligned}
\sum_k S_k^- S_{k+1}^+ S_n^- |1\rangle &= \sum_k (S_k^- S_n^- \underbrace{S_{k+1}^+}_{S_{k+1}^+|1\rangle=0} + 2\delta_{k+1,n} S_k^- S_{k+1}^z) |1\rangle = |n-1\rangle \\
\sum_k S_{k+1}^- S_k^+ S_n^- |1\rangle &= \sum_k (S_{k+1}^- S_n^- S_k^+ + 2\delta_{k,n} S_{k+1}^- S_k^z) |1\rangle = |n+1\rangle \\
\sum_k 2S_k^z S_{k+1}^z S_n^- |1\rangle &= \sum_k (2S_k^z S_n^- S_{k+1}^z - 2\delta_{n,k+1} S_k^z S_{k+1}^-) |1\rangle \\
&= \sum_k (2S_n^- S_k^z S_{k+1}^z - 2\delta_{n,k} S_n^- S_{k+1}^z - 2\delta_{n,k+1} S_{k+1}^-) |1\rangle \\
&\underset{=\frac{H}{-J}|1\rangle=-\frac{E^{(0)}}{J}|1\rangle}{\overset{\sum_k 2S_k^z S_{k+1}^z|1\rangle}{=}} -(\frac{E^{(0)}}{J} + 2) |n\rangle
\end{aligned}$$

one obtains the following equation for the coefficients $a(1), a(2), \ldots, a(N)$ imposing $a(N+1) = a(1)$ through equating the coefficients in the Schrödinger equation: $H |\psi^{(1)}\rangle = E^{(1)} H |\psi^{(1)}\rangle$

$$(E^{(1)} - E^{(0)} - 2J) a(n) + J (a(n+1) + a(n-1)) \quad = \quad 0 \quad \forall n \in \{1; 2; \ldots; N\}.$$

$a_k(n) = \mathrm{e}^{2\pi \mathrm{i} kn/N} \forall k, n \in \{1; 2; \ldots; N\}$ solves this equation and yields for $k \in \{0; 1; \ldots N\}$

$$\begin{aligned}
|\psi_k^{(1)}\rangle &= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \mathrm{e}^{2\pi \mathrm{i} kn/N} |n\rangle \\
E_k^{(1)} &= E^{(0)} + 2J \sum_{n=1}^{N} (1 - \cos(2\pi kn/N)),
\end{aligned}$$

where

$$H |\psi_k^{(1)}\rangle = E_k^{(1)} |\psi_k^{(1)}\rangle .$$

The n linear independent solutions obtained this way correspond to the $\binom{n}{1}$ possible choices for 1 flipped spin. For general $r \in \{0; 1; \ldots; N\}$, one uses the ansatz

$$|\psi^{(1)}\rangle \quad = \quad \sum_{1 \le n_1 < n_2 < \ldots < n_r \le N} a(n_1, n_2, \ldots, n_r) |n_1, n_2, \ldots, n_r\rangle ,$$

where

$$\forall 1 \leq n_1 < n_2 < \ldots < n_r \leq N : |n_1, n_2, \ldots, n_r\rangle \quad := \quad \prod_{k=1}^{r} S^-_{n_k} |1\rangle .$$

Bethe could show in [Bet31] that this procedure leads to 2^N solutions which is the total number of possible spin configurations.

A.2 Proof of the Pauli matrix exponential

Eq. (3.2.12) shall now be deduced. Let $\{\tau_1; \tau_2; \tau_3\}$ be the Pauli matrices and $\tau := (\tau_1, \tau_2, \tau_3)$.

A.2.1 Lemma.

$$\forall a, b \in \mathbb{C}^3 : \quad (a \cdot \tau)(b \cdot \tau) \quad = (a \cdot b) I_2 + \mathrm{i}(a \times b) \cdot \tau$$

Proof. Let $a, b \in \mathbb{C}^3$. Then it is

$$\begin{aligned}(a \cdot \tau)(b \cdot \tau) &= \sum_{i,j=1}^{3} a_i b_j \underbrace{\tau_i \tau_j}_{=\frac{1}{2}(\{\tau_i,\tau_j\}+[\tau_i,\tau_j])} = \sum_{i,j} a_i b_j (\delta_{i,j} I_2 + \mathrm{i} \sum_{k=1}^{3} \epsilon_{ijk} \sigma \tau_k) \\ &= (a \cdot b) I_2 + \mathrm{i} \sum_{k=1}^{3} \underbrace{(\sum_{i,j} \epsilon_{ijk} a_i b_j)}_{=(a \times b)_k} \tau_k = (a \cdot b) I_1 + \mathrm{i}(a \times b) \cdot \tau,\end{aligned}$$

where one used

$$\forall i, j \in \{1; 2; 3\} : \quad \begin{cases} \{\tau_i, \tau_j\} &= 2\delta_{i,j} I_2 \\ [\tau_i, \tau_j] &= 2\mathrm{i} \sum_{k=1}^{3} \epsilon_{ijk} \tau_k \end{cases}$$

and $(\epsilon_{ijk})_{ijk}$ is the Levi-Civita symbol. □

A.2.2 Proposition.

$$\forall \phi \in \mathbb{R}^3 \setminus \{0\} : \quad \mathrm{e}^{\phi \cdot \tau} \quad = \quad \cosh |\phi| + \left(\frac{\phi}{|\phi|} \cdot \tau \right) \sinh |\phi|. \qquad \text{(A.2.1)}$$

Proof. With

$$\left(\frac{\phi}{|\phi|}\cdot\tau\right)^2 \overset{A.2.1}{=} \left(\frac{\phi}{|\phi|}\right)^2 I_2 + \mathrm{i}(\frac{\phi}{|\phi|}\times\frac{\phi}{|\phi|})\cdot\tau = I_2$$

one obtains

$$\begin{aligned}
\mathrm{e}^{\phi\cdot\tau} &= I_2 + \sum_{n=1}^{\infty}\frac{1}{n!}|\phi|^n\left(\frac{\phi}{|\phi|}\cdot\tau\right)^n \\
&= I_2 + \sum_{n=1}^{\infty}\frac{|\phi|^{2n}}{(2n)!}\underbrace{\left(\frac{\phi}{|\phi|}\cdot\tau\right)^{2n}}_{=I_2} + \sum_{n=0}^{\infty}\frac{|\phi|^{2n+1}}{(2n+1)!}\underbrace{\left(\frac{\phi}{|\phi|}\cdot\tau\right)^{2n+1}}_{=\frac{\phi}{|\phi|}\cdot\tau} \\
&= I_2\cosh|\phi| + \left(\frac{\phi}{|\phi|}\cdot\tau\right)\sinh|\phi|
\end{aligned}$$

by the definition of the matrix exponential. □

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Erklärung

Hiermit versichere ich, dass ich diese Arbeit selbständig verfasst und keine anderen, als die angegebenen Quellen und Hilfsmittel benutzt, die wörtlich oder inhaltlich übernommenen Stellen als solche kenntlich gemacht und die Satzung des Karlsruher Instituts für Technologie zur Sicherung guter wissenschaftlicher Praxis in der jeweils gültigen Fassung beachtet habe.

Ort, den Datum