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Geometric dependence of interface fluctuations

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Corpora sunt porro partim primordia rerum,
partim concilio quae constant principiorum.

Lucretius – *De rerum natura*

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Contents

Nomenclature

$\mathcal{D}\phi$	Measure of the path integral, page 16
det'	Determinant omitting the zero mode, page 32
ΔE	Energy splitting, page 20
$\mathrm{erf}(x)$	Gaussian error function, page 43
F	Free energy, page 6
γ	Euler-Mascheroni constant, page 48
$\Gamma(z)$	Γ-function, page 39
$G(r)$	Correlation function, page 18
$H[\phi]$	Hamiltonian of the order parameter field, page 16
k	Boltzmann constant, page 7
$K_t(A)$	Heat kernel of the operator A, page 40
Δ	Two-dimensional Laplacian: $\Delta = -\partial_1\partial^1 - \partial_2\partial^2$, page 38
M	Fluctuation operator, page 28
ϕ	Order parameter, page 12
P	Reflection operator, page 20
q	Square of the nome $q = \mathrm{e}^{2\pi\mathrm{i}\tau}$, page 76
$(\cdot,\cdot)$	Scalar product, page 28
τ	Modular ration., page 59
$\Theta(x)$	Step function, page 47
$\theta(z)$	Jacobi theta-function, page 50
$T^{(a)}$	Translation operator, page 29
T_C	Critical temperature, page 6
$\zeta(z)$	Riemann zeta-function, page 39
$\zeta_A(z)$	Spectral zeta-function of a heat kernel $K_t(A)$, page 40

1 Introduction

Interfaces are ubiquitous phenomena in nature, partitioning a system into regions with disjoined thermodynamic properties like the particle densities in binary-liquid systems or in liquid-gas transitions. This phase separation prohibits the system to establish a global equilibrium, so that the interface vanishes, is not sharp, but rather characterised by a parting region, whose spatial length is indicated by the correlation length. In this region both phases are coexisting in the equilibrium featuring fluctuations permitting the exchange of particles or molecules. Therefore, from the view of applied sciences, interfaces are significant in fields reaching from material sciences to neurophysiology. But they are also important from the point of view of theoretical physics, because the universal behaviour of phase transitions can be applied in many fields of physics. In all physical systems, the geometrical structure as well as the boundary conditions play a role. The simplest and mostly employed geometrical structure in physics is a square, but it shows, that changing the geometric structure (to rectangular or circular structures) often enforces dramatic changes of researched quantities. Obviously, the geometric dependence of interface fluctuations that shall be investigateded in this thesis is an evident task not explicitly calculated yet.

Theoretical models for continuous phase transitions in different dimensions have been proposed for a lot of experimental evidences in particular fields of physics, like the liquid-vapour transition, the ferromagnetic transition or the superconducting transition offering new applications because of the universal behaviour of the principal models. The most promising model for phase transitions set up by elementary physical laws is the Ising model, where interface fluctuations have been studied since it's first analytic solution in two dimensions [Ons44]. However, as in most applications, the physical nature is characterised by three spatial dimensions. Consequently, the most interesting systems for investigating interfaces in everyday life are three dimensional, but until now there is no analytic solution of the Ising model in three dimensions. In contrast, there are suitable approximate solutions obtained from phenomenological considerations of phase transitions, like the Landau theory. From the Landau theory, the first profile of an interface, the *kink* profile, could be derived by J.W. Cahn and J.E. Hilliard [CH58]. As the Landau theory does not involve interface fluctuations, the Ginzburg-Landau theory [LG50] has been used for instance by V. Privman and M.E. Fisher [PF83] to offer an expression proposing the structural behaviour of the correlation length for arbitrary dimensions. Making use of the structural analogy between statistical mechanics and quantum field theory, a more accurate calculation in four dimensions by G. Münster [Mün89] offered an explicit result in first loop order approximation of the Ginzburg-Landau theory. Later, the same methods were applied to calculate these expression in higher orders as well as in the three dimensional setup [Mün90], still restricted on a quadratic basal area $L \times L$ of the underlying box.

Apparently, the use of field theoretical methods has been fruitful for phase transitions. The analogy between statistical mechanics and quantum field theory is identified by the Wick rotation as well as by the similar structural behaviour – the scale invariance – of the statistical mechanical systems and field theories. As the correlation length tends to diverge near the critical point, where the phase transition takes place, wide range fluctuations dominate the system. Additionally, in quantum field theory this large-scale behaviour is identified with massless field theories. Therefore, in this thesis the same field theoretical methods will be used in order to investigate interface fluctuations in three dimensions imposing new geometric structures.

Firstly, in chapter 2, the Ising model will be motivated by a microscopic analysis of elementary physical laws on atomic scales. Moreover, recognising that the behaviour of macroscopic physical quantities can be observed in the thermodynamic limit, in the succeeding, a phenomenological theory, the Landau theory will be proposed, motivated by a mean field approximation near the critical point. Deduced only from macroscopic symmetry considerations, the Landau theory, the so-called *symmetry breaking* will be observed, occurring when the system passes through the critical point. While this theory does not involve fluctuations, it will be expanded to the Ginzburg-Landau theory. In the derivation of this theory, the component that is responsible for the geometric dependence will be identified. Furthermore, the relationship of the parameters used in the Ginzburg-Landau theory to physical parameters from statistical mechanics and quantum field theory is examined. The correlation length of a system performing a phase transition is identified by the energy gap of a particle tunneling from one quantum state to another. The relationship between statistical theories and quantum field theories will be explained in the end of the chapter, so that conclusively, a massless field theory is encouraged for phase transitions by statistical mechanical considerations in this chapter.

Secondly, in chapter 3, this analogy will be used to present a ϕ^4 field theory of phase transitions that satisfies the boundary conditions on a new geometric structure, e.g. $L_1 \times L_2 \times T$. Moreover, using the path integral formalism introduced by R.P. Feynman [Fey48], the above mentioned kink profile established in the T direction will be identified with the most probable path (see figure 1.1). Imposing fluctuations around this classical trajectory, the system can be studied in a Gaussian approximation, resulting in determinants. As the massless case is studied, certain divergences are treated with the method of collective coordinates [GS75] effecting in a *ghost* contribution, compara-

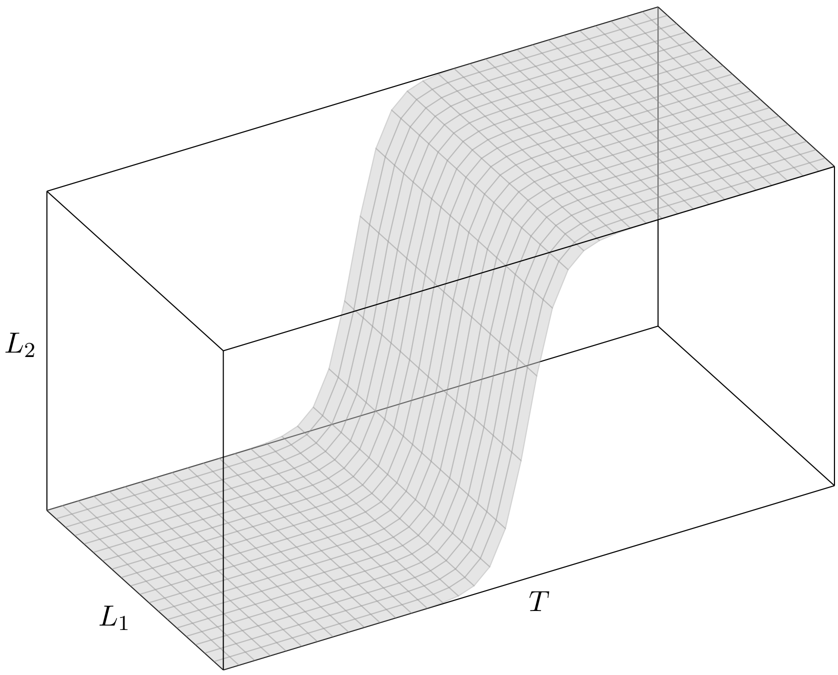

Figure 1.1.: A three dimensional box. The indicated interface can be seen as density transition from one liquid to another.

ble to the Faddeev-Popov ghost in quantum field theories. Consequently, this massless particle is identified with a quasi-particle called *instanton* in quantum chromo dynamics, thus the tunneling amplitude for these instantons is calculated in a dilute gas approximation, described by S. Coleman [Col85]. Finally, this tunneling amplitude delivers an expression for the energy splitting, so that for the behaviour of the correlation length, a ϕ^4 theory will be achieved.

The arising expression is evaluated in detail in chapter 4. This chapter is more of technical nature, transforming the involved determinants into integrals applying zeta regularization techniques. Therefore, the zeta regularization and heat kernel methods, firstly described and systematically used in theoretical physics by S. Hawking [Haw77] are introduced in the beginning of the chapter. As a result of these methods, the expression for the energy splitting will be split off into a normal mode corresponding to the T direction and a transversal mode corresponding to the $L_1 \times L_2$ plane. As the calculation of the normal mode is universal for different geometries as long as T is large, the achieved expressions will be compared to the results obtained by similar methods in [Mün90,Hop93] in order to identify the part that has to be recalculated imposing other geometric structures. The transversal mode is identified by the Laplacian introduced by imposing fluctuations in the derivation of the Ginzburg-Landau theory. Consequently, the evaluation of the critical fluctuations is reduced to the evaluation of the determinant of the Laplacian on different geometries.

Finally, in chapter 5, the determinant of the two dimensional Laplacian is calculated explicitly for a box with rectangular basal area $L_1 \times L_2$. For interface fluctuations, this determinant has been proposed to relate to the Dedekind eta function in [Mün97]. This proposal was motivated by calculations of the two dimensional Laplacian in Bosonic string theories (see e.g. [DFMS97]) that involve conformal field theories. The Dedekind eta function is recognized to fulfil a certain modular invariance that is also needed in the rectangular case, because the solution must be invariant under the transformation $L_1/L_2 \to L_2/L_1$. Successively, the solution involving the eta function needs to satisfy the functional equation $f(\tau) = f(1/\tau)$. The calculation of the determinant of the Laplacian will be done using three different methods. As the calculation is older, known as the modular discriminant, calculated by D.B. Ray and I.M. Singer [RS73] in mathematics, applied by C. Itzykson and J.-B. Zuber [IZ86] for the Bosonic string originally known as the Kronecker limit formula. This method was developed in the 18th century by L. Kronecker [Sie61]. This thesis will, in the first part of chapter 5, follow this approach. The second method, using the Sommerfeld-Watson transformation, was motivated by J. Polchinski [Pol86] for a similar problem. As the calculation in this paper is very shortly described, this method will be evaluated in detail. In a third method, proposed by J. Baez in his weekly blog [Bae98a, Bae98b], the action of the Bosonic string will be recalculated as an infinite setup of harmonic oscillators, because of the structural analogy between the Laplacian and the Klein-Gordon equation for scalar fields. All methods are therefore expected to give the same solution. Subsequently, the obtained solution will be inserted for calculating the correlation length and compared with the previous results for a quadratic setup, investigating the change of the correlation length in the explicit case of a box with rectangular basal area.

2

Theory of phase transitions and critical phenomena

In the introduction, the theory of interfaces was proposed to be a theory of phase transitions. The aim of this thesis is to investigate a theory of interfaces in a cuboid of Volume V, given a certain geometric structure $L_1 \times L_2 \times T$, see figure 1.1. Interfaces can be seen as limit behaviour between different phases of a material. The following chapter will develop the theory of phase transitions basing on theories of phase transitions like the gas-liquid transition or the ferromagnetic transition known from statistical mechanics.

First basic characteristics of phase transitions will be given and then two main aspects of statistical mechanics will be outlined: a microscopic description founded on the elementary physical laws of the model and a macroscopic description. Therefore, a three dimensional model can be given by some macroscopic theory adapted only from symmetry considerations inferred from the macroscopic world. The macroscopic description will be given in a continuous theory, the Ginzburg-Landau theory, which includes fluctuations around the phase transition as well. In both categories, the microscopic and the macroscopic models, the correlation length determines these fluctuations. It will be shown, that there is certain universality between different theories due to the similar behaviour of the correlation length and therefore a connection of the microscopic and macroscopic theories will be outlined in the last section of this chapter. Finally the structural analogy between fluctuations of physical quantities and fluctuations of observables in quantum field theory (QFT) will be outlined. In this chapter a continuous field theory of phase transitions is developed.

2.1. Basic characteristics of phase transitions and statistical mechanics

Phase transitions are characterized by a drastic change of certain macroscopic values called *order parameters* in a thermodynamic system when another quantity, the *control* *parameter*, is varied. According to the value of the order parameters in a thermodynamic system, the different phases can be discriminated. Heuristically, a thermodynamic phase transition can be described as a reason of a competition between the internal energy U and the entropy S of the system [NO11] in the following definition of the free energy

$$F = U - TS. \tag{2.1}$$

When the temperature rises, the free energy changes its sign at a certain *critical temperature* T_C. A physical interpretation could be, that this last term favours disorder depending on the value of T, whereas the internal energy favours order [NO11]. Conclusively, the value of the external control parameter T can be varied to control the competition between the internal energy and the entropy so that the order parameter, here determined by the free energy, discriminates between the phases of the system.

The graduate thesis [vdW73] of Johannes Diderik van der Waals is often identified as the genesis of modern theory of phase transition [Nol14]. It is commonly seen as the first thermodynamic argumentation because later on, van der Waals formulated his famous theory of the realistic gas, which mentions a phase transition between phases at different temperatures. The transition between different phases could be described and interpreted with the Maxwell construction [vdW12] by a coexistence of the two phases, which cannot be distinguished. In 1893, van der Waals transferred his work from the description of two phase systems to interfaces, where he could predict the thickness of a surface [Row79]. As the van der Waals theory is a continuous theory, interfaces can be described by a phase transition.

At about the same time, in 1872, Ludwig Boltzmann developed a first statistical interpretation of an ideal gas following Maxwell's heuristic construction of the speed distribution of the gas particles [Bol72]. In 1877, Boltzmann then re-derived the probability distribution in the framework of statistical mechanics [Bol77] by evaluating the relationship between the Second Law of Thermodynamics and probability calculus. In statistical mechanics, the behaviour at a microscopic level is described by classical (or later quantum physical) laws. In contrast to the macroscopic world, on the microscopic level observables like the temperature or entropy do not exist. The main argument of the statistical description is the *equal a priori argument*:

> "By this we mean that the phase point for a given system is just as likely to be in one region of the phase space as in any other region of the same extent which corresponds equally well with what knowledge we do have as to the condition of the system" [Tol50].

This means, that a system can be found with equal probability for any (micro-) state for an isolated system with a known energy and composition. All these microstates are equally probable in the system where the thermodynamics limit leads to the measurable macroscopic observables the thermodynamic limit, i.e. the infinite volume limit $N/V =$ const. is taken. In other words, the thermodynamic properties of a system can be determined by the partition function Z, which is the sum over all possible free energies weighted with the factor $e^{-\beta F}$

$$Z = \mathrm{Tr}\, e^{-\beta H}, \qquad F = -\frac{1}{\beta} \ln Z, \qquad \beta = (kT)^{-1}. \tag{2.2}$$

Here H is the Hamiltonian and $k \approx 1.381 \cdot 10^{-23}$ J/K is the Boltzmann constant. This approach is a very idealized method to regain some properties of physical systems, like the ideal gas. Under less strict assumptions, when particles can interact and have a small volume, the van der Waals gas can be constructed out of the framework of statistical mechanics.

Important for such systems, in which phase transitions occur, is that this is only possible in systems of infinite volume V. This means, there is an infinite number of degrees of freedom N. In simple models, where different phases occur, the thermodynamic limit is taken in each phase. Depending on the value of the control parameter specific ways of thermodynamic limits are taken. Thus for different phases the value of some properties of the system, described by the order parameter, depend on the way the thermodynamic limit is taken [ZJ07]. After the thermodynamic limit is taken, measurable quantities like the magnetization $\mathcal{M}$, the specific heat C, the magnetic susceptibility χ or the correlation length ξ can be calculated. This connects the microscopic theories to the macroscopic world.

According to Paul Ehrenfest, phase transitions can be classified by considering thermodynamic parameters such as volume or temperature. Under this scheme, phase transitions are labelled by the lowest derivative of the free energy that is discontinuous at the transition. In the modern classification scheme, phase transitions are divided into two broad categories [Nol14].

When the first-order derivative in the order parameter shows a discontinuity, these phase transitions are called first-order phase transitions. When, by contrast, the first-order derivative is continuous, but the second- or higher-order derivative shows a discontinuity or divergence, these phase transitions are called second-order or continuous phase transitions. Observing the behaviour around the point, where two or more phases coexist and become indistinguishable, anomalous phenomena appear, because the correlation length diverges. As this is universal for different models, continuous phase transitions are often called critical phenomena [NO11], where the behaviour of the order parameters around the critical point can be described by universal scaling laws.

The most common example for phase transitions is the ferromagnetic transition. A simple approach, which involves only the symmetry of the spins in the magnetic material, is the Ising model. More generally, a mean field approximation can be applied to phase transitions, where the phenomenological Landau theory serves equivalent results as the Ising model after the thermodynamic limit is taken. All these models have in common, that they inhibit a phase transition. The critical exponents describe similar behaviour of the system close to the critical point. In a ferromagnet, the above mentioned physical quantities can be measured experimentally.

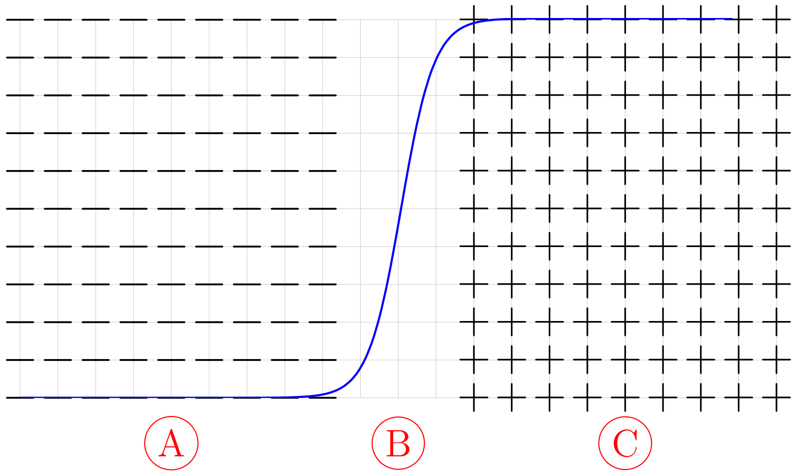

Figure 2.1.: Ising model for interfaces, where the spins are localized at lattice points. In region A all spin values are uniformly -1, in region B all spin values are $+1$. Region C is the transition.

2.2. Microscopic description of phase transitions

The simplest way to construct an interface is to impose a model, in which microscopic symmetries are used in order to describe the system. This model is based upon the idea that in a ferromagnet the magnetic moments of the atoms can have only two opposing orientations $S_i \in \{-1, 1\}, i = 1, \dots N$ and a potential energy exist only between next-neighbours, which favours a parallel position. An interface can be constructed by this model by assuming, that in two distinct regions ((A) and (C) in figure 2.1) these spins are uniformly orientated. Therefore an interface is established in the region (C) between (A) and (B), when all spins in (A) are in the opposite orientation to the spins in (B). The main reason to formulate a continuous theory later is, that there is no analytical solution of the three dimensional Ising model. In the 1920ies, W. Lenz constructed this model to explain ferromagnetic transition, which is a transition between an ordered and a disordered phase in the material. Lenz proposed this model to his student E. Ising as subject for his graduate thesis. Ising examined the model in one dimension, but there is also an analytical solution for a two dimensional model.

2.2.1. Ising model

In the Ising model each spin (indexed by $i = 1, \dots, N$) in the ferromagnet is localized on symmetric crystal lattice, like an equidistant chain of spins in one dimension or a quadratic lattice of spins in two dimensions. The simplest Hamiltonian representing the spins with the coupling constant J between next-neighbouring spins in presence of an external magnetic field h can be written as

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i, \qquad J > 0. \tag{2.3}$$

The brackets indicate that the sum is only taken over nearest neighbouring spins. The partition function for a free system, where the external magnetic field is switched off ($h = 0$), is given by

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\beta H} = \left(\sum_{S_1=\pm 1} \cdots \sum_{S_N=\pm 1} \right) \mathrm{e}^{\beta J \sum_{(i,j)} S_i S_j}.$$

In one dimension this partition function can be evaluated by taking the sum over N neighbouring spins $(i, i+1)$. The result of Ising [Isi25] is

$$Z = 2^N \cosh^{N-1}(\beta J). \tag{2.4}$$

From the knowledge of the partition function, the free energy per spin can be determined by (2.2)

$$\mathcal{F} \equiv \frac{F}{N} = \frac{1}{\beta} \ln \left(\frac{1}{2} \cosh(\beta J) \right).$$

According to the Ehrenfest classification, the derivatives of the free energy could be calculated now in order to search for phase transitions. In the introduction the role of the correlation length for phase transitions was proposed, since the correlation length diverges as the critical point due to wide range fluctuations. The correlation function

$$G(r) = \langle S_i S_{i+r} \rangle$$

can be calculated after some basic transformations [NO11]. The result is

$$G(r) = \tanh^r(\beta J).$$

This indicates some exponential behaviour of the correlation. A value to determine the fluctuations could be a correlation length, defined as the exponential decreasing of the correlation function. The correlation length of the one dimensional Ising model can be given now

$$\xi = -\frac{1}{\ln(\tanh(\beta J))}. \tag{2.5}$$

In the low temperature limit ($\beta \to \infty$) the correlation lenght diverges exponentially $\xi \approx \exp(2\beta J)/2$. Since ξ diverges at the absolute minimum $T = 0$, there is no phase transition observed, thus there is no spontaneuous magnetisation in the one dimensional Ising model.

This observation was generalised by Peierl's, who proved, "that for sufficiently low temperatures the Ising model in two dimensions shows ferromagnetism and the same holds a fortiori also for the three-dimensional model" [Pei36]. This argumentation also maintains for higher dimensions.

This leads to the need for a solution of the two-dimensional Ising model, which is a much more ambitious and subtle endeavour. The first solution was given by L. Onsager in 1944 with the transfer matrix method [Ons44]. His solution for the spontaneous magnetization $\mathcal{M}$ of the two-dimensional Ising model on a quadratic lattice in absence of an external magnetic field is given by

$$\mathcal{M} = \left[1 - \sinh^{-4}(2\beta J)\right]^{1/8}. \tag{2.6}$$

In general, the spontaneous magnetisation is given by

$$\mathcal{M} = \langle S_i \rangle = \lim_{h \to 0} \frac{\mathrm{d}\mathcal{F}}{\mathrm{d}h}. \tag{2.7}$$

As a discontinuity can be found in the derivatives of the free energy at

$$\sinh(2\beta J_C) = 1 \quad \Leftrightarrow \quad kT_\mathrm{C} = \frac{2J}{\ln(1+\sqrt{2})} \approx 2.27J,$$

this temperature is the critical temperature of the two dimensional Ising model.

Onsager's solution is considered to be "one of the landmarks in theoretical physics" and was consequently awarded with the Nobel Prize in 1968 [BK95]. In general, phase transitions occur only in discrete models above dimension one ($D \geq 2$) for discrete symmetry groups and above dimension two ($D \geq 3$) for continuous symmetry groups [ZJ07]. There has yet not been any analytical solution of the three dimensional Ising model, but the following mean field theory of the Ising model can be evaluated in arbitrary dimensions.

2.2.2. Mean field theory of the Ising model

Before Onsager presented a solution of the two dimensional Ising model, a different theory, the mean field (or molecular field theory) was proposed by Pierre-Ernest Weiss in 1907. This theory can be applied to the D-dimensional Ising model for the Hamiltonian (2.3). The value of a single spin S_j can be decomposed in the mean value and their fluctuations according to

$$S_j = \langle S_j \rangle + (S_j - \langle S_j \rangle).$$

The local energy of spin S_i then reads

$$\begin{aligned} E_i &= -S_i \left(J \sum_{j \neq i} S_j + h \right) \\ &= -S_i(\sum_j \langle S_j \rangle + h) - JS_i \sum_{j \neq i}(S_j - \langle S_j \rangle) \end{aligned}$$

The mean field approximation is the negation of wide range fluctuations

$$(S_j - \langle S_j \rangle) = 0$$

which are set to zero. Then the interaction is restricted on a local field. Only the nearest-neighbouring spins are taken into account. For the two possible configurations $S_i = \pm 1$ there are two possible energy levels

$$E_i^+ = -J \sum_j \langle S_j \rangle - h \qquad \text{and} \qquad E_i^- = J \sum_j \langle S_j \rangle + h,$$

which by the definition of the local magnetisation $\mathcal{M} = \langle S_j \rangle$ give

$$E_i^\pm = \mp (qJ\mathcal{M} + h),$$

where q denotes the number of nearest neighbouring spins. The local energy E_i is the

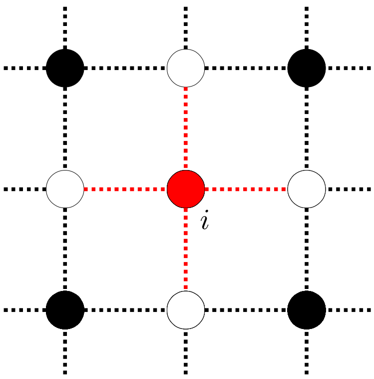

Figure 2.2.: Two dimensional Ising model with spin S_i and the $q = 4$ nearest neighbouring spins.

energy of the local field at the lattice point i. In two dimensions, $q = 4$ spins S_j are in equal distance to the spin S_i (see Figure 2.2). Thus, the partition function becomes

$$Z = \operatorname{Tr} e^{-\beta H} = e^{\beta(qJ\mathcal{M}+h)} + e^{-\beta(qJ\mathcal{M}+h)} = 2 \cosh\left(\beta(qJ\mathcal{M} + h)\right). \tag{2.8}$$

From here on the self-consitent equation

$$\mathcal{M} = \tanh\left(\beta(qJ\mathcal{M} + h)\right) \tag{2.9}$$

for the magnetisation is reached, since the magnetisation was also defined as the derivative of the free energy with respect to the external magnetic field (2.7). This equation could be evaluated now in the limit $h \to 0$. As the above equation serves no analytic expression for $\mathcal{M}$, this expression is now evaluated for small values of $\mathcal{M} = \mathcal{M}_0$, when $\beta \to \beta_C$ as the series expansion for $\mathcal{M} \to 0$ of the hyperbolic tangent is

$$\mathcal{M} = \tanh(q(\beta - \beta_C)J\mathcal{M}) \approx qJ(\beta - \beta_C)\mathcal{M}_0 - \frac{1}{3}(qJ(\beta - \beta_C)\mathcal{M}_0)^3 + \mathcal{O}(\mathcal{M}_0^5)$$

and because the left hand side is also close to zero, it's value is set to $\mathcal{M} = 0$. Then

$$\mathcal{M}_0 = \pm\sqrt{\frac{3}{qJ(\beta - \beta_C)}} \tag{2.10}$$

can be found, implying, that the spontaneous magnetisation diverges according to

$$\mathcal{M}_0 \sim |\beta - \beta_C|^{-1/2} \tag{2.11}$$

when the critical temperature is reached from below. Obviously, this result is wrong in one dimension, since in the corresponding Ising model no critical temperature $T_C > 0$ could be found. The expression (2.9) indicates, that the critical temperature β_C can be found in any dimension

$$\beta_C qJ = 1 \quad \Rightarrow \quad T_C = \frac{qJ}{k}$$

when $q = 2$ in one dimension. Therefore, the mean field expansion is qualitatively wrong in one dimension, but in two dimensions it is qualitatively right, but quantitatively wrong. Because in higher dimensions, the interactions between more nearest-neigbouring spins become more important, the deviation from the analytical or numerical solution decreases.

2.3. Phenomenological theories for phase transition

The previous mean field approximation indicated that there could be a continuous description of phase transition near the critical point. The Landau theory is a phenomenological description of phase transitions, which is independent from the elementary degrees of freedom, like the lattice structure or the spins. It will be shown, that the mean field approximation and the Landau theory, named after L.D. Landau [Lan37], are equivalent to each other near the critical point. Because the mean field approximation neglects fluctuations, the theory will be expanded to the Ginzburg-Landau theory that includes wide range interactions as well.

In a phenomenological theory, the thermodynamic potential is written as a function of an order parameter ϕ only from symmetric considerations. In the ferromagnetic case, the free energy is chosen as the thermodynamic potential. The free energy then is a function of the magnetisation, which is the order parameter $\phi = \mathcal{M}$. In absence of the external magnetic field, the magnetisation $\mathcal{M} = \langle S_i \rangle$ changes its sign under a transformation that changes the sign of all spins, so the order parameter transforms as

$$\phi \to -\phi \qquad \text{as} \qquad S_i \to -S_i \qquad \text{for all } i.$$

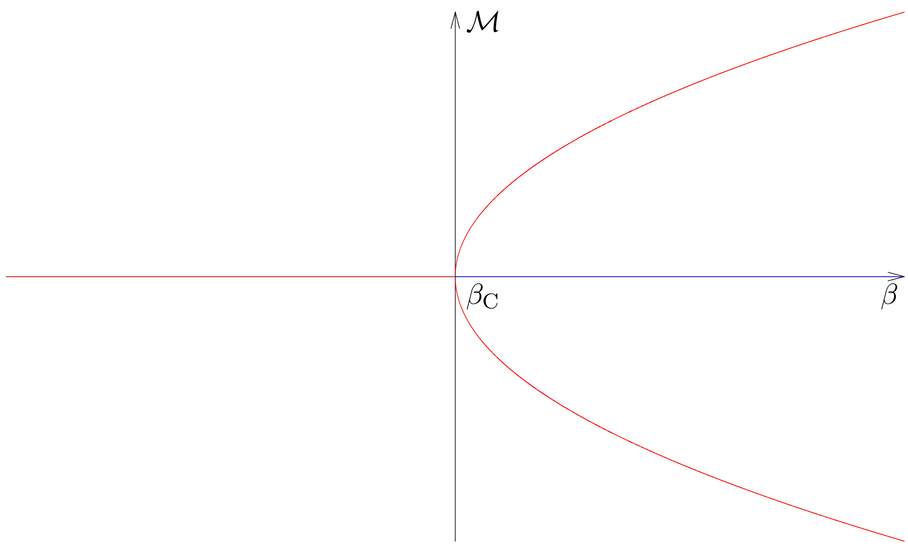

Figure 2.3.: The ferromagnetic transition, where the red line indicated the stable branches, whereas the blue line indicates the unstable branch. Above β_C there are two branches corresponding to a magnetic material, whereas below β_C no magnetisation is observed.

This transformation leaves the Hamiltonian of the Ising-model invariant. Furthermore this transformation represents a global symmetry and the free energy must be an even function of the magnetisation, so that the invariance of the thermodynamic potential (the free energy $\mathcal{F}$) is preserved

$$\mathcal{F}(\phi) = \mathcal{F}(-\phi).$$

2.3.1. Landau-Theory

As the rigorous calculation of the Ising model shows that $\mathcal{M}$ is small when T is near its critical value T_C, the free energy of the system can be assumed keeping only the smallest values in $\mathcal{M}$. By the above argument, that the free energy is invariant under parity transformation, the free energy expansion with arbitrary parameters $\alpha, \beta \in \mathbb{R}$ can be written as[1]

$$\mathcal{F}(\phi) = \mathcal{F}_0 + \frac{1}{2!}\alpha\phi^2 + \frac{1}{4!}\beta\phi^4,$$

where the smallest orders preserved insure that all relevant symmetries of the microscopic level are preserved at a *coarse-grained level* [NO11]. Graphically, the location of the minima can be understood by the potential theory. A negative factor $\beta \leq 0$ implies instability for $\phi \to \pm\infty$ because the function decreases infinitely, this parameter is set

[1] Not to be confused with the Boltzmann factor $\beta^{-1} = kT$.

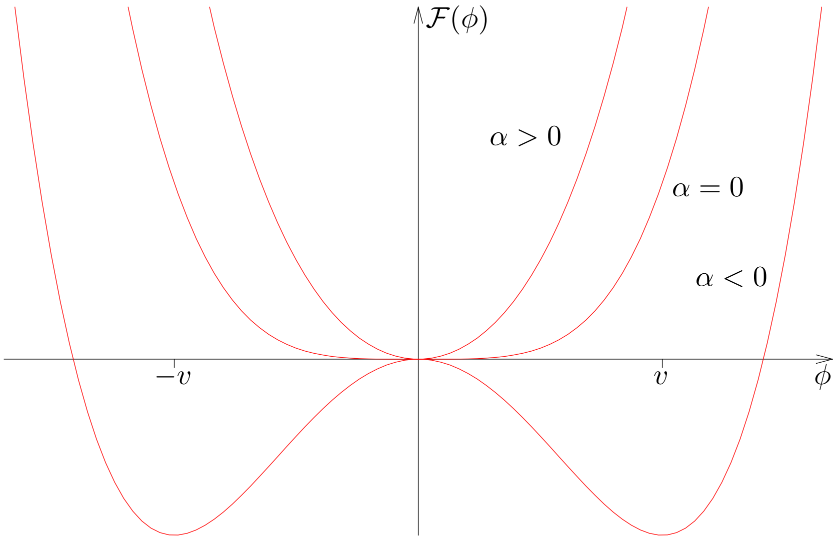

Figure 2.4.: Symmetry breaking of the Landau theory where different signs of α force different fixed points.

$\beta > 0$. For the coefficient α there are three possible regions in which $\mathcal{F}(\phi)$ shows different behaviour. In figure 2.4 it is shown, that for $\alpha = 0$ the expansion starts in fourth order, implying that $\mathcal{F}(\phi)$ is flat in the origin. For $\alpha > 0$ the quadratic term supports the increasing of $\mathcal{F}(\phi)$ so that the curve is similar to a curve of a second order function. Interestingly for $\alpha < 0$, there are two minima and the minimum from before is inverted to a maximum. In words of potential theory there are two stable fixed points at $\mathcal{F}(\bar{\phi}) = \mathcal{F}(\pm v)$ and one unstable fixed point at $\mathcal{F}(0)$ when $\alpha < 0$, whereas there is only one stable fixed point at $\mathcal{F}(0)$ when $\alpha \leq 0$. This dramatic change of the behaviour of the system in the two different phases is called *symmetry-breaking*, because the global behaviour of the system changes. Every particle in the potential approaches the minimum at $\mathcal{F}(0)$ when $\alpha > 0$ and when $\alpha < 0$ the particles of the positive site approach the right minimum while the others approach the left minimum. Therefore, this global symmetry is broken.

This implies that the critical temperature T_C can be identified with α

$$\alpha \sim \frac{T - T_\mathrm{C}}{T} =: t,$$

because in the critical point the value of this so-called *reduced temperature* is $t = 0$. In the equilibrium, the free energy depends only on the temperature and on the magnetic field. This is obtained by minimizing the above equation of the free energy according to the order parameter. Direct minimisation leads to

$$\left.\frac{\partial \mathcal{F}}{\partial \phi}\right|_{\phi=\bar{\phi}} = 0 \qquad \Rightarrow \qquad \bar{\phi} \equiv \pm v \pm \sqrt{-\frac{6\alpha}{\beta}} \quad \vee \quad \bar{\phi} = 0. \tag{2.12}$$

The second derivative shows that for $\alpha < 0$ the minimum is approached at $\bar{\phi} = \pm v$ whereas the maximum is found in $\mathcal{F}(0)$.

2.3.2. Ginzburg-Landau theory

The last section showed, that the Landau theory is equivalent to the mean field approximation near the critical point. Since in the mean field approximation fluctuations were neglected, there will be no fluctuations in the Landau theory. This theory, the Ginzburg-Landau theory [LG50], is named after V.L. Ginzburg und L.D. Landau, who found a phenomenological description of superconductivity in 1950. For this theory V.L. Ginzburg was awarded with the Nobel Prize in 2003. Here the theory will be formulated in three (real) space dimensions following [LBB91].

The aim is now to reformulate the Landau theory as a continuous field theory in three dimensions. Obviously, the Landau theory must be reproduced by the new theory using an approximation, because the behaviour near the critical point was qualitatively correctly described by the mean field approximation in three dimensions. In order to reproduce the Landau theory by means of a Hamiltonian $H(\phi)$ depending on a continuous random variable ϕ with values in $\phi \in \mathbb{R}$, the expectation value $\langle\phi\rangle = \bar{\phi} = \mathcal{M}$ is fixed, because the magnetisation of the whole system shall be finite. The invariances under parity $H(\phi) = H(-\phi)$ preserve the imposed symmetry, so that the polynomial structure of the free energy expansion can be used. This means, the equation depends on two coefficients and the following Hamiltonian is constructed

$$H(\phi) = \frac{1}{2}\alpha\phi^2 + \frac{1}{4!}\beta\phi^4.$$

The partition function can than be written as

$$Z = \operatorname{Tr} \mathrm{e}^{-H(\phi)} = \int \mathrm{d}\phi \mathrm{e}^{-H(\phi)},$$

where the Boltzmann factor is set to $\beta = 1$ as it is assumed to be constant in the critical point. The factor β in the expansion again must be positive, because this integral shall converge.

The Landau theory can be regained by a saddle point approximation. In this case, this means replacing the integral by the minimum value $\bar{\phi} = \mathcal{M}$ of H

$$Z \approx \mathrm{e}^{-H(\bar{\phi})}.$$

With equation (2.2), the free energy is given by

$$\mathcal{F} = H(\bar{\phi}) = \frac{1}{2}\alpha\mathcal{M}^2 + \frac{1}{4!}\beta\mathcal{M}^4.$$

Using the saddle point approximation on the Ginzburg-Landau Hamiltonian regains the Landau Free energy expansion. Thus this procedure will be called *Landau approximation*.

In order to formulate a theory that involves interactions, a step back is necessary. These interactions in the Ising model were defined by the interactions between spins, an elementary degree of freedom. Generalising the above Hamiltonian to N sites (elementary degrees of freedom), one imposes periodicity conditions

$$\phi(x_i + aN) = \phi(x_i),$$

where a is the lattice spacing. Defining a discretization

$$\partial\phi(x_i) = \frac{\phi(x_i + a) - \phi(x_i)}{a}$$

which is the differential quotient and for small a, the derivative with respect to x. Interactions between next-neighbouring spins can be expressed as

$$\sum_i \frac{1}{a^2} \left(\phi(x_i + a) - \phi(x_i)\right)^2 = \sum_i \left(\partial\phi(x_i)\right)^2$$

The Hamiltonian can be postulated in analogy to the free energy expansion

$$H_{\mathrm{GL}} = a \sum_{i=1}^{N} \left[\frac{1}{2}(\partial\phi_i)^2 + \frac{1}{2}\alpha\phi_i^2 + \frac{1}{4!}\beta\phi_i^4\right],$$

where $\phi_i \equiv \phi(x_i)$. Going over to a continuum, when $N \to \infty$ and $a \to 0$ leads to a continuous variable $x_i \to x$. Furthermore, in three dimensions, the continuous variable is $x \to \mathbf{x}$. This means the order parameter ϕ_i in the discrete setup is replaced by the order parameter $\phi(\mathbf{x})$ in three dimensions. In the continuum limit, the Hamiltonian reads

$$H_{\mathrm{GL}}[\phi] = \int \mathrm{d}^3x \left[\frac{1}{2}(\nabla\phi(\mathbf{x}))^2 + \frac{1}{2}\alpha\phi^2(\mathbf{x}) + \frac{1}{4!}\beta\phi^4(\mathbf{x})\right].$$

Moreover the integral in the partition function becomes a path integral

$$\begin{aligned} Z &= \int \prod_{i=1}^{N} \mathrm{d}\phi_i \exp\left(-a^3 \int \mathrm{d}^3x \left[\frac{1}{2}(\nabla\phi_i)^2 + \frac{1}{2}\alpha\phi_i^2 + \frac{1}{4!}\beta\phi_i^4\right]\right) \\ &= \int \mathcal{D}\phi(x) \exp(-H_{\mathrm{GL}}[\phi(\mathbf{x})]), \end{aligned} \tag{2.13}$$

where the square brackets indicate, that H_{GL} is a functional of ϕ. In the above limit the measure is a measure of a path integral, which indicates that over all possible configurations $\mathrm{d}\phi_i$ is integrated. In words of quantum field theory, this is the integral over all possible paths. Introducing a potential $\mathcal{V}(\phi)$, the Hamiltonian is rewritten

$$\begin{aligned} H[\phi] &= \int \mathrm{d}^3x \left[\frac{1}{2}(\nabla\phi)^2 + \mathcal{V}(\phi)\right] \\ &= \int \mathrm{d}^3x \mathcal{H}[\phi] \end{aligned} \tag{2.14}$$

where $\mathcal{H}[\phi]$ is the Hamiltonian density and the potential

$$\mathcal{V}(\phi) = \frac{1}{2}\alpha\phi^2 + \frac{1}{4!}\beta\phi^4$$

is used. Considering the minimum of this potential being at $\bar{\phi} = \pm v = \pm\sqrt{\frac{-6\alpha}{\beta}}$ (see equation (2.12)), the factor β can be identified by the mean field approximation with the coupling constant J in (2.10), so that β will be given by a dimensionless coupling constant g of field theories. The factor α will be identified with a "mass" according to

$$\alpha = -\frac{m^2}{2},$$

which will be explained in the next section. Then the potential is

$$\mathcal{V}(\phi) = -\frac{m^2}{2}\phi^2 + \frac{g}{4!}\beta\phi^4.$$

The value of the potential in the minimum

$$\bar{\phi} = \pm v = \pm\sqrt{\frac{3m^2}{g}} \tag{2.15}$$

is then given by

$$\begin{aligned}\mathcal{V}(\bar{\phi}) &= -\frac{m^2}{4}v^2 + \frac{g}{4!}v^4 = -\frac{3}{4}\frac{m^4}{g} + \frac{3}{8}\frac{m^4}{g}\\ &= -\frac{3}{8}\frac{m^4}{g} = -\frac{g}{4!}v^4.\end{aligned}$$

In a last step, as the energy integral does not change under addition of a constant factor, the potential is rewritten in order to ensure that the minima of the potential are zero in the minima

$$\begin{aligned}V(\bar{\phi}) := \mathcal{V}(\bar{\phi}) + \frac{g}{4!}v^4 &= -\frac{1}{2}m^2\phi^2 + \frac{g}{4!}\phi^4 + \frac{g}{4!}v^4\\ &= \frac{g}{4!}(\phi^2 - v^2)^2.\end{aligned} \tag{2.16}$$

In the formulation of this theory, the interactions were defined over a derivative. Since this derivative will lead to a Laplacian operator, this fact is a first hint, that in the calculation of the critical fluctuations, the Laplacian will be responsible for the geometric dependence of these critical fluctuations.

2.4. Critical behaviour in field theories

All studied theories in the last sections showed a certain critical behaviour near the critical point. This behaviour is characterised by the divergence of the macroscopic parameters, like the magnetisation.

The degree of divergence can be described by some power-law, so that an exponent describes the total behaviour of the system [NO11]. These exponents are called *critical exponents* that define a certain degree of divergence in the critical point. Moreover, the critical exponents of different physical quantities are linked by scaling laws [Kad66, Wil75]. Experiments confirm these power-law singularities as a function of the control parameter and its critical value for macroscopic observables, like the susceptibility χ, the magnetisation $\mathcal{M}$, the specific heat C or the correlation length ξ. Using the above defined reduced temperature, the following critical exponents can be found approaching the critical temperature [NO11]:

$$\begin{aligned} C &\sim |t|^{-\alpha} \quad t > 0 \\ \mathcal{M} &\sim |t|^{\beta} \quad t < 0 \\ \chi &\sim |t|^{-\gamma} \quad t > 0 \\ \xi &\sim |t|^{\nu'} \quad t < 0. \end{aligned}$$

Here the exponents $\alpha, \beta, \gamma, \nu'$ are the critical exponents. In the one dimensional Ising model, the correlation length was found to to have the critical exponent $\nu' = 1$, (2.5). For the mean field theory and also for the Landau theory, the value $\beta = 1/2$ was found in any dimension (2.11).

2.4.1. The interface tension and the correlation length

The reason for the divergence near the critical point is given by the divergence of the correlation length. Whereas far away from the critical point interactions play only a role on microscopic length scales, the divergence of the correlation length ξ is related to wide range thermic fluctuations. Therefore, microscopic details of the system play no role close to the critical point and physical quantities of different system are universal with a characteristic large-scale behaviour. Furthermore, the behaviour of systems within a certain *universality class* can be identified by the global characteristics like symmetry and dimension of the system [NO11]. This fact has been used in the last sections, where the behaviour of the system was just given by a macroscopic value, the order parameter ϕ.

The correlation function, defined by the covariance of the system, is a measure for fluctuations around the expectation value of a random variable. It has been used before in order to evaluate the correlation length of the one dimensional Ising model (2.5). Defining

$$G(r) := \langle \phi(r)\phi(0) \rangle$$

for a continuous random variable $\phi(\mathbf{x})$, the fluctuations of the continuous theories can be evaluated. As indicated in section 2.2, the correlation length can be given as an exponential function. Indeed, according to the Ornstein-Zernike theory [OZ14], the correlation function is given by

$$G(r) \approx \mathrm{e}^{-r/\xi}.$$

According to this expression the correlation length defines the spatial length of fluctuations. In the literature this correlation length is often called *bulk-correlation* length.

Another definition of a correlation length that linked to the interface tension is the *longitudinal* or *tunneling* correlation length (see e.g. [PF83])

$$\xi_{||}^{-1} = C \exp(-\sigma_\infty L_1 L_2) \tag{2.17}$$

where σ_∞ is the interface tension defined for large systems ($L_1 \to \infty, L_2 \to \infty$). The interface tension is equivalently given for the Ising model by the free energy. According to figure 2.1, the free energy of the system with interface is F_{-+}, while the free energy of the system without an interface is F_{++}. The gap in the free energy then defines the interface tension

$$\sigma_\infty = \lim_{\substack{L_1\to\infty \\ L_2\to\infty}} \left(-\frac{F_{-+} - F_{++}}{\beta L_1 L_2} \right), \tag{2.18}$$

where β is again the Boltzmann factor. This definition is equivalent to the definition of an energy gap ΔE between the two states. Using the partition function, the following can be written

$$\sigma_\infty = \lim_{\substack{L_1\to\infty \\ L_2\to\infty}} \left(-\frac{1}{L_1 L_2} \ln \frac{Z_{-+}}{Z_{++}} \right).$$

2.4.2. Quantum fluctuations

In quantum field theories (QFT) fluctuations are known as well. One example is the Lamb shift, originating from fluctuations of the electron around its mean value in the hydrogen atom. As a result a shift of the spectral lines by some energy ΔE takes place. In QFT these diverging quantities depend on a large momentum scale, the ultraviolet cut-off. With the Heisenberg uncertainty principle this means that the divergent quantities depend on small distance scale in position space. This can be seen analogue to the continuum description of the Ginzburg-Landau theory above, using a continuous field ϕ as order parameter. In QFT, this cut-off is typical at the scale of atomic distances [PS95]. By understanding the physics at these small scales, the parameters for systems on larger scales can be determined. Nevertheless, in QFT, the nature of the physics on atomic scale cannot be determined by elementary physical laws, as all quantities of observables only have statistical meaning. Large distance physics in QFT involve particles whose masses are very small in comparison to the cut-off scale. Therefore, it is useful to describe the statistical theory of critical fluctuation as a quantum field theory of particles with zero mass m. With the above assumptions, this would mean

$$\xi_{||} \sim m^{-1}. \tag{2.19}$$

Considering a time evolved system with a Hamiltonian $\hat{H}$, one finds for the correlation function [DFMS97]

$$\begin{aligned}\langle\phi(r,0)\phi(r,\tau)\rangle &= \langle 0|\phi(r,0)\mathrm{e}^{-\hat{H}\tau}\phi(r,0)\mathrm{e}^{\hat{H}\tau}|0\rangle \\ &= \sum_n \langle 0|\phi(r,0)\mathrm{e}^{-\hat{H}\tau}|n\rangle\langle n|\phi(r,0)\mathrm{e}^{\hat{H}\tau}|0\rangle \\ &= \sum_n \mathrm{e}^{-(E_n-E_0)\tau}|\langle 0|\phi(r,0)|n\rangle|^2.\end{aligned}$$

For a system with two eigenstates, the ground state and the excited state E_a, where $\Delta E = E_a - E_0$ reads in the limit of large times T

$$\langle\phi(r,0)\phi(r,\tau)\rangle \sim \mathrm{e}^{-\Delta E T} \tag{2.20}$$

In the previously defined statistical theory of phase transitions, two vacuum expectation values can be found in the broken phase: $|+\rangle$ that corresponds to $\bar{\phi} = +v$ and $|-\rangle$ corresponding to $\bar{\phi} = -v$. The Hamiltonian $\hat{H}$ is associated with the quantum mechanical Hamiltonian with the eigenstates $|+\rangle$ and $|-\rangle$. Furthermore, there is a symmetric ground state $|0_s\rangle$ with energy E_s via the symmetry transformation $\bar{\phi} \to -\bar{\phi}$ performed by an operator P and an anti-symmetric ground state $|0_a\rangle$, whose energy E_a is exactly ΔE higher than E_s.

This can be imagined as the transition of a quantum mechanical particle from one potential well into the other. This energy splitting has been introduced in the last section, in order to define the interface tension by the free energy of the anti-symmetric system F_{+-} corresponding to the state $|0_a\rangle$ and the symmetric system system F_{++} corresponding to $|0_s\rangle$.

The reflection symmetry can be performed by the reflection operator P whose action on a state $|\psi\rangle = \psi(x)$ is given by

$$P\psi(x) = \psi(-x)$$

implying for the ground states $P\bar{\phi} = -\bar{\phi}$. The commutator $[\hat{H}, P] = 0$ vanishes, because the potential (2.16) is even under this symmetry. This means, $\hat{H}$ and P can be diagonalised simultaneously. The two eigenstates of the reflection operator will be

$$\begin{aligned}|0_s\rangle &= \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right) \\ |0_a\rangle &= \frac{1}{\sqrt{2}}\left(|+\rangle - |-\rangle\right).\end{aligned}$$

The linear combination of these states deliver the vacuum expectation values

$$|+\rangle = \frac{1}{\sqrt{2}}\left(|0_s\rangle + |0_a\rangle\right) \tag{2.21}$$

$$|-\rangle = \frac{1}{\sqrt{2}}\left(|0_s\rangle - |0_a\rangle\right). \tag{2.22}$$

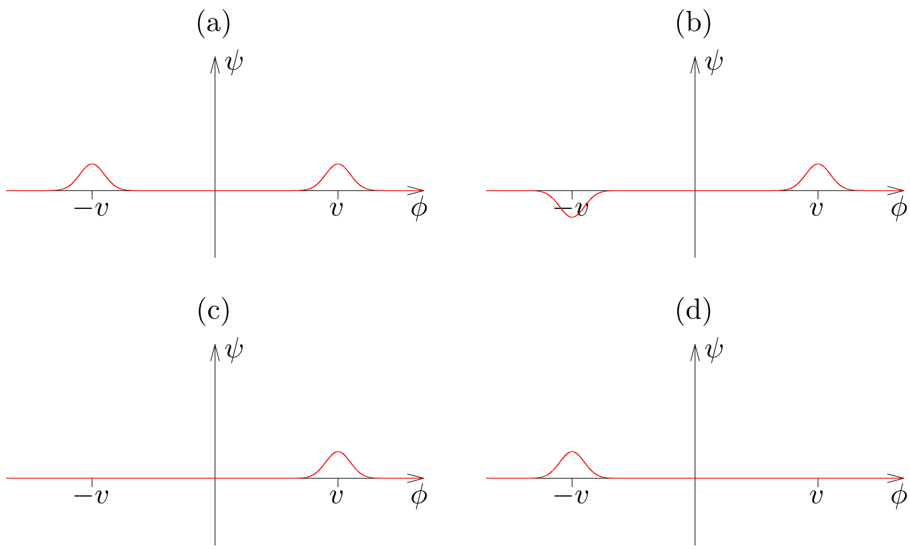

Figure 2.5.: Schematic representation of the symmetric (a) and anti-symmetric (b) state and their linear combinations (c), (d), motivated by [Mün10].

These states and their linear combinations are shown schematically in figure 2.5. The symmetric and anti-symmetric state give the demanded symmetry

$$P|0_s\rangle = |0_s\rangle, \qquad P|0_a\rangle = -|0_a\rangle.$$

In the path integral formalism, the time evolution (2.20) can be represented by [Das93]

$$\begin{aligned}\langle +|\mathrm{e}^{-\hat{H}T}|-\rangle &= \int \mathcal{D}\phi \mathrm{e}^{-S_E[\phi]} \\ &= \int \mathcal{D}\phi \mathrm{e}^{-H[\phi]},\end{aligned}$$

where H is the Hamiltonian (2.14) of statistical field theory, associated with the Euclidean action via Wick rotation [LBB91]. Analogous to the Boltzmann factor, the Planck constant $\hbar$ is set to $\hbar = 1$, since the theory is evaluated near the critical point. The z-direction is identified with the Euclidean time in the field theory. Using this structural analogy, the transition amplitude can be defined equivalently to the previously defined partition function of the Ginzburg-Landau theory (2.13)

$$Z = \langle +|\mathrm{e}^{-\hat{H}T}|-\rangle = \int \mathcal{D}\phi \mathrm{e}^{-H[\phi]}. \tag{2.23}$$

This is analogous to the transfer matrix of a particle tunneling from the initial state $|-\rangle$ at time $-T/2$ to the final state $|+\rangle$ at time $T/2$. If the quantum field theoretical

Hamiltonian $\hat{H}$ can be expanded into a complete set of eigenstates, the left hand side of (2.23) with the states (2.21) and (2.22) give the transition amplitude

$$\begin{aligned} \langle + | \mathrm{e}^{-\hat{H}T} | - \rangle &= \frac{1}{2}\left(\mathrm{e}^{-E_a T} + 0 + 0 - \mathrm{e}^{-E_s T}\right) \\ &= \frac{1}{2}\left(\mathrm{e}^{-E_a T} - \mathrm{e}^{-(E_a + \Delta E)T}\right) \\ &= \frac{1}{2}\mathrm{e}^{-E_a T}\left(1 - \mathrm{e}^{-\Delta E T}\right). \end{aligned} \tag{2.24}$$

The mixed states vanish, because in this Hilbert space of symmetric and anti-symmetric functions, the states $|0_s\rangle$ and $|0_a\rangle$ are orthogonal.

This gives a good connection to derive the tunneling correlation length by the energy splitting

$$\xi_{||}^{-1} = \Delta E. \tag{2.25}$$

Moreover, the energy gap ΔE is the mass m of the quantum field, as it is the mass of the particle in rest. Because the correlation length diverges at the critical point, the theory of critical phenomena is equivalent to a massless field theory. Therefore, the mass m can be used as the control parameter deviated from the Landau theory, since the zero value of that control parameter α was reason for the symmetry-breaking.

3

Interfaces in ϕ^4 theory

As shown, the Ginzburg-Landau functional serves as a universal approach on phase transitions as well as on interfaces. In the end of the last chapter, the structural analogy of statistical mechanics and quantum field theory was outlined. Given a field $\phi(\mathbf{x})$, the following chapter drafts out the theory in the setup of a quantum field theory and path integrals, often called statistical field theory [LBB91]. The theory corresponds to a ϕ^4-theory in QFT. Therefore, reasonable boundary conditions for the field will be determined first in order to apply this Hamiltonian to the interface in a cuboid box $L_1 \times L_2 \times T$, see figure 1.1. This setup will be investigated in the Landau approximation, which means, the vacuum expectation value and the statistically most probable configuration of a field ϕ_0 satisfying the demanded boundary conditions will be calculated. This will lead to a classical solution, the *kink*-solution, which was first given by J.W. Cahn and J.E. Hilliard in 1958 [CH58]. Additionally the transition energy of the kink will be derived. It will be shown, that the system is invariant under translations in z-direction from a physical point of view because the form and transition energy of the interface shall be invariant under different positions of the interfaces in the box.

For the field $\phi(\mathbf{x})$ there is no general analytic expression. Therefore, a more suitable approximation, involving fluctuations will be necessary. One way is to perturb the Hamiltonian (2.14)

$$H[\phi] = \int\limits_{L_1 \times L_2 \times T} \mathrm{d}^3x \left\{ \frac{1}{2}(\nabla\phi)^2 + V(\phi) \right\} \tag{3.1}$$

$$= \int \mathrm{d}^3x \mathcal{H}[\phi] \tag{3.2}$$

with the ϕ^4 potential

$$V[\phi] = \frac{g}{4!}(\phi^2 - v^2)^2 \tag{3.3}$$

by a small fluctuation η around the classical trajectory ϕ_0. Then a series expansion will allow a reconsideration of the path, involving small fluctuations in a Gaussian approximation. These fluctuations will be identified by a fluctuation operator.

In the last chapter the correlation length was observed corresponding to the energy splitting between the symmetric and anti-symmetric state. The transition through the interface will be formulated as the tunneling of a particle from an initial state to a final state through the potential barrier. Under some quantum field theoretical considerations involving pseudo particles called *instantons*, this treatment goes back to S. Coleman [Col85]. The upcoming zero mode will be handled with the method of collective coordinates, where the translational invariance of the system is used to split off the zero-mode. The system is translationary invariant from a physical point of view because the form and transition energy of the interface shall be invariant under different positions of the interfaces in the box.

Conclusively, this chapter will lead to an expression for the interface energy of the system, which can be evaluated by methods of zeta-regularization later on.

3.1. Boundary conditions for the interface

The system that is going to be modeled must be restricted by the following constraints:

- There must be at least one interface. This means the energetic more favourable constant solution of the system must be avoided and the phase transition is enforced.

- It must be finite in the plane of the interface, so that the boundary conditions establish an interface. In the other direction the system must be infinite, so that the phase transition can take place and the proposed kink solution can be established.

An interface can, as described in the last chapter, only exist in the broken phase of the Ginzburg-Landau theory where the two potential minima exist. Furthermore, the geometry must be fixed by the following conditions to enhance the restrictions on the volumina stated in the previous chapter: one direction must be able to be extended to infinity, because for finite volumes, symmetry breaking cannot occur, and the further two dimensions are restricted to a finite spatial volume $A = L_1 L_2$. To make this clear the following conventions will be used:

- The site with infinitely extended length will be referred to by the z-coordinate, with $z \in \mathbb{R}$, the length of the site will be named T, while later on the limit $T \to \infty$ will be taken.

- The finite special volume will be referred to by $A = L_1 \times L_2$ and it will be described by the vector $\vec{x} = (x_1, x_2) \in \mathbb{R}^2$ with $0 < x_1 < L_1$ and $0 < x_2 < L_2$.

Summarizing these geometric restrictions, a volume of $L_1 \times L_2 \times T$ has been constructed for a field $\phi(\mathbf{x}) = \phi(\vec{x}, z) = \phi(x_1, x_2, z)$, where $T \to \infty$. Moreover, realistic boundary conditions are demanded.

Remembering that the Ginzburg-Landau theory is a field theory, a field $\phi(\mathbf{x})$ plays the role of the order parameter. For this field, the interface, established in (x_1, x_2)-direction, takes place in the infinitely large z direction when fixed boundary conditions are used. This can equally be described by anti periodic boundary conditions

$$\phi(\vec{x}, z) = -\phi(\vec{x}, z + T). \tag{3.4}$$

The two ground states of the infinite volume system in broken symmetry phase system can be characterized by a vacuum expectation value $v > 0$ of the field

$$\bar{\phi} \equiv \langle \pm | \phi(\mathbf{x}) | \pm \rangle = \pm v. \tag{3.5}$$

To exclude surface phenomena the boundary conditions in the $\vec{x}$ directions are chosen to be periodic:

$$\phi(x_1, x_2, z) = \phi(x_1 + L_1, x_2, z) = \phi(x_1, x_2 + L_2, z). \tag{3.6}$$

These conditions establish at least one transition between $\bar{\phi} = -v$ and $\bar{\phi} = v$. To be accurately, more than one transitions satisfy these boundary conditions as long as the number of transitions is odd. However, these transitions will be dominated by the one-transition setup, because in every interface, a transition of the potential barrier must be overcome. The energetic most favourable states that are dominated by their statistical weight, the Boltzmann probability, will establish only one interface. This interface profile originates due to the most probable or – in words of quantum field theory – due to the classical path. To begin with, the vacuum expectation value needs to be calculated. This has been already done in the last chapter (2.15), resulting in $\bar{\phi} = \pm v = \pm\sqrt{\frac{3m^2}{g}}$, and can be also achieved by minimizing the Hamiltonian in the framework of variational calculus (see appendix A.1).

3.2. The kink solution obtained from Landau approximation

In the Landau approximation, the system contains merely the state of maximum probability, which is the state of minimum transition energy over the potential barrier. The interface profile is therefore a field ϕ_0 which minimizes the transition energy, where the Hamiltonian $H[\phi(\mathbf{x})]$ is minimized. Consequently, the variational calculus leads to the classical Euler-Lagrange equation

$$\left.\frac{\delta H[\phi(\mathbf{x})]}{\delta \phi(\mathbf{x})}\right|_{\phi=\phi_0} = \frac{1}{2}(-2\nabla^2\phi_0) + \frac{g}{4!}4\phi_0^3 - \frac{m^2}{4}2\phi_0 = 0. \tag{3.7}$$

The derivative used here is the *Fréchet derivative*, serving as the functional derivative of an operator (see e.g. [LBB91, PS95]). Taking the above mentioned boundary conditions into consideration, which imply the appearance of one or more interfaces that gives

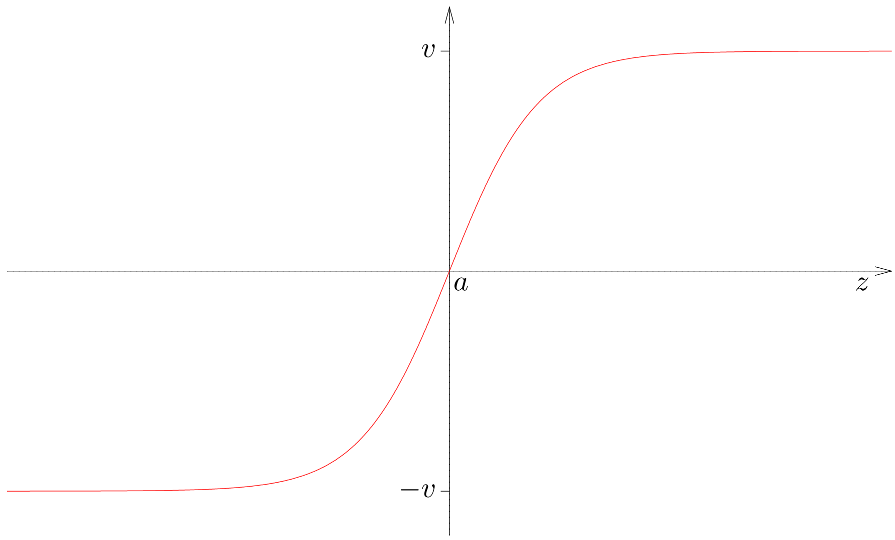

Figure 3.1.: The kink profile.

the most probable path through the double well potential, these conditions lead to the Cahn-Hilliard [CH58] profile

$$\phi_0^{(a)}(z) = v \tanh\left[\frac{m}{2}(z-a)\right] \tag{3.8}$$

for one kink (see appendix A.1), where the parameter $a \in \mathbb{R}$ can be chosen arbitrarily because it is an integral constant and manifests the position of the profile on the z-axis. Solutions of the form (3.8) are called kink solutions. It shows the form presented in figure 3.1. The energy of the transition is an integral over the Hamiltonian density according to equation (3.2), where the explicit profile, the kink-profile (3.8) is inserted. Since the integration in z has to be performed over whole $\mathbb{R}$, the arbitrary parameter a can be eliminated by substitution.

Furthermore, this means, the energy is independent from the position of the kink. This translational invariance will be used later in detail in order to handle the zero mode using the method of collective coordinates. Let for now be $\phi_0 \equiv \phi_0^{(0)}$, because a can be chosen arbitrarily.

Changing the sign of the boundary conditions $\phi_0 \underset{z\to\pm\infty}{=} \mp v$ leads to the *anti-kink* $\phi_0(z) = -v\tanh(mz/2)$. The energy of one kink thus is calculated by integrating the Hamiltonian density (see appendix A.2) and results in

$$H_0 \equiv H\left[\phi_0(\mathbf{x})\right] = 2L_1L_2\frac{m^3}{g}. \tag{3.9}$$

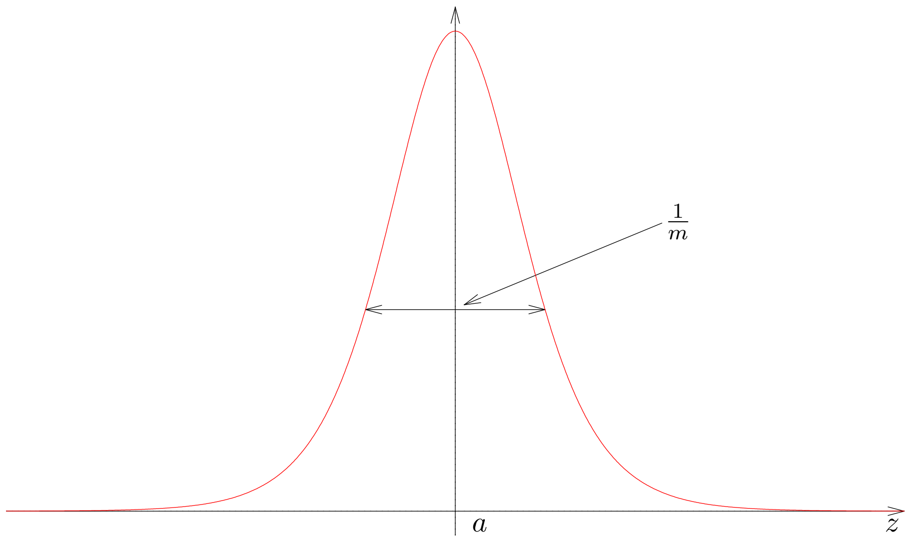

Figure 3.2.: Localization of the kinetic energy of a kink, obtained in appendix A.2.

3.3. Perturbing the Hamiltonian with fluctuations

In quantum field theory, the Euler-Lagrange equation gives the most probable classical trajectory satisfying the Hamiltonian principle of the least action. Small fluctuations $\eta(\mathbf{x})$ are added to the classical trajectory (3.8) $\phi_0(\mathbf{x})$

$$\phi(\mathbf{x}) = \phi_0(\mathbf{x}) + \eta(\mathbf{x}). \tag{3.10}$$

The Hamiltonian therefore is given by

$$H\left[\phi(\mathbf{x})\right] = H\left[\phi_0(\mathbf{x}) + \eta(\mathbf{x})\right].$$

The Taylor series of the Hamiltonian $H\left[\phi\right]$ around the kink solution with fluctuations η is given by

$$\begin{aligned} H\left[\phi(\mathbf{x})\right] &= H\left[\phi_0(\mathbf{x}) + \eta(\mathbf{x})\right] \\ &= H\left[\phi_0(\mathbf{x})\right] + \int \mathrm{d}^3x \left.\frac{\delta H\left[\phi\right]}{\delta\phi(\mathbf{x})}\right|_{\phi_0} \eta(\mathbf{x}) \\ &\quad + \frac{1}{2}\int \mathrm{d}^3x\mathrm{d}^3x' \left.\frac{\delta^2 H\left[\phi\right]}{\delta\phi(\mathbf{x})\delta\phi(\mathbf{x}')}\right|_{\phi_0} \eta(\mathbf{x})\eta(\mathbf{x}') + \dots . \end{aligned}$$

The potential has the maximal order $\mathcal{O}(\phi^4)$, thus all functional derivatives of the functional H above the fourth order vanish. As discussed before, the classical trajectory satisfies the classical Euler Lagrange equation (3.7), so the second term in the expansion also vanishes. The contribution of orders above two, the so-called interactions, will be ignored, as they do not contribute to the Gaussian approximation. This leaves to evaluate the second order of the expression

$$\left.\frac{\delta^2 H\left[\phi\right]}{\delta\phi(\mathbf{x})\delta\phi(\mathbf{x}')}\right|_{\phi=\phi_0} = -\left[\nabla^2 - V''(\phi_0)\right]\delta(\mathbf{x}-\mathbf{x}') \equiv M_{xx'}[\phi_0]. \tag{3.11}$$

So, the expanded Hamiltonian is

$$H\left[\phi_0+\eta\right] = H_0 + \frac{1}{2}\left(\eta, M[\phi_0]\eta\right), \tag{3.12}$$

where $(\cdot,\cdot)$ denotes the scalar product, here defined by

$$(f,g) = \int \mathrm{d}^3x f(\mathbf{x})g(\mathbf{x})$$

for square integrable functions $f,g : \mathbb{R}^3 \to \mathbb{R}$. In this case, the operator $M[\phi_0]$, defined above, represents the contribution of the fluctuations around the classical solution. Therefore, it is called fluctuation operator and will be given explicitly later. The corresponding partition function reads

$$Z = \int \mathcal{D}\phi \mathrm{e}^{-H[\phi]} = \mathrm{e}^{-H_0}\int \mathcal{D}\eta \mathrm{e}^{-\frac{1}{2}(\eta, M[\phi_0]\eta)}. \tag{3.13}$$

This partition function contains a Gaussian integral. A naive way to evaluate this integral would be

$$Z = \frac{\mathcal{N}}{\sqrt{\det(M[\phi_0])}}\mathrm{e}^{-H_0} \tag{3.14}$$

with a normalizing constant $\mathcal{N}$ due to the Gaussian integral. The Gaussian integral in d dimensions is given by

$$\int \mathrm{d}y^d \mathrm{e}^{-\frac{1}{2}\sum_{n=1}^{d} y_n^2} = (2\pi)^{d/2}. \tag{3.15}$$

The partition function in (3.13) can only be determined this way, when all eigevalues are strictly positive. Because of the eigenvalue $\lambda_0 = 0$ the Gaussian integral diverges. In other words, as the determinant is a product over all eigenvalues, the determinant in (3.13) delivers a zero value and the partition function diverges. There is a connection between the previously mentioned translational invariance of the kink and the zero mode. This will be evaluated in detail in the next section with the method of collective coordinates.

In order to evaluate the fluctuations, the operator $M[\phi_0]$ is studied in detail now. It is specially relevant that the operator possesses explicitly one eigenmode with zero eigenvalue called zero mode. This zero mode is described by the function Ψ_0. Observing the fluctuations again, the same extremal condition (3.7) delivers the following expression for the fluctuation operator.

Varying the extrema of the Hamiltonian by a small fluctuation around a classical trajectory, imposing the same extremal condition (3.7) as before

$$\left.\frac{\delta H[\phi]}{\delta\phi(\mathbf{x})}\right|_{\phi=\phi_0+\eta} = 0.$$

Whereas this means

$$\begin{aligned}\left.\frac{\delta H[\phi]}{\delta\phi(\mathbf{x})}\right|_{\phi=\phi_0+\eta} &= -\nabla^2(\phi_0+\eta) - \frac{m^2}{2}(\phi_0+\eta) + \frac{g}{3!}(\phi_0+\eta)^3 \\ &= \left.\frac{\delta H[\phi]}{\delta\phi(\mathbf{x})}\right|_{\phi=\phi_0} - \nabla^2\eta - \frac{m^2}{2}\eta + \frac{g}{2!}\phi_0^2\eta + \mathcal{O}(\eta^2) \\ &= 0 + \left[-\nabla^2 - \frac{m^2}{2} + \frac{g}{2}\phi_0^2\right]\eta + \mathcal{O}(\eta^2).\end{aligned}$$

Recalling, that the classical trajectory satisfies condition (3.7), the first term equals zero. By neglecting higher orders of η, the calculation leads to

$$\left[-\nabla^2 - \frac{m^2}{2} + \frac{g}{2}\phi_0^2\right]\eta = 0, \tag{3.16}$$

with the fluctuation operator which is defined by

$$M[\phi_0] \equiv -\nabla^2 - \frac{m^2}{2} + \frac{g}{2}\phi_0^2 = -\left[\nabla^2 - V''(\phi_0)\right]. \tag{3.17}$$

The last step can be shown by calculating the second derivative of the potential (3.3) with respect to ϕ_0

$$\begin{aligned}V''(\phi_0) &= \frac{g}{2}\left(\phi_0^2 - \frac{1}{3}v^2\right) \\ &= \frac{g}{2}\phi_0^2 - \frac{m^2}{2}.\end{aligned}$$

That is exactly the operator defined in (3.11). The fluctuation η solving the condition (3.16) is identified with the zero-mode Ψ_0, since the Gaussian integral in the partition function (3.14) diverges by this mode. The connection of this zero-mode to the invariance under translations of the kink $\phi_0(z)$ on the z-axis is outlined now. The translational operator $T^{(a)}$ is defined by small translations a:

$$\phi_0(z+a) = T^{(a)}\phi_0(z) = \left(1 + a\frac{\partial}{\partial z}\right)\phi_0(z) = \phi_0(z) + a\phi_0'(z) + \mathcal{O}(a^2). \tag{3.18}$$

The prime here indicates a derivative with respect to z. By omitting the higher orders of a, this can be written as

$$T^{(a)}\phi_0(z) = \phi_0(z) + c(a)\Psi_0(z),$$

where Ψ_0 corresponds to a translation in functional space induced by the translation of the position in z-direction. For the classical solution

$$c(a)\Psi_0(z) = a\partial_z\phi_0(z) = a\frac{mv}{2}\,\mathrm{sech}^2\left(\frac{m}{2}z\right) \tag{3.19}$$

is obtained. Assuming Ψ_0 to be normalized, the scalar product provides

$$(c(a)\Psi_0(z), c(a)\Psi_0(z)) = c^2(a)||\Psi_0||^2 = c^2(a).$$

From (3.19), the constant can be derived

$$\begin{aligned} c^2(a) &= (c(a)\Psi_0(z), c(a)\Psi_0(z)) = a^2(\phi_0'(z), \phi_0'(z)) \\ &= a^2\int \mathrm{d}^3x(\phi_0'(z))^2 = a^2H_0 \end{aligned}$$

according to the calculations of the kink energy in appendix A.2. Consequently, in the limit of infinitesimal a, the translation is given by

$$T^{(a)}\phi_0(z) = \phi_0(z+a) = \phi_0(z) + a\sqrt{H_0}\Psi_0(z). \tag{3.20}$$

Comparing (3.18) with (3.20) the following zero mode can be found

$$\Psi_0(z) = \frac{\phi_0'(z)}{\sqrt{H_0}}.$$

Inserting the zero-mode Ψ_0 of the operator $M[\phi_0]$ for η in the left hand equation (3.16) gives zero. Because of the above connection between the zero mode and the translation along the z-axis, the zero mode delivers a contribution to all one-kink solutions. The following treatment applied here is called method of collective coordinates [GS75]. Defining

$$\xi(a) := \int \mathrm{d}^3x\,[\phi(\mathbf{x}) - \phi_0(z-a)]\,\frac{\phi_0'(z-a)}{\sqrt{H_0}}$$

for a field $\phi(\mathbf{x})$. By the properties of the Dirac delta function follows

$$1 = \int \mathrm{d}\xi\delta(\xi) = \int \mathrm{d}a\frac{\mathrm{d}\xi}{\mathrm{d}a}\delta(\xi(a)),$$

where a shift and the derivative give

$$\begin{aligned} \frac{\mathrm{d}\xi}{\mathrm{d}a} &= \frac{\mathrm{d}}{\mathrm{d}a}\int \mathrm{d}^3x\,[\phi(\vec{x}, z+a) - \phi_0(z)]\,\frac{\phi_0'(z)}{\sqrt{H_0}} \\ &= \int \mathrm{d}^3x\frac{\mathrm{d}\phi(\vec{x}, z+a)}{\mathrm{d}a}\frac{\phi_0'(z)}{\sqrt{H_0}}, \end{aligned}$$

because there $\phi_0(z)$ and $\phi_0'(z)$ do not depend on a any more. Furthermore, the derivative with respect to a in $\phi(\vec{x}, z+a)$ can as well be written as a derivative with respect to z. Therefore the path integral over an arbitrary configuration $\phi(\mathbf{x})$ is given by

$$\begin{aligned}\int \mathcal{D}\phi \mathrm{e}^{-H[\phi]} &= \int \mathcal{D}\phi \left[\int \mathrm{d}a \frac{\mathrm{d}\xi}{\mathrm{d}a} \delta(\xi(a))\right] \mathrm{e}^{-H[\phi]} \\ &= \int \mathrm{d}a \int \mathcal{D}\phi \int \mathrm{d}^3x \left[\phi'(\vec{x}, z+a) \frac{\phi_0'(z)}{\sqrt{H_0}}\right. \\ &\quad \left. \times\, \delta\left(\int \mathrm{d}^3x \left[\phi(\vec{x}, z+a) - \phi_0(z)\right] \frac{\phi_0'(z)}{\sqrt{H_0}}\right)\right] \mathrm{e}^{-H[\phi]}.\end{aligned}$$

As there is no difference in evaluating all configurations $\phi(\vec{x}, z+a)$ or $\phi(\vec{x}, z)$, the expression becomes

$$\begin{aligned}\int \mathcal{D}\phi \mathrm{e}^{-H[\phi]} = \int \mathrm{d}a \int \mathcal{D}\phi \int \mathrm{d}^3x &\left[\phi'(\mathbf{x}) \frac{\phi_0'(z)}{\sqrt{H_0}}\right. \\ &\left. \times\, \delta\left(\int \mathrm{d}^3x \left[\phi(\mathbf{x}) - \phi_0(z)\right] \frac{\phi_0'(z)}{\sqrt{H_0}}\right)\right] \mathrm{e}^{-H[\phi]}\end{aligned}$$

On a symmetric support $a \in [-T/2, T/2]$, the first integral becomes T, because the rest of the integral is independent of a. Setting now $\phi = \phi_0 + \eta$, the integral becomes

$$\begin{aligned}\int \mathcal{D}\phi \mathrm{e}^{-H[\phi]} = T \int \mathcal{D}\phi \int \mathrm{d}^3x &\left[(\phi_0'(\mathbf{x}) + \eta'(\mathbf{x})) \frac{\phi_0'(z)}{\sqrt{H_0}}\right. \\ &\left. \times\, \delta\left(\int \mathrm{d}^3x \left[\phi_0(\mathbf{x}) + \eta(\mathbf{x}) - \phi_0(z)\right] \frac{\phi_0'(z)}{\sqrt{H_0}}\right)\right] \mathrm{e}^{-H[\phi_0(\mathbf{x})+\eta(\mathbf{x})]},\end{aligned}$$

where the last expression can be substituted by the series expansion (3.11) because only small fluctuations are considered. The expression inside the delta function simplifies and

$$\delta\left(\left(\eta, \frac{\phi_0'}{\sqrt{H_0}}\right)\right) \tag{3.21}$$

is gained. This means, the integral has only a meaning, when

$$\left(\eta, \frac{\phi_0'}{\sqrt{H_0}}\right) = 0. \tag{3.22}$$

Because of the energy integral $\int \mathrm{d}^3x (\phi_0')^2 = H_0$ the whole integral simplifies to

$$\int \mathcal{D}\phi \mathrm{e}^{-H[\phi]} = T\sqrt{H_0}\mathrm{e}^{-H_0} \int \mathcal{D}\eta \left[\left[1 + \frac{1}{H_0}(\eta, \phi_0'')\right] \delta\left(\left(\eta, \frac{\phi_0'}{\sqrt{H_0}}\right)\right)\right] \mathrm{e}^{\frac{1}{2}(\eta, M\eta) + \mathcal{O}(\eta^3)}.$$

Evaluating the derivatives of the classical trajectory $\phi_0(z)$ deliver

$$\begin{aligned}\phi_0'(z) &= \frac{mv}{2}\,\mathrm{sech}^2\left(\frac{m}{2}z\right)\\ \phi_0''(z) &= \frac{m^2 v}{4}\tanh\left(\frac{m}{2}z\right)\mathrm{sech}^2\left(\frac{m}{2}z\right)\\ &= \frac{m}{2}\tanh\left(\frac{m}{2}z\right)\phi_0'(z).\end{aligned}$$

This means, the scalar product (3.22) vanishes, if

$$\int \mathrm{d}^3x\eta(\mathbf{x})\phi'(z) = 0.$$

Explicitly this means

$$(\eta, \phi_0'') = \frac{m}{2}\left(\eta, \tanh(mz/2)\phi_0'(z)\right) = 0.$$

Then the above equation simplifies to

$$\int \mathcal{D}\phi \mathrm{e}^{-H[\phi]} \approx T\sqrt{H_0}\mathrm{e}^{-H_0}\int \mathcal{D}\eta \mathrm{e}^{\frac{1}{2}(\eta,M\eta)} \tag{3.23}$$

in second order expansion. By condition (3.21) follows, that only the fluctuations orthogonal to the zero mode are included in the integral (3.23). To be explicit, the eigenvalues $\lambda_0 < \lambda_1 < \ldots < \lambda_n$ of the eigenfunctions η in (3.16) the integral is evaluated according to

$$\begin{aligned}\int \mathcal{D}\eta \mathrm{e}^{-(\eta,M\eta)} &= \int \prod_{n\geq 0} \mathrm{d}c_n \mathrm{e}^{-\frac{1}{2}\sum_{n\geq 0}\lambda_n c_n^2}\\ &= \int \mathrm{d}c_0 \int \prod_{n>0} \mathrm{d}c_n \mathrm{e}^{-\frac{1}{2}\sum_{n>0}\lambda_n c_n^2}\\ &= \sqrt{\frac{H\left[\phi_0\right]}{2\pi}}\int \mathrm{d}a \int \prod_{n>0} \mathrm{d}c_n \mathrm{e}^{-\frac{1}{2}\sum_{n>0}\lambda_n c_n^2}\\ &= \sqrt{\frac{H\left[\phi_0\right]}{2\pi}}\frac{\mathcal{N}\int \mathrm{d}a}{\sqrt{\det\text{'}(M(\phi_0))}},\end{aligned}$$

where the apostrophe denotes that the determinant is evaluated omitting the zero mode $\lambda_0 = 0$. The factor $\sqrt{2\pi}$ is inserted due to the collective coordinate c_0 in the Gaussian integral

$$\int \mathcal{D}\eta = \mathcal{N}\int \prod_i \frac{dc_i}{\sqrt{2\pi}}$$

$$\int \frac{\mathrm{d}c_0}{\sqrt{2\pi}}\delta(c_0) = (2\pi)^{-1/2}.$$

The partition function (3.13) reads

$$Z = \mathcal{N}\sqrt{\frac{H\left[\phi_0\right]}{2\pi}}\frac{\mathrm{e}^{-H[\phi_0]}\int \mathrm{d}a}{\sqrt{\det'(M[\phi_0])}}, \tag{3.24}$$

with $H[\phi_0]$ given in (3.9).

3.4. The energy splitting

From statistical field theory it is known, that the partition function for the broken phase of the Ginzburg Landau theory corresponds to a transition amplitude in quantum field theory induced by a time-evolution operator $\mathrm{e}^{-\hat{H}T}$. In the broken phase, there is no degeneracy at finite volume. Furthermore, there is a symmetric ground state $|0_s\rangle$ with energy E_s via the symmetry transformation $\phi_0 \to -\phi_0$ performed by an operator P and an anti-symmetric ground state $|0_a\rangle$

Using the analogy between the partition function and the particle tunneling from one state to the other, the following contribution for one kink on symmetric support $[-T/2, T/2]$ is followed by (2.23) and (3.24)

$$\langle +|\mathrm{e}^{-\hat{H}T}|-\rangle = \mathcal{N}T\sqrt{H_0}(\det' M)^{-1/2}\mathrm{e}^{-H_0} \tag{3.25}$$

with $M \equiv M[\phi_0]$.

3.4.1. Multi kink contribution

A next step is the introduction of a sharp kink approximation, often called dilute gas approximation. From equation (A.7) it can be inferred, that the kinetic energy of kinks are precisely localized with a size for order $1/m$ for large T around $z = a$, see as well Figure 3.2. This form is often called soliton in nonlinear-physics and resembles a pseudo-particle in quantum field theory, called instanton. This means, there are, as stated previously, more than only one kink. There are n kinks playing a role on a large T scale. If the time is large $T \to \infty$, the characteristic intervals become $T \gg m^{-1}$ and the corresponding Hamiltonian corresponding to such a configuration is nH_0, where H_0 is the Hamiltonian of one kink. This can be seen in Figure 3.3. This means, most contribution of the multi kink energy splitting result from decreases and increases on the states with $\phi_0 = \pm v$, which is due to

$$M_0 = -\nabla^2 + m^2.$$

This expression is comparable to the harmonic oscillator in quantum mechanics. From quantum mechanics is known, that the spectrum of the harmonic oscillator is strictly positive. Therefore, no correction due to a zero mode will be necessary. The path integral in this case is similar to the previous path integral, giving

$$\langle +|\mathrm{e}^{-\hat{H}T}|-\rangle = \mathcal{N}(\det M_0)^{-1/2}\mathrm{e}^{-H_0},$$

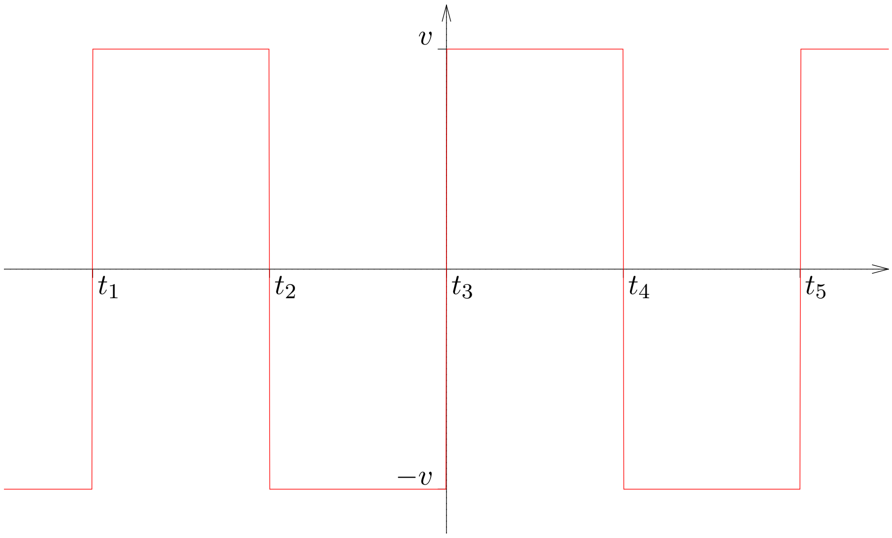

Figure 3.3.: Multi kinks in a sharp kink approximation.

where $\hat{H}_0$ corresponds to the symmetric functions. If the kinks are in sharp kink approximation and the time is large enough, the functional integral can be evaluated summing over all these configurations for widely separated objects go to $H \approx nH_0$, which gives according to [Col85]

$$\mathrm{e}^{-H} = K^n \mathrm{e}^{-nH_0} \tag{3.26}$$

with a constant K to be determined later, with n objects centered at times $t_1, t_2, \ldots, t_n$, where

$$-T/2 < t_1 < t_2 < \ldots < t_n < T/2.$$

All multi kink configurations which fulfill the boundary conditions are the configurations with an odd number of kink and anti kinks following each other. This means the integral over all these configurations gives

$$\int \mathrm{d}a = \int\limits_{-T/2}^{T/2} \mathrm{d}t_n \cdots \int\limits_{-T/2}^{t_3} \mathrm{d}t_2 \int\limits_{-T/2}^{t_2} \mathrm{d}t_1 = T^n/n!,$$

which can be easily computed and proven by induction. Likewise, n must be odd by definition of the boundary conditions. The determinant then is considered being only the determinant over a product of separated harmonic oscillators, resembling the wells of the double well potential. For n widely separated kinks, the result is

$$\begin{aligned}\langle +|\mathrm{e}^{-\hat{H}T/\hbar}|-\rangle &= \mathcal{N}(\det M_0)^{-1/2}\sum_{n\text{ odd}}\frac{\left(K\mathrm{e}^{-H_0}T\right)^n}{n!} \\ &= \mathcal{N}(\det M_0)^{-1/2}\frac{\exp\left(K\mathrm{e}^{-H_0}T\right)-\exp\left(-K\mathrm{e}^{-H_0}T\right)}{2} \\ &= \mathcal{N}(\det M_0)^{-1/2}\frac{1}{2}\exp\left(K\mathrm{e}^{-H_0}T\right)\left[1-\exp\left(-2K\mathrm{e}^{-H_0}T\right)\right],\end{aligned} \tag{3.27}$$

where the last expression can be compared with the initial equation (2.24), so that

$$\Delta E = 2K\mathrm{e}^{-H_0}.$$

The degeneracy of the two energy eigenvalues is broken by tunneling amplitude, the difference is given by a Gamov factor e^{-H_0}. This can be compared with the prior statement, giving (3.25) and (3.27) for $n=1$

$$\mathcal{N}(\det M_0)^{-1/2}Ke^{-H_0}T = \mathcal{N}T\sqrt{\frac{H_0}{2\pi}}(\det' M)^{-1/2}\mathrm{e}^{-H_0},$$

so that

$$K = \sqrt{\frac{H_0}{2\pi}}\left(\frac{\det' M}{\det M_0}\right)^{-1/2},$$

where the factor $\sqrt{2\pi}$ is due to the zero mode.

Conclusively

$$\begin{aligned}\Delta E &= 2K\mathrm{e}^{-H_0} \\ &= 2\sqrt{\frac{H_0}{2\pi}}\left|\frac{\det' M}{\det M_0}\right|^{-1/2}\mathrm{e}^{-H_0},\end{aligned} \tag{3.28}$$

where the absolute value is used because the determinants are positive.

This solution indicates, that the energy splitting can be given in the proposed form using the interface tension (2.18)

$$\Delta E = C\exp(-\sigma(L_1,L_2)L_1L_2).$$

Then, the interface tension is given by

$$\sigma(L_1,L_2)L_1L_2 = -\ln\Delta E + \ln C.$$

4

Expressing the energy splitting by integrals

The aim of this chapter is to find an expression to calculate the previously assessment for the energy splitting

$$\Delta E = 2e^{-H_0}\sqrt{\frac{H_0}{2\pi}}\left|\frac{\det' M}{\det M_0}\right|^{-1/2}. \tag{4.1}$$

Riemann zeta functions and heat kernels can express the determinants involved in (4.1). By taking into account, that there is a zero mode in $\det' M$, asymptotic behaviours of heat kernels can be used which go back to H. Weyl in 1911 [Wey11]. In this approach, the divergences can be handled. Especially, the heat kernels transform the problem into a problem of zeta-functions, which can be calculated via zeta-function regularization methods. It will be shown, that the expression

$$\ln\left|\frac{\det' M}{\det M_0}\right| \tag{4.2}$$

can be transformed into integrals, following [Mün89]. The calculation is explicitly given for $L \times L$ in the diploma thesis of P. Hoppe [Hop93]. This calculation will be redone, in order to ensure, that the structure of these integrals also hold in the geometric dependent setup. Finally, this chapter will show that only one of the three integrals must be recalculated in order to satisfy the geometric dependence for $L_1 \times L_2, L_1 \neq L_2$. This calculation is brought up in chapter 5.

In the preceding chapters, the expression for the fluctuation operator (3.17) was obtained:

$$
\begin{aligned}
M &= -\nabla^2 - \frac{m^2}{2} + \frac{g}{2}\phi_0^2 \\
&= -\nabla^2 - \frac{m^2}{2} + \frac{gv^2}{2}\tanh^2\left(\frac{m}{2}z\right) \\
&= -\nabla^2 - \frac{m^2}{2} + \frac{3}{2}m^2\tanh^2\left(\frac{m}{2}z\right) \\
&= -\nabla^2 + m^2 - \frac{3}{2}m^2 + \frac{3}{2}m^2\tanh^2\left(\frac{m}{2}z\right) \\
&= -\nabla^2 + m^2 - \frac{3}{2}m^2\operatorname{sech}^2\left(\frac{m}{2}z\right).
\end{aligned}
$$

The operator M_0 corresponds to the previously mentioned dilute gas approximation

$$M_0 = -\nabla^2 + m^2.$$

Defining the two dimensional Laplacian for the transverse modes

$$\Delta := -\partial_1\partial^1 - \partial_2\partial^2,$$

the fluctuation operator can be expressed as

$$M = \Delta + Q, \quad M_0 = \Delta + Q_0$$

with the z-component (in QFT time-like component) of the fluctuation operator

$$
\begin{aligned}
Q &= -\partial_z\partial^z + m^2 - \frac{3}{2}m^2\operatorname{sech}^2\left[\frac{m}{2}z\right], \\
Q_0 &= -\partial_z\partial^z + m^2.
\end{aligned}
$$

First of all, the methods for the following chapters shall be introduced.

4.1. Zeta function regularization and heat kernel methods

In order to evaluate the determinant of an operator, the spectrum of the operator can be used. For a matrix A the determinant is given in the following manner

$$\det A = \prod_{i=1}^{n} \lambda_i, \tag{4.3}$$

where $\lambda_i \in \mathbb{R}, i \in \{1, 2, \ldots, n\}$ is the discrete spectrum of A containing a finite number of eigenvalues $\lambda_i > 0$. The Riemann zeta function is defined as

$$\zeta(z) = \sum_{k=1}^{\infty} \frac{1}{k^z}$$

for $\Re(z) > 1$. An integral representation of the zeta-function is

$$\zeta(z) = \sum_k k^{-z} = \frac{1}{\Gamma(z)} \int_0^\infty \frac{\mathrm{d}t t^{z-1}}{\mathrm{e}^t - 1} = \frac{1}{\Gamma(z)} \sum_k \int_0^\infty \mathrm{d}t t^{z-1} \mathrm{e}^{-kt},$$

where the Γ-Function is defined as

$$\Gamma(z) = \int_0^\infty \mathrm{d}t t^{z-1} \mathrm{e}^{-t}.$$

Via analytic continuation (see reflection formula in appendix B.3) the zeta function for $z \in \mathbb{C} \backslash \{1\}$ can as well be defined. The derivative of the zeta function provides

$$\frac{\mathrm{d}}{\mathrm{d}z} \zeta(z) = -\sum_{k=1}^\infty \frac{\ln k}{k^z} \underset{z \to 0}{\longrightarrow} -\sum_{k=1}^\infty \ln k,$$

which means the zeta function can be used to evaluate the determinant of a matrix A defining a spectral version of the zeta function, in short *spectral zeta function*

$$\zeta_A(z) := \sum_{i=1}^n \frac{1}{\lambda_i^z}$$

by

$$\frac{\mathrm{d}}{\mathrm{d}z} \zeta_A(z) \Big|_{z=0} = -\sum_{i=1}^\infty \ln \lambda_i = -\ln \prod_{i=1}^\infty \lambda_i = -\ln \det A \tag{4.4}$$

using (4.3) in the last step because A is self-adjoint and thus independent from the chosen base.

By analogy with the handling of the matrix A, the same approach can be used for self-adjoint operators O. The product of the eigenvalues gives the determinant of this operator

$$\det O = \prod_i \lambda_i,$$

where $\lambda_i, i \in \mathbb{N}$ is the spectrum with $\lambda_i > 0$ for all $i \in \mathbb{N}$, which is independent from the chosen base, because O was defined to be self-adjoint. Often the spectrum of an operator is neither discrete nor finite, the main idea in order to evaluate the determinant, is to rewrite this expression in terms of an operator zeta function. This zeta function is defined by analogy with (4.3) for the operator O, where for a continuous spectrum the spectral density will be used

$$\zeta_O(z) := \mathrm{Tr}(O^{-z}) = \sum_{i=1}^\infty \frac{1}{\lambda_i^z}. \tag{4.5}$$

If the spectrum is not strictly positive, a shift can be done by adding a regularizing mass μ^2 to the eigenvalues. Nevertheless, the trace is also defined for continuous spectra. The last step in (4.5) is only defined for discrete finite spectra and to be understood symbolically, or as a definition, in other cases.

By taking the derivative at $z = 0$, the previous expression (4.4) can be regained for operators

$$\left.\frac{\mathrm{d}\zeta_O(z)}{\mathrm{d}z}\right|_{s=0} = \lim_{z\to 0} -\sum_{i=1}^{\infty} \lambda_i^{-s} \ln \lambda_i$$
$$= -\sum_{i=1}^{\infty} \ln \lambda_i = -\ln\left(\prod_{i=1}^{\infty} \lambda_i\right) = -\ln \det O.$$

Compendiously,

$$\ln \det O = \operatorname{Tr} \ln O \tag{4.6}$$
$$= -\left.\frac{\mathrm{d}\zeta_O(z)}{\mathrm{d}z}\right|_{z=0} \tag{4.7}$$

is achieved, as long as the operator zeta-function $\zeta_O(z)$ is well defined. Moreover, it is useful to define a *heat kernel*

$$K_t(A) := \operatorname{Tr} \mathrm{e}^{-tA}, \tag{4.8}$$

so that a suitable $t \in \mathbb{R}$ insures that the trace is well defined. The kernel defines a zeta function

$$\zeta_{K_t(A)}(z) = \frac{1}{\Gamma(z)} \int_0^{\infty} \mathrm{d}t t^{z-1} K_t(A), \tag{4.9}$$

because

$$\zeta'_{K_t(A)}(0) = -\ln \det A = -\ln \prod \lambda_i = -\sum \ln \lambda_i.$$

And with (4.7), it can be determined that

$$\operatorname{Tr} \ln A = -\zeta'_A(0) \tag{4.10}$$
$$= -\int_0^{\infty} \mathrm{d}t t^{-1} K_t(A), \tag{4.11}$$

where from now on, the operator zeta function of a heat kernel will be identified by $\zeta_A(z) := \zeta_{K_t(A)}(z)$.

As there are more operators involved in the following sections, the factorization properties of heat kernels will be useful. For two operators O_1 and O_2 the heat kernel factorizes due to the Baker-Campbell-Hausdorff formula

$$K_t(O_1 + O_2) = \operatorname{Tr} \mathrm{e}^{-t(O_1+O_2)} = \operatorname{Tr}\left(\mathrm{e}^{-tO_1} \mathrm{e}^{-tO_2} \mathrm{e}^{t^2[O_1,O_2]/2+\dots}\right).$$

Here, the last factor depends on convoluted commutators of the operators, so that for commutating operators

$$\begin{aligned} K_t(O_1 + O_2) &= \operatorname{Tr}\left(e^{-tO_1} e^{-tO_2}\right) = \operatorname{Tr}\left(e^{-tO_1}\right) \operatorname{Tr}\left(e^{-tO_2}\right) \\ &= K_t(O_1) K_t(O_2) \end{aligned} \tag{4.12}$$

the properties of the trace $\operatorname{Tr}(O_1 \otimes O_2) = \operatorname{Tr}(O_1)\operatorname{Tr}(O_2)$ in the last step are used. In this case, the exponential function provides the direct sum, which is the sum of the eigenvalues of the operators O_1 and O_2.

4.2. Transforming the determinants into integrals

From (4.1), the evaluation of the fraction of the determinants needs to be calculated. In the last section, it could be made obvious, that it is common for the evaluation determinants of operators containing an unbounded spectrum to use zeta function-regularizing techniques for expressions like

$$\ln \left| \frac{\det' M}{\det M_0} \right| \tag{4.13}$$

instead of using the expression in (4.1). For equation (4.13), there exists a representation in integrals, which will be developed in the following theorem.

Theorem 4.1: Transforming the determinants in integrals
The determinants in (4.1) *can be transformed in integrals according to*

$$\ln \left| \frac{\det' M}{\det M_0} \right| = - \frac{\mathrm{d}}{\mathrm{d}z} \zeta(z) \bigg|_{z=0} \tag{4.14}$$

with

$$\begin{aligned} \zeta(z) &= \zeta_1(z) + \zeta_2(z) + \zeta_3(z), \\ \zeta_1(z) &= \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \frac{L_1 L_2}{4\pi t} \left[\tilde{K}_t(Q) - 1\right], \\ \zeta_2(z) &= \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \left[K_t(\Delta) - 1\right], \\ \zeta_3(z) &= \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \left[\tilde{K}_t(\Delta) - \frac{L_1 L_2}{4\pi t}\right] \left[\tilde{K}_t(Q) - 1\right], \end{aligned}$$

where $\zeta_1(z)$ and $\zeta_2(z)$ are defined for $\Re(z) > 1$ and analytically continued to $z = 0$ and $\zeta_3(z)$ is valid for all z and the difference of the heat kernels $\tilde{K}_t(M) = K_t(M) - K_t(M_0)$.

The proof of this theorem will take several transformations, which involve studying the zero-modes of the operator M and M_0 as well as investigating the asymptotic behaviour of the involved heat kernels. At first, the zero-mode will be removed and the factorization property will be used.

LEMMA 4.2: FACTORIZATION OF HEAT KERNELS

Introducing a regularizing mass $\mu^2 > 0$ the expression (4.2) *can be rewritten in*

$$\ln \frac{\det' M}{\det M_0} = - \lim_{\mu \to 0} \left[\int_0^\infty \mathrm{d}t t^{-1} \tilde{K}_t(M + \mu^2) - \ln \mu^2 \right], \tag{4.15}$$

$$= - \frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \tilde{K}_t(M + \mu^2) \tag{4.16}$$

with where $\tilde{K}_t(M + \mu^2)$ is defined as

$$\tilde{K}_t(M + \mu^2) = \mathrm{e}^{-t\mu^2} K_t(\Delta) \left[K_t(Q) - K_t(Q_0) \right]. \tag{4.17}$$

Proof of lemma 4.2. In order to handle the zero mode, a regularizing mass μ^2 is introduced which is chosen to be arbitrary large to dissolve the zero mode of M. The shift in the spectrum of M and M_0 with μ^2 has been carried out in order to ensure that the spectrum is always positive. In order to calculate the left hand side of (4.14) the determinants are transformed into a trace according to (4.15) and the zero mode of M is split off

$$\ln \frac{\det' M}{\det M_0} = \mathrm{Tr}' \ln \frac{M}{M_0} \tag{4.18}$$

$$= \lim_{\mu \to 0} \left[\mathrm{Tr} \ln \left(\frac{M + \mu^2}{M_0 + \mu^2} \right) + \ln \mu^2 \right] \tag{4.19}$$

and following (4.11) the heat kernel can be identified

$$\ln \frac{\det' M}{\det M_0} = - \lim_{\mu \to 0} \left[\int_0^\infty \mathrm{d}t t^{-1} \tilde{K}_t(M + \mu^2) - \ln \mu^2 \right], \tag{4.20}$$

where $\tilde{K}_t(M + \mu^2)$ is defined as the difference of the heat kernels

$$\tilde{K}_t(M + \mu^2) := K_t(M + \mu^2) - K_t(M_0 + \mu^2) \tag{4.21}$$

$$= \mathrm{e}^{-t\mu^2} K_t(\Delta) \tilde{K}_t(Q), \tag{4.22}$$

where the fact that heat kernels factorize (4.12) was used, because all commutators are zero

$$K_t(M + \mu^2) = \mathrm{e}^{-t\mu^2} K_t(\Delta) K_t(Q). \tag{4.23}$$

□

In [Hop93] a proof is given, that expression (4.15) exists for $t \to \infty$ and $\mu \to 0$. The asymptotic behaviour of this expression for $t \to 0$ will be investigated later on. To achieve this, the heat kernel of the operator Q will be calculated at first.

Lemma 4.3: Heat kernel for the operator Q

Using the spectrum and the spectral densities of Q the limit $T \to \infty$ the heat kernel $\tilde{K}_t(Q)$ is given by

$$\tilde{K}_t(Q) = \operatorname{erf}(m_0\sqrt{t}) + \mathrm{e}^{-\frac{3}{4}m_0^2 t}\operatorname{erf}\left(\frac{m_0}{2}\sqrt{t}\right),$$

where $\operatorname{erf}(x)$ *denotes the Gaussian error function.*

Proof of lemma 4.3. First, the spectrum of Q is evaluated. Following [Hop93] and [MF53] the spectrum of Q and Q_0 can be evaluated, which is given by the eigenmode for translation

$$\epsilon_1 = 0 \tag{4.24}$$

and the discrete eigenmode

$$\epsilon_2 = \frac{3}{4}m^2, \tag{4.25}$$

corresponding to vibrational modes. The continuous part is given by

$$\epsilon_k = m^2 + k^2, \tag{4.26}$$

with the spectral density

$$g_0(p) = \frac{1}{2\pi}\left[T - 3m\frac{p^2 + \frac{1}{2}m^2}{\left(p^2 + \frac{1}{4}m^2\right)(p^2 + m^2)}\right] + \mathcal{O}(T^{-1}).$$

The spectrum of Q_0 can be obtained by solving the wave equation

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}\psi_n(z) = (\epsilon_n + m^2)\psi_n(z)$$

which gives

$$\epsilon_n = \left(\frac{2\pi}{T}n\right)^2 + m^2, \quad n \in \mathbb{Z}.$$

For large T, the spectrum goes over to a quasi-continuous spectrum

$$\epsilon_p = p^2 + m^2 \tag{4.27}$$

with the following spectral density

$$\tilde{g}_0(p) = \frac{T}{2\pi}.$$

The difference of the spectra is given by

$$g_0(p) - \tilde{g}_0(p) = \frac{1}{2\pi}\left[-3m\frac{p^2 + \frac{1}{2}m^2}{\left(p^2 + \frac{1}{4}m^2\right)(p^2 + m^2)}\right] + \mathcal{O}(T^{-1}), \tag{4.28}$$

where the lower orders can be neglected in the limit $T \to \infty$.

Using the eigenvalues ϵ_1 and ϵ_2 from (4.24) and (4.25) as well as spectral densities of Q and Q_0 from (4.28), the heat kernel $\tilde{K}_t(Q)$ in the limit $T \to \infty$ reads

$$\begin{aligned}\tilde{K}_t(Q) &= 1 + \mathrm{e}^{-3m^2/4} + \int_{-\infty}^{\infty} \mathrm{d}p \, [g_0(p) - \tilde{g}_0(p)] \, \mathrm{e}^{-t(p^2+m^2)} \\ &\overset{T\to\infty}{=} 1 + \mathrm{e}^{-\frac{3}{4}m^2 t} + \int_{-\infty}^{\infty} \mathrm{d}p g(p) \mathrm{e}^{-t(p^2+m^2)},\end{aligned} \tag{4.29}$$

where the spectral densities (4.28) can be used in the limit $T \to \infty$

$$g(p) = -\frac{m}{2\pi}\left(\frac{2}{p^2 + m_0^2} + \frac{1}{p^2 + \frac{m_0^2}{4}}\right). \tag{4.30}$$

These integrals (as shown in the appendix C) are given by

$$\int_{-\infty}^{\infty} \mathrm{d}x \frac{\mathrm{e}^{-t(x^2+a^2)}}{x^2 + a^2} = \frac{\pi}{a}\left[1 - \mathrm{erf}(a\sqrt{t})\right].$$

This simplifies the heat kernel to

$$\begin{aligned}K_t(Q) &= 1 + \mathrm{e}^{-\frac{3}{4}m^2 t} - \frac{2m}{2\pi}\frac{\pi}{m}(1 - \mathrm{erf}(m\sqrt{t})) - \mathrm{e}^{-\frac{3}{4}m^2 t}\frac{m}{2\pi}\frac{2\pi}{m}\left[1 - \mathrm{erf}(\frac{m}{2}\sqrt{t})\right] \\ &= \mathrm{erf}(m\sqrt{t}) + \mathrm{e}^{-\frac{3}{4}m^2 t}\,\mathrm{erf}\left(\frac{m}{2}\sqrt{t}\right).\end{aligned} \tag{4.31}$$

□

Remark 4.4. The asymptotic behaviour in the area $x \approx 0$ of the error function are given as

$$\mathrm{erf}(x) = \frac{2x}{\sqrt{\pi}} - \frac{2x^3}{3\sqrt{\pi}} + \mathcal{O}(x^5),$$

so that (4.31) conducts

$$\tilde{K}_t(Q) = \frac{3m}{\sqrt{\pi}}\sqrt{t} - \frac{3m^3}{3\sqrt{\pi}}t^{3/2} + \mathcal{O}(t^{5/2}), \tag{4.32}$$

where the series expansion of the exponential function

$$\exp(-x) = 1 - x - \mathcal{O}(x^2)$$

is used as well.

In the limit $t \to 0$, the asymptotic behaviour of the heat kernels are given by the Weyl law [Wey11]. A physical reasoning of this law can be found in the article 'Can one hear the shape of a drum?' by Marc Kac [Kac66]. Heat kernels can be treated like the integral kernel of the heat equation, therefore, physically, the limit $t \to 0$ represents the initial state. Imagining, that the initial state of a heat source can be described by a Dirac δ-function, the boundaries of the system play no role in the limit $t \to 0$. This is similar to a diffusion equation in statistical physics, where these thoughts can be as well applied.

Lemma 4.5: Asymptotic behaviour of the heat kernel
In the limit $t \to 0$ the asymptotic expression of the heat kernels are given by

$$\tilde{K}_t(M + \mu^2) = \frac{L_1 L_2}{\sqrt{4\pi t}}(a_1 + a_0 t) + \mathcal{O}(t^{3/2}),$$

with

$$a_1 = \frac{3m}{2\pi}, \qquad a_0 = -\frac{3m}{2\pi}\left(\frac{1}{2}m_0^2 + \mu^2\right).$$

Proof of lemma 4.5. In Remark 4.4, the heat kernel of $\tilde{K}_t(Q)$ was observed to behave like

$$\tilde{K}_t(Q) \quad \overset{t\to 0}{\sim} \quad t^{1/2}.$$

The limit for the $\mathrm{e}^{-t\mu^2}$ part is due to the exponential function

$$\mathrm{e}^{-t\mu^2} = 1 - t\mu^2 - \mathcal{O}(t^2) \tag{4.33}$$

so that

$$e^{-t\mu^2} \overset{t\to 0}{\sim} 1.$$

This leads to the fact that the heat kernel of the Laplacian is viewed asymptotically. Here, the Weyl formula applies [ANPS09]

$$K_t(\Delta) = \frac{|\Omega|}{4\pi t} + \alpha + \mathcal{O}(t), \tag{4.34}$$

where $\Omega = L_1 L_2$ is the area of integration and α is a constant not needed. Consequently,

$$K_t(\Delta) \overset{t\to 0}{\sim} t^{-1}.$$

Therefore, combing the above asymptotic behaviour for $t \to 0$ leads to

$$\frac{\tilde{K}(M+\mu^2)}{t} \overset{t\to 0}{\sim} t^{-3/2},$$

implying the integral diverges at $t = 0$. To handle this divergency, the asymptotic behaviour is examined later on in detail.

Combining the asymptotic expression of the heat kernel of Q (4.32) and the series expansion of $e^{-t\mu^2}$ (4.33)

$$e^{-\mu^2 t}\tilde{K}_t(Q) = \left[\frac{3m}{\sqrt{\pi}}\sqrt{t} - \frac{3m}{\sqrt{\pi}} t^{3/2}\left(\frac{1}{2}m^2 + \mu^2\right)\right] + \mathcal{O}(t^{5/2})$$

with (4.34), the term

$$\tilde{K}_t(M+\mu^2) = \frac{L_1 L_2}{\sqrt{4\pi t}}\left[\frac{3m}{2\pi} - \frac{3m}{2\pi} t\left(\frac{1}{2}m^2 + \mu^2\right)\right] + \mathcal{O}(t^{3/2})$$

is found. For the integrand of the zeta function with

$$a_1 = \frac{3m}{2\pi}, \qquad a_0 = -\frac{3m}{2\pi}\left(\frac{1}{2}m_0^2 + \mu^2\right)$$

is

$$t^{z-1}\tilde{K}_t(M+\mu^2) = \frac{L_1 L_2}{\sqrt{4\pi}} t^{z-1/2}\left(a_1 \frac{1}{t} + a_0 + a_{-1} t + \mathcal{O}(t^2)\right).$$

□

Sequentially, the determined expression for the asymptotic expansion of the heat kernels will be used to split the integrands diverging parts from the non diverging parts in the limits $t \to 0$ and $\mu^2 \to 0$

Lemma 4.6: Separating the diverging parts

Using the asymptotic expansion derived in Lemma 4.5 the searched expression can be transformed into

$$\ln \frac{\det' M}{\det M_0} = -\left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0} \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \left[\tilde{K}_t(M) - 1\right], \tag{4.35}$$

where $\tilde{K}_t(M)$ is the difference of the heat kernels of $K_t(M)$ and $K_t(M_0)$.

Proof of lemma 4.6. The asymptotical observations in Lemma 4.5 mean, that the divergencies, which come from $\mu \to 0$, can be isolated. The terms diverging for $t \to 0$ are separated with $\hat{a}_1 := a_1 \frac{L_1 L_2}{\sqrt{4\pi}}$ from (4.35) reads

$$\zeta_{M+\mu^2}(z) = \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \tilde{K}_t(M+\mu^2) \tag{4.36}$$

$$\begin{aligned} &= \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \Big\{ \tilde{K}_t(M+\mu^2) - \mathrm{e}^{-t\mu^2} \\ &\qquad - \Theta(1-t) \left[\hat{a}_1 t^{-1/2} - \mathrm{e}^{-t\mu^2}\right] \Big\} \\ &\quad + \underbrace{\frac{1}{\Gamma(z)} \hat{a}_1 \int_0^1 \mathrm{d}t t^{z-3/2}}_{=:I_1(z)} + \underbrace{\frac{1}{\Gamma(z)} \int_1^\infty \mathrm{d}t t^{z-1} \mathrm{e}^{-t\mu^2}}_{=:I_2(z)}, \end{aligned} \tag{4.37}$$

where Θ denotes the step function with $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for $x \le 0$. The separation has been executed between the $t \in [0,1]$ interval and the $t \in [1,\infty]$ interval. In the $t \in [0,1]$ interval the asymptotic behaviour of Lemma 4.5 has been used. Combining the two intervals (4.36) is regained. Incidentally, the derivative

$$\begin{aligned} \left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0} \frac{1}{\Gamma(z)} I(z) &= \lim_{z=0} \left(\frac{1}{\Gamma'(z)} I(z) + \frac{1}{\Gamma(z)} I(z) \right) \\ &= \lim_{z=0} I(z) \end{aligned}$$

with an integral $I(z)$ will often be used, where the identities of the gamma function were used according to appendix B.1.

The last integral now will be evaluated. Since it converges for $z = 0$, the derivative can be taken

$$\begin{aligned} \left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0} I_2(z) = \left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0} \frac{1}{\Gamma(z)} \int_1^\infty \mathrm{d}t t^{z-1} \mathrm{e}^{-t\mu^2} &= \int_1^\infty \mathrm{d}t t^{-1} \mathrm{e}^{-t\mu^2} \\ &= -\gamma - \ln \mu^2 + \mathcal{O}(\mu^2). \end{aligned} \tag{4.38}$$

The last step results from the exponential integral Ei(x) and it's series expansion (see e.g. [BMMS13])

$$\mathrm{Ei}(x) = -\int_{-x}^{\infty} \mathrm{d}t \frac{\mathrm{e}^{-t}}{t} \approx \gamma + \ln x + \mathcal{O}(x),$$

where $\gamma = 0.5772\ldots$ is the Euler-Mascheroni constant. The second integral in (4.37) will be evaluated for $z > 1/2$

$$I_1(z) = \frac{1}{\Gamma(z)} \hat{a}_1 \int_0^1 \mathrm{d}t t^{z-3/2} = \frac{1}{\Gamma(z)} \hat{a}_1 \frac{2}{2z-1} \tag{4.39}$$

The derivative at $z = 0$ is with abuse of the condition $\Re(z) > 1/2$ (for details see Remark 4.7)

$$\left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0} \frac{2}{2z-1} = -4$$

so that

$$\left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0} I_1(z) = \left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0} \frac{1}{\Gamma(z)} \hat{a}_1 \int_0^1 \mathrm{d}t t^{z-3/2} = -4\hat{a}_1. \tag{4.40}$$

The first integral of (4.37) is renamed

$$\tilde{\zeta}_\mu(z) = \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \Big\{ \tilde{K}_t(M+\mu^2) - \mathrm{e}^{-t\mu^2} - \Theta(1-t) \left[\hat{a}_1 t^{-1/2} - \mathrm{e}^{-t\mu^2} \right] \Big\},$$

where the index shows the value of the regularising mass μ^2. Furthermore, it defines a new zeta function $\tilde{\zeta}'_\mu(z)$. For $t > 1$, the above integral gives, due to the properties of the step function,

$$\tilde{\zeta}'_\mu(z) := \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \left[\tilde{K}_t(M+\mu^2) - \mathrm{e}^{-t\mu^2} \right]. \tag{4.41}$$

This means, that including the values for $t \leq 1$ from the step function

$$\tilde{\zeta}'_\mu(z) = \tilde{\zeta}_\mu(z) + \frac{1}{\Gamma(z)} \int_0^1 \mathrm{d}t t^{z-1} \left[\hat{a}_1 t^{-1/2} - \mathrm{e}^{-t\mu^2} \right]$$

and, because the diverging parts have been split off, the limit $\mu = 0$ can be taken here

$$\tilde{\zeta}'_0(z) = \tilde{\zeta}_0(z) + \frac{1}{\Gamma(z)} \int_0^1 \mathrm{d}t t^{z-1} \left[\hat{a}_1 t^{-1/2} - 1 \right]$$

where again for $\Re(z) > 1/2$

$$\frac{1}{\Gamma(z)} \int_0^1 \mathrm{d}t t^{z-1} \left[\hat{a}_1 t^{-1/2} - 1\right] = \frac{1}{\Gamma(z)} \left(\frac{2\hat{a}_1}{2z-1} - \frac{1}{z} \right)$$
$$= \frac{1}{\Gamma(z)} \frac{2\hat{a}_1}{2z-1} - \frac{1}{\Gamma(z+1)},$$

using $z\Gamma(z) = \Gamma(z+1)$. Now taking the derivative, the first part equals (4.39), giving

$$\frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \left(\frac{1}{\Gamma(z)} \frac{2\hat{a}_1}{2z-1} - \frac{1}{\Gamma(z+1)} \right) = -4\hat{a}_1 - \gamma. \tag{4.42}$$

(see appendix B.1). This concludes

$$\frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \tilde{\zeta}'_0(z) = \frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \tilde{\zeta}_0(z) - 4\hat{a}_1 - \gamma. \tag{4.43}$$

Remembering (4.15),

$$\begin{aligned}
\ln \frac{\det' M}{\det M_0} &= - \lim_{\mu \to 0} \left[\int_0^\infty \mathrm{d}t t^{-1} \tilde{K}_t(M + \mu^2) - \ln \mu^2 \right] \\
&\overset{(4.36)}{=} - \lim_{\mu \to 0} \left[\frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \zeta_{M+\mu^2}(z) - \ln \mu^2 \right] \\
&\overset{(4.37)(4.38)}{=} - \frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \tilde{\zeta}_0(z) + 2\hat{a}_1 + \gamma + \lim_{\mu \to 0} \left(\ln \mu^2 - \ln \mu^2 \right) \\
&\overset{(4.43)}{=} - \frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \tilde{\zeta}'_0(z)
\end{aligned}$$

can be found. Conclusively, this means, with the definition of (4.41), in the limit $\mu \to 0$

$$\ln \frac{\det' M}{\det M_0} = - \frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \left[\tilde{K}_t(M) - 1 \right], \tag{4.44}$$

which concludes Lemma 4.6. □

Remark 4.7. The integrals in (4.40) and (4.42) were not defined for $z = 0$, thus the solution

$$\frac{\mathrm{d}}{\mathrm{d}z}\bigg|_{z=0} \int_0^1 \mathrm{d}t t^{z-3/2} = 4$$

is not valid for $\Re(z) < 1/2$ and requires a study of their analytic continuation to $\Re(z) < 1/2$ or a dimensional renormalisation. But this is not necessary, because in the final conclusion both of these integrals indicated with value 4 cancel out.

Now a simple expression of the heat kernel is found that can be used to separate the z-direction from the other directions. The following proof will complete Theorem 4.1.

Proof of theorem 4.1. With $K_t(M) = K_t(Q)K_t(\Delta)$ the z-direction can be split off far away from the other spatial directions

$$\tilde{\zeta}'(z) = \zeta_1(z) + \zeta_2(z) + \zeta_3(z) \tag{4.45}$$

where

$$\zeta_1(z) = \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \frac{L_1 L_2}{(4\pi t)} \left[\tilde{K}_t(Q) - 1\right], \tag{4.46}$$

$$\zeta_2(z) = \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \left[K_t(\Delta) - 1\right], \tag{4.47}$$

$$\zeta_3(z) = \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \left[\tilde{K}_t(\Delta) - \left(\frac{L_1 L_2}{4\pi t}\right)\right] \left[\tilde{K}_t(Q) - 1\right], \tag{4.48}$$

where in the symmetric case $L \times L$ the heat kernel of the Laplacian $K_t(\Delta)$ can be identified with the Jacobi θ-function

$$\theta(z) = \sum_{n \in \mathbb{Z}} \mathrm{e}^{-\pi n^2 z} = z^{-1/2} \theta(1/z).$$

The left hand side of (4.45), the zeta function (4.44), can be achieved by summing the three above integrals. ∎

4.3. Calculating the interface tension

In the following, the previously obtained integrals will be evaluated. It can be seen, that the structure of the integrals ζ_1 and ζ_3 is not changing by reconsidering the geometry of the system. Thus, the solution of these integrals can be taken from the previous literature.

Contribution of $\zeta_1(z)$

From (4.29) with $A := L_1 L_2$ the integration can be done

$$\begin{aligned}
\zeta_1(z) &= \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} L_1 L_2 (4\pi t)^{-1} \left[\tilde{K}_t(Q) - 1\right] \\
&= \frac{L_1 L_2}{4\pi\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-2} \mathrm{e}^{-3m^2 t/4} + \frac{L_1 L_2}{4\pi\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-2} \int_{-\infty}^\infty \mathrm{d}p g(p) \mathrm{e}^{-t(m^2+p^2)}
\end{aligned}$$

This integral is solved in [Mün89] in four dimensions and in [Mün90] in three dimensions for the case $L = L_1 = L_2$. Another approach involving residue calculus and the properties of the complex logarithm will be shown in appendix D. This provides the solution

$$\left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0} \zeta_1(z) = -\frac{L_1 L_2}{4\pi} m^2 \left(3 + \frac{3}{4}\ln 3\right) \tag{4.49}$$

With $L_1 = L_2 = L$, it can be observed that the geometrical dependence does not change the solution, which was obtained before.

Contribution of $\zeta_2(z)$

The contribution of $\zeta_2(z)$ is given by

$$\zeta_2(z) = \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} \left[K_t(\Delta) - 1\right]. \tag{4.50}$$

The heat kernel $K_t(\Delta)$, which is by knowing the eigenvalues of the Laplacian

$$\begin{aligned} K_t(\Delta) &= \mathrm{Tr}\, \mathrm{e}^{-t\Delta}, \\ &= \sum_{n_1,n_2} \mathrm{e}^{-\lambda_{n_1,n_2} t}, \end{aligned} \tag{4.51}$$

where the eigenvalues are given by

$$\lambda_{n_1,n_2} = (2\pi)^2 \left[\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2}\right].$$

In (4.50), the zero-mode of (4.51) for $n_1 = n_2 = 0$ is avoided by the subtraction of 1, so ζ_2 reads

$$\begin{aligned} \zeta_2(z) &= \frac{1}{\Gamma(z)} \sum_{n_1,n_2}{}' \int_0^\infty \mathrm{d}t t^{z-1} \mathrm{e}^{-\lambda_{n_1,n_2} t} \\ &= \frac{1}{\Gamma(z)} \sum_{n_1,n_2}{}' \lambda_{n_1,n_2}^{-z} \int_0^\infty \mathrm{d}t t^{z-1} \mathrm{e}^{-t}, \end{aligned}$$

where the integral is exactly the gamma function that cancels out. Therefore,

$$\begin{aligned} \zeta_2(z) &= \sum_{n_1,n_2}{}' \lambda_{n_1,n_2}^{-z} \\ &= (2\pi)^{-2z} \sum_{n_1,n_2}{}' \left[\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2}\right]^{-z} \end{aligned} \tag{4.52}$$

needs to be calculated. In the case of $L_1 = L_2 = L$, this function is called Epstein-Zeta function and has been calculated before. In the diploma thesis [Hop93], an explicit calculation can be found. In [Eli95], another approach can be found. The result in this literature is

$$\left.\frac{\mathrm{d}\zeta_2}{\mathrm{d}z}\right|_{z=0} = -\ln\frac{L^2}{4\pi} + 2\ln\left[\sqrt{2}\frac{\Gamma(3/4)}{\Gamma(1/4)}\right]. \tag{4.53}$$

$$\approx -\ln\frac{L^2}{4\pi} - 1.47634\ldots. \tag{4.54}$$

The result implies, that there will be a similar first term $\sim \ln L_1L_2$ and a term, which is depending on the geometric dependence of the problem, which must result in the second term of (4.53) for $L_1 = L_2$. Thus for $L_1 \neq L_2$ equation (4.52) needs another calculation which will be done in the next chapter, including this geometric dependence.

Contribution of $\zeta_3(z)$

The $\zeta_3(z)$ contribution in [Mün90] is given by

$$\left.\frac{\mathrm{d}}{\mathrm{d}z}\right|_{z=0}\zeta_3(z) = 2\sqrt{\frac{\sqrt{3}Am}{\pi}}\mathrm{e}^{-\sqrt{3}mA/2} + \text{faster decreasing terms.}$$

In this calculation the properties of the Jacobi θ function were used, which do not apply in the present case, because there is no fixed L in both spacial directions. Nevertheless, it can be observed, that for large L, therefore for large $L \sim \sqrt{A} = \sqrt{L_1L_2}$ this term vanishes. This observation will not be proved in detail here. These calculations of $\zeta_1(z)$ and $\zeta_3(z)$ leave the $\zeta_2(z)$ contribution to be calculated.

4.3.1. Dimensional renormalization

The interface tension shall now be evaluated in dependence of physical quantities. These are given by the system area L_1L_2, the inverse mass m_R^{-1} as the correlation length, and the renormalized coupling g_R. In the proceeding, the broken phase is observed in first loop order. The relevant renormalization was derived in one loop order in [Mün90], explicit calculations are given for instance in [GKM96] and in the diploma thesis of M. Köpf [Köp08]. Setting the extra dimension $d = 4 - \epsilon$ in $L = \sqrt{L_1L_2}$, all equations in these works stay invariant. Therefore, the calculations will not be given in detail here. The renormalized coupling is given by

$$g = g_R\left(1 + \frac{7}{4}\frac{u_R}{8\pi}\right),$$

the renormalized mass is given by

$$m^2 = m_R^2\left(1 - \frac{3}{8}\frac{u_R}{8\pi}\right)$$

with the dimensionless coupling

$$u_R = \frac{g_R}{m_R}.$$

The aim is to give the dimensionless coupling u_R in first order. In this one loop scheme, no orders above $\mathcal{O}(u_R)$ fall into place. The energy of a kink

$$H_0 = \frac{2Am^3}{g}$$

shall be expressed by the renormalized values. Therefore, a series expansion up to the first order is used for the mass

$$\begin{aligned} m &= m_R\sqrt{1 - \frac{3}{8}\frac{u_R}{8\pi}} = 1 - \frac{3}{128\pi}u_R + \mathcal{O}(u_R^2) \qquad (4.55)\\ \Rightarrow \quad m^3 &= m_R^3\left(1 - \frac{3}{128\pi}u_R + \mathcal{O}(u_R^2)\right)^3 \\ &= m_R^3\left(1 - \frac{9}{128\pi}u_R + \mathcal{O}(u_R^2)\right) \end{aligned}$$

and the coupling constant

$$\frac{1}{g} = \frac{1}{g_R}\left(1 - \frac{7}{32\pi}u_R + \mathcal{O}(u_R^2)\right).$$

Now the dimensionless constant becomes

$$\begin{aligned} \frac{m^3}{g} &= \frac{m_R^3}{g_R}\left(1 - \frac{9}{128\pi}u_R + \mathcal{O}(u_R^2)\right)\left(1 - \frac{7}{32\pi}u_R + \mathcal{O}(u_R^2)\right) \\ &= \frac{m_R^3}{g_R}\left(1 - \frac{37}{128\pi}u_R + \mathcal{O}(u_R^2)\right). \qquad (4.56) \end{aligned}$$

4.3.2. Geometric independence of the interface tension

The contributions of to the energy splitting of $\zeta_1(z)$ and $\zeta_3(z)$ were obtained before. The contribution of $\zeta_2(z)$ contained a term dependent on the system size and another term independent of the system size for $L_1 = L_2 = L$. Assuming, for the setup $L_1 \neq L_2$, this will lead to a part depending on the system size and another term depending on the aspect ratio L_1/L_2 of the system. The contribution of $\zeta_2(z)$ has as well been seen only in the prefactor. Thus, in this section, it will be assumed that again only the prefactor changes because the analytic calculation of $\zeta_2(z)$ in [Mün90] was similar. The derivative of the sum over the eigenvalues λ_{n_1,n_2} will as well give a logarithmic contribution, depending on the geometric dependence of the system which will expressed by the aspect ratio $\tau = \mathrm{i}L_1/L_2$. Thus, the prefactor is $C(\tau)$ in [Mün90]

$$\Delta E = C(\tau)\exp(-\sigma(A)A), \qquad (4.57)$$

setting $A := \sqrt{L_1 L_2}$. In conclusion, the exponent of the energy splitting (4.1)

$$\Delta E = 2\mathrm{e}^{-H_0}\sqrt{\frac{H_0}{2\pi}}\left|\frac{\det' M}{\det M_0}\right|^{-1/2}$$

can be calculated now depending only on $\zeta_1(z)$. Here, $H_0 = 2Am^3/g$ and

$$\ln\left|\frac{\det' M}{\det M_0}\right| = -\frac{\mathrm{d}}{\mathrm{d}z}\zeta_1(z)\bigg|_{z=0} - \frac{\mathrm{d}}{\mathrm{d}z}\zeta_2(z)\bigg|_{z=0} - \frac{\mathrm{d}}{\mathrm{d}z}\zeta_3(z)\bigg|_{z=0}.$$

It has been observed that $\zeta_3(z)$ contains no relevant contribution to the interface tension. The following results were obtained for

$$\zeta_1'(0) = -\frac{A}{4\pi}m^2\left(3 + \frac{3}{4}\ln 3\right)$$

with $A = L_1 L_2$. and in [Mün90]

$$\zeta_2'(0) = -\ln\frac{A}{4\pi} - B(\tau),$$

where $B(\tau)$ is still to be calculated, because of the geometric dependence of this factor. Therefore, the determinants become

$$\begin{aligned}\left|\frac{\det' M}{\det M_0}\right|^{-1/2} &= \exp\left[-\frac{A}{8\pi}m^2\left(3 + \frac{3}{4}\ln 3\right) - \frac{1}{2}\ln\frac{A}{4\pi} - \frac{B(\tau)}{2} + \dots\right] \\ &= \frac{\mathrm{e}^{-B(\tau)/2}}{\sqrt{\frac{A}{4\pi}}}\exp\left[-\frac{A}{8\pi}m^2\left(3 + \frac{3}{4}\ln 3\right) + \dots\right].\end{aligned}$$

This means, the energy splitting is given by

$$\begin{aligned}\Delta E &= 2\sqrt{\frac{2Am^3}{2\pi g}}\frac{\mathrm{e}^{-B(\tau)/2}}{\sqrt{\frac{A}{4\pi}}}\exp\left[-\frac{2Am^3}{g} - \frac{A}{8\pi}m^2\left(3 + \frac{3}{4}\ln 3\right) + \dots\right] \\ &= 4\sqrt{\frac{2m^3}{g}}\frac{\mathrm{e}^{-B(\tau)/2}}{\sqrt{2}}\exp\left[-\frac{2Am^3}{g} - \frac{A}{8\pi}m^2\left(3 + \frac{3}{4}\ln 3\right) + \dots\right] \\ &= C(\tau)\exp(\sigma_\infty A),\end{aligned}$$

where

$$\begin{aligned}\sigma_\infty &= \lim_{A\to\infty}\frac{1}{A}\sigma(A) = \lim_{A\to\infty}\left(\frac{2m^3}{g} + \frac{m^2}{8\pi}\left(3 + \frac{3}{4}\ln 3\right) + \dots\right) \\ &= \frac{2m^3}{g} + \frac{m^2}{8\pi}\left(3 + \frac{3}{4}\ln 3\right).\end{aligned}$$

In a last step, this interface tension is expressed by the physical variables achieved by dimensional renormalization. It follows with (4.56) and (4.55)

$$\begin{aligned}
\sigma_\infty &= \frac{2m^3}{g} + \frac{m^2}{8\pi}\left(3 + \frac{3}{4}\ln 3\right) \\
&= 2\frac{m_R^3}{g_R}\left(1 - \frac{37}{128\pi}u_R + \mathcal{O}(u_R^2)\right) + m_R^2\left(1 - \frac{3}{128\pi}u_R\right)8\pi\left(3 + \frac{3}{4}\ln 3\right) \\
&= 2\frac{m_R^2}{u_R} - \frac{37}{64\pi}m_R^2 + m_R^2\frac{1}{8\pi}\left(3 + \frac{3}{4}\ln 3\right) - m_R^2 u_R \frac{3}{128\pi}\frac{1}{8\pi}\left(3 + \frac{3}{4}\ln 3\right) \\
&= 2\frac{m_R^2}{u_R}\left(1 - \frac{u_R}{4\pi}\left(\frac{13}{32} + \frac{3}{16}\ln 3\right) + \mathcal{O}(u_R^2)\right).
\end{aligned}$$

This is precisely the result obtained in [Mün90]. Nevertheless, the precise calculation for the case $L_1 = L_2 = L$ in [Hop93] indicates, that the interface tension will not change under other geometries. But the prefactor C can contain a dramatic change for the energy splitting, thus for the correlation length of the system. With these calculations it should be clear, that for the case with geometric dependence on a $L_1 \times L_2$ geometry, the prefactor must follow two restrictions:

- It must provide the result (4.53) for $L_1 = L_2$, which means for the aspect ratio $\tau = \mathrm{i}$. This indicates, that the theory can still be evaluated in the scheme of zeta regularization techniques.
- A certain modular invariance must be given, as the system is invariant under the change of $L_1 \leftrightarrow L_2$, which means, that the prefactor must be the same for $\tau \to 1/\tau$.

These considerations will lead to the formulation of the theory for the geometric dependence of the Laplace operator under the modular invariance $\tau \to 1/\tau$.

5

The determinant of the Laplace operator

In the last chapter, the integral ζ_2, which is the determinant of the two dimensional Laplacian, was identified to play the key role for the geometric dependence. In the literature, there are some approaches to calculate the determinant of the Laplacian that will be used here. The first approach is due to D. B. Ray and I. M. Singer [RS73] and in physics C. Itzykson and J.-B. Zuber [IZ86]. Mathematically, this approach is even older, going back to the Kronecker limit formula [Sie61]. Thus, this calculation will need a deep knowledge of special functions, many properties are given in the appendix B. Then, the calculation is some kind of straight forward and easy to understand. By this connection it this calculation will be subsumed under the title Kronecker limit formula.

The second approach uses less constructions over special functions, but a many properties of complex integrals and complex analysis, mostly governed by the Cauchy residue theorem. The key idea is due to [Pol86] a Sommerfeld-Watson transformation. Therefore, this section is named after this transformation.

The last approach on the determinant differs completely from the other two. In this approach the structural analogy to a Bosonic string will be used in order to evaluate the upcoming expressions and the Laplacian will be identified with an infinite set of harmonic oscillators coming from the massless Klein-Gordon equation. This approach is motivated by J. Baez [Bae98a, Bae98b].

Calculating the determinant of the Laplacian on an infinite plane, the plane is equivalent to a sphere, which is a Riemanian surface. In the context of critical phenomena, the simplest non-spherical case of a Riemanian surface is a torus, which is identical to a plane with periodic boundary conditions in two directions. The two directions are separated in a holomorphic and anti-holomorphic sector. The interactions between these sectors are revealed by modular transformations [DFMS97]. The torus can be imagined as the plane with periodic boundaries, where one direction is transformed by an exponential transformation into a circle, which leads to a cylinder. In the other direction, the periodic boundary conditions also apply, so that the endings of the cylinder are connected leaving the form of a torus (see figure 5.1). This transformation is a conformal mapping,

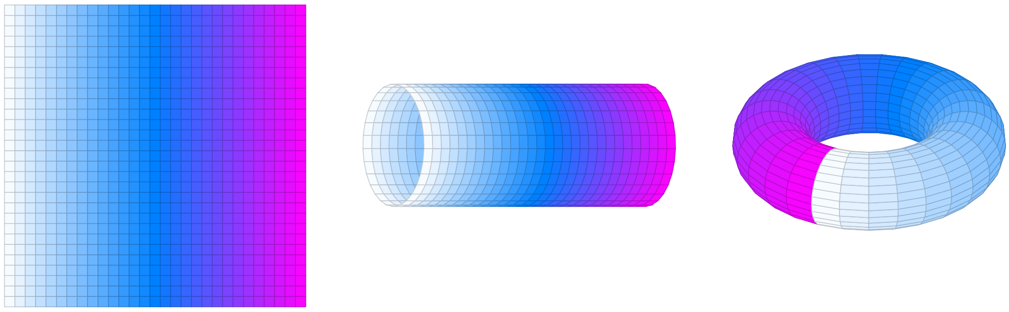

Figure 5.1.: Transforming a plane with periodic boundary conditions into a torus.

leaving angles and local distances preserved but not distances at all. Thus, the torus can be defined by two independent lattice vectors on a plane. On the complex plane, these vectors are represented by two complex numbers ω_1 and ω_2, where the area of the torus is $A = \Im(\omega_2\bar{\omega}_1)$. The modular ratio therefore is $\tau = \omega_2/\omega_1$. Under the imposed periodic conditions in x_1 and x_2, direction the functional is invariant with respect to translations by the periods ω_1 and ω_2.

5.1. Kronecker limit formula

In this system, the function is restricted on asymmetric domains $L_1 \times L_2$ periodic boundaries. This calculation follows the work of C. Itzykson and J.-B. Zuber [IZ86] and is presented more detailed in the textbook [DFMS97]. Historically this method follows an approach in mathematics outlined by D. B. Ray and I. M. Singer 'Analytic Torsion on two dimensional manifold' using the Selberg trace [Sel56] which serves as an analogy to the Poisson summation formula used in [Mün89]. The eigenfunctions of the Laplacian Δ for a system with periodic boundaries are given by the equation

$$\Delta\varphi(x_1, x_2) = \lambda_{n_1,n_2}\varphi(x_1, x_2)$$

where the eigenvalues λ_{n_1,n_2} are given by

$$\lambda_{n_1,n_2} = (2\pi)^2 \left[\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2}\right]. \tag{5.1}$$

By introducing the values

$$\begin{aligned} & \omega_1 = L_1, \qquad \omega_2 = \mathrm{i}L_2 \\ \text{with} \quad & \bar{\omega}_1 = \omega_1, \qquad \bar{\omega}_2 = -\omega_2 \end{aligned}$$

a lattice Λ can be defined on a torus $\mathbb{T} = \mathbb{C}/\Lambda$

$$\Lambda = \{\omega_1 n + \omega_2 m | n, m \in \mathbb{Z}\}.$$

The dual lattice Λ^* is then given by the generators

$$k_1 = -i\frac{\omega_2}{A}, \qquad k_2 = i\frac{\omega_1}{A}$$
$$\text{with} \qquad \bar{k}_1 = k_1, \qquad \bar{k}_2 = -k_2,$$

where $A = \operatorname{Im}\omega_2\overline{\omega_1}$ is the area $A = L_1 L_2$, which remains invariant under the modular transformation. The eigenvalues take the form

$$(2\pi)^2 \left[\left(\frac{n_1 L_2}{A}\right)^2 + \left(\frac{n_2 L_1}{A}\right)^2\right] = (2\pi)^2 \left[\left(\frac{i n_1 \omega_2}{A}\right)^2 + \left(\frac{n_2 \omega_1}{A}\right)^2\right]$$

which can be rewritten in terms of the dual lattice

$$\left(\frac{2\pi}{A}\right)^2 \left[-n_1^2{\omega_2}^2 + n_2^2\omega_1^2\right] = \left(\frac{2\pi}{A}\right)^2 |n_1\omega_2 - n_2\omega_1|^2 . \tag{5.2}$$

Keeping in mind that $\omega_2 \in \mathrm{i}\mathbb{R}$, resulting in $\bar{\omega}_2 = -\omega_2$, now the eigenvalues (5.1), become

$$\lambda_{n_1,n_2} = (2\pi)^2 |n_1 k_1 + n_2 k_2|^2 = (2\pi/A)^2 |n_1\omega_2 - n_2\omega_1|^2 .$$

The modular ratio is given by $\tau = \omega_2/\omega_1 = iL_1/L_2$, which can be transformed in the following way

$$\tau^{-1} = \omega_1/\omega_2 = -k_2/k_1 = \tau_k.$$

Introducing the modular ratio $\tau = \omega_2/\omega_1$, the sum over the eigenvalues (4.52) can be expressed by

$$-\frac{1}{2}\ln\det{}'\Delta = \sum \ln \lambda_{n_1,n_2}^{-1/2} = \frac{1}{2}G'(0) \tag{5.3}$$

with the Eisenstein series

$$G(s) = \left|\frac{A}{2\pi\omega_1}\right|^{2s} \sum_{m,n}{}' \frac{1}{|m+n\tau|^{2s}}. \tag{5.4}$$

Now the equivalence of the right hand side of (5.3) to (4.52) can be proven

$$\frac{1}{2}G'(s) = \left|\frac{A}{2\pi\omega_1}\right|^{2s} \log\left(\frac{A}{2\pi\omega_1}\right) \sum_{m,n}{}' \frac{1}{|m+n\tau|^{2s}} - \left|\frac{A}{2\pi\omega_1}\right|^{2s} \sum_{m,n}{}' \frac{\log|m+n\tau|}{|m+n\tau|^{2s}}$$

and

$$\frac{1}{2}G'(0) = \sum_{m,n}{}' \log\frac{A}{2\pi\omega_1|m+n\tau|},$$

so that

$$\exp(\frac{1}{2}G'(0)) = \prod_{m,n} \frac{\frac{A}{2\pi\omega_1}}{|m+n\tau|}.$$

Conclusively, the Eisenstein series given in (5.4) can be used to evaluate the sum. The function $G(s)$ is analytic for $\operatorname{Re} s > 1$ but can be continued [DFMS97]. Defining

$$\begin{aligned} G(s) &= \left(\frac{4\pi^2}{\tau_2^2}\right)^{-2s} \sum_{n,m}{}' \left[(m+n\tau)\right]^{-2s} \\ &= \left(\frac{4\pi^2}{\tau_2^2}\right)^{-2s} \left\{ 2\zeta(2s) + \sum_n{}' \left(\sum_m \left[(m+n\tau)\right]^{-2s} \right) \right\}, \end{aligned} \tag{5.5}$$

where $\zeta(s)$ is the Riemann ζ-function with $\tau = \tau_1 + i\tau_2$. Due to the representations of the cotangent [BMMS13], the first step is achieved by

$$\pi\cot(\pi z) = \frac{1}{z} + \sum_{d=1}^{\infty} \left(\frac{1}{z-d} + \frac{1}{z+d} \right)$$

$$\pi\cot(\pi z) = \pi i - 2\pi i \sum_{m=0}^{\infty} q^m(z), \quad q(z) = \mathrm{e}^{2\pi \mathrm{i} z}.$$

Differentiating both representations $(k-1)$ times with respect to z gives

$$\begin{aligned} (-1)^{k-1}\Gamma(k) \sum_{d=1}^{\infty} \left(\frac{1}{z+d}\right)^k &= -(2\pi i)^k \sum_{m=1}^{\infty} m^k q^m \\ \Rightarrow \quad \sum_{d=1}^{\infty} \left(\frac{1}{z+d}\right)^k &= \frac{(2\pi i)^k}{\Gamma(k)} \sum_{m=1}^{\infty} m^{k-1} q^m, \end{aligned}$$

where the fact can be used, that k is even. Therefore, the lattice consists for any $cz+d$

$$\sum_{c,d}{}' \left(\frac{1}{cz+d}\right)^k = \sum_d{}' \frac{1}{d^k} + \sum_c{}' \left(\sum_d \frac{1}{(cz+d)^k} \right)$$

This has been used in (5.5). The sum over m is periodic in the real part of $n\tau$ with period 1. With $\tau = \tau_1 + i\tau_2$ the following can prove,

$$\begin{aligned} f(n\tau_1) &= \sum_{m=-\infty}^{\infty} \frac{1}{|m+n(\tau_1+i\tau_2)|^{2s}} \\ &= \ldots + \frac{1}{|-1+n(\tau_1+i\tau_2)|^{2s}} + \frac{1}{|n(\tau_1+i\tau_2)|^{2s}} + \frac{1}{|1+n(\tau_1+i\tau_2)|^{2s}} + \ldots \\ &= \sum_{m-1=\infty}^{\infty} \frac{1}{|m+(n\tau_1+1)+i\tau_2|^{2s}} \\ &= \sum_{m=\infty}^{\infty} \frac{1}{|m+(n\tau_1+1)+i\tau_2|^{2s}} = f(n\tau_1+1), \end{aligned}$$

because the sum goes over all $m \in \mathbb{Z}$. A function $f(x)$ periodic in $[0,1]$ can now be expressed by a Fourier expansion

$$f(x) = \sum_{n\in\mathbb{Z}} c_n \mathrm{e}^{2\pi i n x}, \qquad c_n = \int_0^1 \mathrm{d}x f(x) \mathrm{e}^{-2\pi i n x}.$$

As it was proven, the function $f(n\tau_1)$ above is a periodic in $[0,1]$, so the Fourier expansion reads

$$\begin{aligned} f(n\tau_1) &= \sum_{p\in\mathbb{Z}} \mathrm{e}^{2\pi i p n\tau_1} \int_0^1 \mathrm{d}(n\tau_1) \sum_m \frac{1}{|m+n(\tau_1+i\tau_2)|^{2s}} \mathrm{e}^{-2\pi i p n\tau_1} \\ &= \sum_{p\in\mathbb{Z}} \mathrm{e}^{2\pi i p n\tau_1} \int_0^1 \mathrm{d}y \sum_m \frac{1}{|m+y+in\tau_2|^{2s}} \mathrm{e}^{-2\pi i p y} \end{aligned}$$

and

$$\begin{aligned} \sum_m \frac{1}{|m+n\tau|^{2s}} &= \sum_l \mathrm{e}^{2i\pi l n\tau_1} \int_0^1 \mathrm{d}y \mathrm{e}^{-2i\pi l y} \sum_m \frac{1}{|m+y+in\tau_2|^{2s}} \\ &= \sum_l \int_{-\infty}^{\infty} \mathrm{d}y \mathrm{e}^{2i\pi l(n\tau_1-y)} \frac{1}{|m+y+in\tau_2|^{2s}} \\ &= \frac{1}{\Gamma(s)} \sum_l \int_{-\infty}^{\infty} \mathrm{d}y \int_0^{\infty} \mathrm{d}t t^{s-1} \mathrm{e}^{2i\pi l(n\tau_1-y)-t(y^2+n^2\tau_2^2)} \end{aligned}$$

where the last transformation is due to the representation of the gamma function

$$\frac{1}{z^k} = \frac{1}{\Gamma(k)} \int_0^{\infty} \mathrm{d}t t^{k-1} \mathrm{e}^{-zt},$$

so that

$$\frac{1}{|m+y+in\tau_2|^{2s}} = \frac{1}{\Gamma(s)} \int_0^{\infty} \mathrm{d}t t^{s-1} \mathrm{e}^{-t(y^2+n^2\tau_2^2)}.$$

Evaluating the integral with respect to y leads to

$$\begin{aligned} \sum_m \frac{1}{|m+n\tau|^{2s}} &= \frac{\pi^{1/2}}{\Gamma(s)} \sum_l \int_0^{\infty} \mathrm{d}t t^{s-3/2} \mathrm{e}^{-(tn^2\tau_2^2+\pi^2 l^2/t-2i\pi l n\tau_1)} \\ &= \sqrt{\pi}\frac{\Gamma(s-1/2)}{\Gamma(s)} |n\tau_2|^{1-2s} \\ &\quad + \frac{\sqrt{\pi}}{\Gamma(s)} \sum_l{}' \mathrm{e}^{2i\pi l n\tau_1} \left|\frac{\pi l}{n\tau_2}\right|^{s-1/2} \int_0^{\infty} \mathrm{d}t t^{s-3/2} \mathrm{e}^{-\pi|ln|\tau_2(t+1/t)}, \end{aligned} \tag{5.6}$$

because for $l = 0$

$$\int_0^\infty \mathrm{d}t t^{s-3/2} \mathrm{e}^{-tn^2\tau_2^2} = \int_0^\infty \frac{\mathrm{d}t}{n^2\tau_2^2} \left(\frac{t}{n^2\tau_2^2}\right)^{s-3/2} \mathrm{e}^{-t}$$
$$= \left(\frac{1}{n^2\tau_2^2}\right)^{s-1/2} \int_0^\infty \mathrm{d}t t^{s-3/2} \mathrm{e}^{-t}$$
$$= |n\tau_2|^{1-2s} \Gamma(s-1/2)$$

with

$$\Gamma(z) = \int_0^\infty \mathrm{d}t t^{z-1} \mathrm{e}^{-t}.$$

For the second term in (5.6), the substitution $t \to |\pi l/(n\tau_2)| t$ is used as succeeding

$$\sum_l{}' \int_0^\infty \mathrm{d}t t^{s-3/2} \mathrm{e}^{-(tn^2\tau_2^2 + \pi^2 l^2/t - 2i\pi l n \tau_1)}$$
$$= \sum_l{}' \mathrm{e}^{2i\pi l n \tau_1} \int_0^\infty \left|\frac{\pi l}{n\tau_2}\right| \mathrm{d}t \left|\frac{\pi l}{n\tau_2} t\right|^{s-3/2} \mathrm{e}^{-\pi n l \tau_2 (t+1/t)}$$
$$= \sum_l{}' \mathrm{e}^{2i\pi l n \tau_1} \left|\frac{\pi l}{n\tau_2}\right|^{s-3/2} \int_0^\infty \mathrm{d}t\, |t|^{s-1/2}\, \mathrm{e}^{-\pi n l \tau_2 (t+1/t)}.$$

Consequently, the term results in

$$G(s) = \left|\frac{4\pi^2}{\tau_2^2}\right|^{-2s} \Bigg\{ 2\zeta(2s)$$
$$+ \sqrt{\pi} \frac{\Gamma(s-1/2)}{\Gamma(s)} \sum_n{}' |n\tau_2|^{1-2s}$$
$$+ \frac{\sqrt{\pi}}{\Gamma(s)} \sum_n{}' \sum_l{}' \mathrm{e}^{2i\pi l n \tau_1} \left|\frac{\pi l}{n\tau_2}\right|^{s-1/2} \int_0^\infty \mathrm{d}t t^{s-3/2} \mathrm{e}^{-\pi |ln| \tau_2 (t+1/t)} \Bigg\}. \tag{5.7}$$

Summing the second term over n, subsequent functional relation (reflection formula B.3) can be used

$$\pi^{-s/2}\Gamma(s/2)\zeta(s) = \pi^{1/2-s/2}\Gamma(1/2 - s/2)\zeta(1-s)$$

with the definition of the zeta function

$$\sqrt{\pi} \frac{\Gamma(s-1/2)}{\Gamma(s)} \sum_n{}' |n\tau_2|^{1-2s} = 2\sqrt{\pi} \frac{\Gamma(s-1/2)}{\Gamma(s)} |\tau_2|^{1-2s} \zeta(2s-1)$$
$$= \frac{2}{\Gamma(s)} \pi^{s-1/2} |\tau_2|^{1-2s} \Gamma(1-s) \zeta(2-2s).$$

In order to find the value of the derivative $G'(s)$ at $s = 0$, the function $G(s)$ is expanded to first order around $s = 0$. For the first term in (5.7), this leads to

$$\begin{aligned} 2\zeta(2s) &= 2\zeta(0) + 2s\zeta'(0) + \mathcal{O}(s^2) \\ &= -1 - 2s\ln(2\pi) + \mathcal{O}(s^2) \end{aligned}$$

with $\zeta(0) = -1/2$ from (B.22) and $2\zeta'(0) = -\ln(2\pi)$. The value of the second term in (5.6) becomes

$$\begin{aligned} \frac{\Gamma(1-s)\zeta(2-2s)}{\Gamma(s)} &= (1 + s\Gamma'(1) + \mathcal{O}(s^2))\left(\frac{\pi^2}{6} + 2s\zeta'(2) + \mathcal{O}(s^2))(s + \mathcal{O}(s^2)\right) \\ &= \frac{\pi^2}{6}s + \mathcal{O}(s^2), \end{aligned}$$

where the value $\zeta(2) = \pi^2/6$ (B.23), the value of the derivative (B.24) and the series expansion $1/\Gamma(s) = s + s^2 + \mathcal{O}(s^3)$ is used. The third term can as well be expanded around $s = 0$. The integral (see for instance [Sch81])

$$\int_0^\infty \mathrm{d}t t^{-3/2}\mathrm{e}^{-\alpha(t+1/t)} = \sqrt{\frac{\pi}{\alpha}}\mathrm{e}^{-2\alpha}$$

together with the series expansion gives in the last term of (5.7)

$$\begin{aligned} &\frac{1}{\Gamma(s)}\mathrm{e}^{2i\pi ln\tau_1}\int_0^\infty \mathrm{d}t t^{s-3/2}\mathrm{e}^{-\pi|ln|\tau_2(t+1/t)} \\ &= s\mathrm{e}^{2i\pi ln\tau_1}\sqrt{\frac{\pi}{\pi|ln|\tau_2}}\mathrm{e}^{-2\pi|ln|\tau_2} + \mathcal{O}(s^2). \end{aligned}$$

These calculations lead to

$$\begin{aligned} G(s) = -1 - 2s\ln\left|\frac{A}{2\pi\omega_1}\right| - 2s\ln 2\pi + \frac{\pi}{3}s\tau_2 \\ + s\sum_n{}' \sum_l{}' \frac{1}{|l|}\mathrm{e}^{2i\pi ln\tau_1 - 2\pi|ln|\tau_2} + \mathcal{O}(s^2). \end{aligned}$$

With the definition

$$q(\tau) = \mathrm{e}^{2\pi i\tau}, \qquad \eta(\tau) = q^{1/24}(\tau)\prod_{n=1}^\infty(1 - q^n(\tau))$$

of the Dedekind eta function $\eta(\tau)$ and because of $|A/\omega_1| = \sqrt{A\tau_2}$, the derivative of $G(s)$ close to $s = 0$ reads

$$\begin{aligned} G'(s) &= -\ln \tau_2 + \frac{\pi}{3}\tau_2 + \eta(\tau)\overline{\eta(\tau)} \\ G'(0) &= -2\ln\left(\sqrt{A\tau_2}|\eta(\tau)|^2\right) \\ &= -2\ln\left(\sqrt{L_1 L_2}\sqrt{\frac{L_1}{L_2}}|\eta(\tau)|^2\right) \\ &= -\ln\frac{L_1 L_2}{4\pi} - 2\ln\left(\sqrt{4\pi}\sqrt{\frac{L_1}{L_2}}|\eta(\tau)|^2\right). \end{aligned}$$

For $L_1 = L_2 = L$

$$\begin{aligned} G'(0) &= -\ln\frac{L^2}{4\pi} - 2\ln\left(\sqrt{4\pi}|\eta(\mathrm{i})|^2\right) \\ &= -\ln\frac{L^2}{4\pi} - 2\ln\left(\sqrt{4\pi}|\eta(\mathrm{i})|^2\right) \\ &\approx -\ln\frac{L^2}{4\pi} - 1.47634\ldots \end{aligned}$$

is found.

5.2. Sommerfeld-Watson transformation

A second way of calculating the determinant follows J. Polchinski [Pol86]. In this calculation, the Sommerfeld-Watson transformation plays a key role. The aim of this transformation is to convert a slowly converging series into an contour integral using the Cauchy residue theorem. The sum as a sum over the residues corresponds to the integrand's poles and the integral can be evaluated.

The problem of calculating infinite series over complex poles arises in the early 20th century, when wireless communication began to grow. A. Sommerfeld calculated the propagation of electro-magnetic surface-waves and transformed the contour of an integral over infinite poles into a contour excluding only two branch cuts [Som09]. The other related work is due to G. N. Watson on a similar problem, calculating by transforming a sum into a complex integral. This is called Watson transformation. The first usage of this transformation goes back to G. N. Watson [Wat18] who calculated the diffraction of electric fields in presence of the earth. A. Sommerfeld combined both methods. Then a different theory of diffraction, using integrals, where he transformed the integral over infinite poles into an integral using only one branch cut, was created. The present formulation goes back to A. Sommerfeld applying the Watson transform in order to calculate infinite series coming from spherical functions [Som47] arising from the calculation of electro magnetic for the above mentioned problem. It has later been used in order to calculate scattering amplitudes [Reg59]. These calculations became important in the high energy sector of strong interactions, then the Regge theory was succeeded by quantum chromo dynamics.

At first, the present form of ζ_2 needs to be rewritten. The calculation begins with the left side of (5.2) by transforming it to

$$\begin{aligned}\left(\frac{2\pi}{A}\right)^2\left[-n_1^2\omega_2^2+n_2^2\omega_1^2\right] &= \left(\frac{2\pi}{A}\right)^2(n_2\omega_1-n_1\omega_2)(n_2\omega_1+n_1\omega_2)\\ &= \left(\frac{2\pi}{A}\omega_1\right)^2(n_2-n_1\tau)(n_2+n_1\tau)\\ &= \left(\frac{2\pi}{A}\omega_1\right)^2(n_2-n_1\tau)(n_2-n_1\bar{\tau})\\ &= \frac{\tau_2}{A}\frac{4\pi^2}{\tau_2}(n_2-n_1\tau)(n_2-n_1\bar{\tau}),\end{aligned}$$

where in the third step the fact is used that $\tau = \tau_1 + \mathrm{i}\tau_2$ is purely imaginary. The last step is due to comparison reasons with Polchinski. The ζ_2 function (4.52) can now be expressed as

$$\begin{aligned}\zeta_2(s) &= \left(\frac{\tau_2}{A}\right)^{-s}\sum_{n_1,n_2}{}'\left[\frac{4\pi^2}{\tau_2^2}(n_2-n_1\tau)(n_2-n_1\bar{\tau})\right]^{-s}\\ \frac{\mathrm{d}}{\mathrm{d}z}\zeta_2\bigg|_{z=0} &= \ln\frac{\tau_2}{A}-G'(0),\end{aligned} \tag{5.8}$$

where the fact was used, that the sum gives[1]

$$\sum_{n_1=-\infty}^{\infty}{}'\sum_{n_2=-\infty}^{\infty}{}' 1 = 2\zeta(0) = -1$$

to the derivative of the prefactor. The function $G(s)$ is defined as

$$\begin{aligned}G(s) &= -\sum_{n_1,n_2}{}'\left[\frac{4\pi^2}{\tau_2^2}(n_2-n_1\tau)(n_2-n_1\bar{\tau})\right]^{-s}\\ &= -\sum_{n_1,n_2}{}'\left\{\left(\frac{4\pi^2}{\tau_2^2}\right)^{-s}\sum_{n_1,n_2}\left[(n_2-n_1\tau)(n_2-n_1\bar{\tau})+\mu^2-\mu^2\right]^{-s}\right\}\\ &= -\lim_{\mu^2\to 0}\left\{\left(\frac{4\pi^2}{\tau_2^2}\right)^{-s}\sum_{n_1,n_2}\left[(n_2-n_1\tau)(n_2-n_1\bar{\tau})+\mu^2\right]^{-s}-\left(\frac{4\pi^2\mu^2}{\tau_2^2}\right)^{-s}\right\}.\end{aligned}$$

The sum is prevented from diverging because the regularizing mass μ^2 is taken into calculation. The calculations are similar to the ζ-function regularization, meaning here,

[1] there is a small error in [Pol86]

that the derivative of $G(s)$ at the value $s = 0$ is searched.The derivative of $G(s)$ is given by

$$\frac{\mathrm{d}}{\mathrm{d}s}G(s)\Big|_{s=0} = -\lim_{\substack{s\to 0\\ \mu^2\to 0}} \frac{\mathrm{d}}{\mathrm{d}s}\left\{\left(\frac{4\pi^2}{\tau_2^2}\right)^{-s}\sum_{n_1,n_2}\Big[(n_2-n_1\tau)(n_2-n_1\bar{\tau})+\mu^2\Big]^{-s} - \left(\frac{4\pi^2\mu^2}{\tau_2^2}\right)^{-s}\right\}.$$

The simplest part can be evaluated directly, as

$$\begin{aligned}\lim_{s\to 0}\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{4\pi^2\mu^2}{\tau_2^2}\right)^{-s} &= \lim_{s\to 0}\frac{\mathrm{d}}{\mathrm{d}s}\mathrm{e}^{-s\ln\left(\frac{4\pi^2\mu^2}{\tau_2^2}\right)}\\ &= -\lim_{s\to 0}\ln\left(\frac{4\pi^2\mu^2}{\tau_2^2}\right)\left(\frac{4\pi^2\mu^2}{\tau_2^2}\right)^{-s}\\ &= 2\ln\tau_2 - 2\ln 2\pi\mu. \end{aligned} \tag{5.9}$$

The modular ratio was chosen to be a complex number, so splitting $\tau = \tau_1 + i\tau_2$ the summand gets

$$\begin{aligned}(n_2-n_1\tau)(n_2-n_1\bar{\tau})+\mu^2 &= n_2^2 + n_1^2(\tau_1+i\tau_2)(\tau_1-i\tau_2) - 2n_1n_2\tau_1 + \mu^2\\ &= (n_2-n_1\tau_1)^2 + n_1^2\tau_2^2 + \mu^2\\ &= (n_2-n_1\tau_1)^2 + Q^2(n_1,\mu),\end{aligned}$$

where

$$Q^2(n_1,\mu) = n_1^2\tau_2^2 + \mu^2. \tag{5.10}$$

The sum becomes

$$\sum_{n_1,n_2}\Big[(n_2-n_1\tau_1)^2+Q^2(n_1,\mu)\Big]^{-s} = \sum_{n_2=-\infty}^{\infty}\underbrace{\sum_{n_1=-\infty}^{\infty}\Big[(n_2-n_1\tau_1)^2+Q^2(n_1,\mu)\Big]^{-s}}_{=f(n_2)},$$

where the n_2 sum can be evaluated explicitly using the Sommerfeld-Watson transformation. Then

$$\sum_{n=-\infty}^{\infty}(-1)^n g(n) = \frac{1}{2\mathrm{i}}\oint_C \mathrm{d}z\frac{g(z)}{\sin\pi z}.$$

The contour C encloses all poles on the real axis, that are all zeros of $\sin(\pi z)$, which are the numbers $z = n, n\in\mathbb{Z}$. For non-alternating series $f(n)$, this can be converted into into an integral using $g(n) = \mathrm{e}^{-\mathrm{i}\pi n}f(n)$. This choice forces a changing of sign, because

$$\begin{aligned}\frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z} &< -1, &&\text{for}\quad \Im(z) > 0,\\ \frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z} &> 0, &&\text{for}\quad \Im(z) < 0.\end{aligned}$$

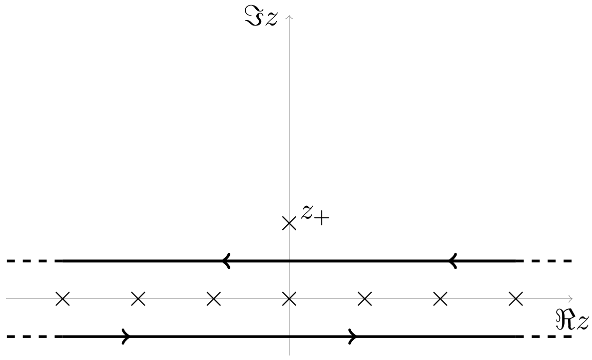

Figure 5.2.: Contour C closing at $z \to \pm\infty$.

Therefore, introducing the substitution

$$\begin{aligned} -\frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z} - \frac{1}{2}, &\qquad \text{for} \quad \Im(z) > 0, \\ \frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z} + \frac{1}{2}, &\qquad \text{for} \quad \Im(z) < 0, \end{aligned}$$

can be used to change the integral into an integral using both contours $C_+ : \{z, \infty + \mathrm{i}\epsilon < z < -\infty + \mathrm{i}\epsilon\}$ and $C_- : \{z, -\infty - \mathrm{i}\epsilon < z < \infty - \mathrm{i}\epsilon\}$, (see Figure 5.2)

$$\begin{aligned} \sum_{n_2=-\infty}^{\infty} f(n_2) &= -\int_{C_+} \mathrm{d}z f(z) \left(\frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z} + \frac{1}{2} \right) + \int_{C_-} \mathrm{d}z f(z) \left(\frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z} + \frac{1}{2} \right) \\ &= \underbrace{\left(\int_{C_-} - \int_{C_+} \right) \frac{\mathrm{d}z}{2} f(z)}_{=:I_1} + \underbrace{\int_{C_-} \mathrm{d}z f(z) \frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z} - \int_{C_+} \mathrm{d}z f(z) \frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z}}_{=:I_2} . \end{aligned}$$

In the succeeding, both integrals will be evaluated and their derivative will be taken.

Evaluating the I_1 integral

For the I_1 integral there is

$$I_1(s) = \frac{1}{2} \sum_{n_1=-\infty}^{\infty} \left(\int_{C_-} - \int_{C_+} \right) \mathrm{d}z \left[(z - n_1\tau_1)^2 + Q^2(n_1, \mu) \right]^{-s},$$

which by a shift of $z \to z + n_1\tau_1$ does not change on account of the infinite integration limits. For this reason, the new function is symmetric $f(z) = f(-z)$ and under a substitution in C_+ with $z \to -z$, it can be lined out that

$$I_1(s) = \sum_{n_1=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}z \left[z^2 + Q^2(n_1, \mu) \right]^{-s}, \tag{5.11}$$

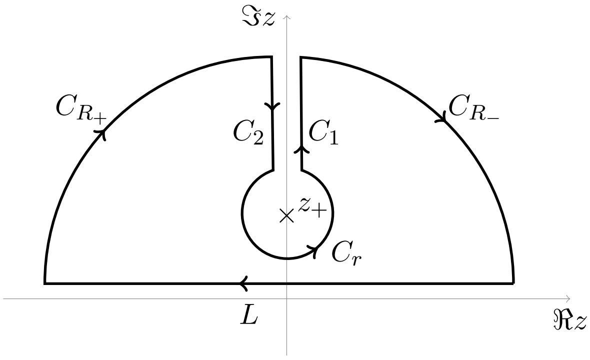

Figure 5.3.: Contour Γ_+ for integration.

where the limit $\epsilon \to 0$ has been taken. This integral can be evaluated using the Euler beta function, what is done in the appendix B.2. Using (5.10), the result is

$$\begin{aligned}\lim_{s\to 0}\frac{\mathrm{d}}{\mathrm{d}s}I_1(s) &= -\sum_{n_1} 2\pi Q(n_1,\mu)\\ &= -2\pi\mu - 2\pi\tau_2 {\sum_{n_1}}' n_1, \end{aligned} \tag{5.12}$$

where, in the last step, the $n_1 = 0$ contribution was split up from the sum, and the limit $\mu^2 \to 0$ has been taken. Using the properties of the Riemann zeta function at $\zeta(-1)$, (see appendix B.3) the contribution is

$$\begin{aligned}\lim_{s\to 0}\frac{\mathrm{d}}{\mathrm{d}s}I_1(s) &= -2\pi\mu - 2\pi\tau_2 2\zeta(-1)\\ &= -2\pi\mu + \frac{\pi\tau_2}{3}. \end{aligned} \tag{5.13}$$

Evaluating the I_2 integral

For the I_2 integral there is

$$\begin{aligned} I_2(s) = &\sum_{n_1=-\infty}^{\infty}\int_{C_-}\mathrm{d}z\frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z}\left[(z-n_1\tau_1)^2 + Q^2(n_1,\mu)\right]^{-s}\\ &-\sum_{n_1=-\infty}^{\infty}\int_{C_+}\mathrm{d}z\frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z}\left[(z-n_1\tau_1)^2 + Q^2(n_1,\mu)\right]^{-s}, \end{aligned}$$

where the contour C_+ is given in Figure 5.2. This integral converges for $s = 0$, so first the derivative can be taken. The derive of the integral over the contour C_+ is given by

$$\lim_{s\to 0}\frac{\mathrm{d}}{\mathrm{d}s}\int_{\infty+\mathrm{i}\epsilon}^{-\infty+\mathrm{i}\epsilon}\mathrm{d}z\left[z^2+\mu^2\right]^{-s}\frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z} = -\int_{\infty+\mathrm{i}\epsilon}^{-\infty+\mathrm{i}\epsilon}\mathrm{d}z\frac{\mathrm{e}^{-\mathrm{i}\pi z}}{2\mathrm{i}\sin\pi z}\ln\left[z^2+\mu^2\right].$$

Furthermore, there is a branch point for the logarithm, when the argument is zero or less. This will be used to deform the contour C_+ to a contour Γ_+, which is given in Figure 5.3. From Cauchy's residue theorem, it is known that for the new contour

$$\oint_{\Gamma_+} = 0$$

because there are no singularities inside the contour Γ_+, but there is a branch point at $\nu_+ = n_1\tau_1 + \mathrm{i}Q(n_1,\mu) = \mathrm{i}z_+$ outside of the contour. While evaluating the integrals, the limits $R \to \infty$ and $r \to 0$ will be taken. The part L of Γ_+ running from $\infty + \mathrm{i}\epsilon$ to $-\infty + \mathrm{i}\epsilon$ is given by

$$-\int_L = \int_{C_{R_1}} + \int_{C_{R_2}} + \int_{C_1} + \int_{C_2} + \int_{C_r} .$$

It can be deduced that (substituting $z = z_+ + r\mathrm{e}^{\mathrm{i}\phi}, \phi \in (0, 2\pi)$)

$$\left| \int_{C_r} \right| \leq 2\pi r \underset{r\to 0}{\to} 0,$$

as well as for the other contributions (substituting $z = R\mathrm{e}^{i\theta_i}, \theta_1 \in (\pi, 3\pi/2), \theta_2 \in (3\pi/2, 2\pi)$), it consequently ends in

$$\left| \int_{C_{R_+}} + \int_{C_{R_-}} \right| \underset{R\to\infty}{\to} 0,$$

due to [AGW96]. This means

$$\int_L = -\int_{C_1} - \int_{C_2}, \tag{5.14}$$

where the contour of C_1 runs from $\mathrm{i}z_+$ to $\mathrm{i}\infty$ and for C_2 from $\mathrm{i}\infty$ to $\mathrm{i}z_+$ with $z_+ > 0$:

$$C_1 : \{y \in \mathrm{i}\mathbb{R} : \mathrm{i}z_+ \leq y < \mathrm{i}\infty\} \qquad \text{and} \qquad C_2 : \{y \in \mathrm{i}\mathbb{R} : \mathrm{i}\infty < y \leq \mathrm{i}z_+\}$$

With a change of variables $y = \mathrm{i}z$ and $\mathrm{d}z = -\mathrm{i}\mathrm{d}y$ for $r \to 0$ the integral using contour C_1 is given by

$$\begin{aligned}\int_{C_1} &= \mathrm{i}\int_{z_+}^{\infty} \mathrm{d}y \frac{\mathrm{e}^{-\pi y}}{2\mathrm{i}\sin(-\pi \mathrm{i}y)} \ln\left[-y^2 + \mu^2\right] \\ &= \mathrm{i}\int_{z_+}^{\infty} \mathrm{d}y \frac{\mathrm{e}^{-\pi y}}{2\sinh(\pi y)} \ln\left[-y^2 + \mu^2\right]\end{aligned}$$

and the integral using C_2 is given by

$$\begin{aligned}\int_{C_2} &= \mathrm{i}\int_{\infty}^{z_+} \mathrm{d}y \frac{\mathrm{e}^{-\pi y}}{2\mathrm{i}\sin(-\pi \mathrm{i}y)} \ln\left[-y^2 + \mu^2\right] \\ &= -\mathrm{i}\int_{z_+}^{\infty} \mathrm{d}y \frac{\mathrm{e}^{-\pi y}}{2\sinh(\pi y)} \ln\left[-y^2 + \mu^2\right] .\end{aligned}$$

To such a degree, the integrals should as well cancel out. This is not the case, as there is a gap of 2δ over the branch cut of the logarithm. The complex logarithm will give a contribution of $2\pi\mathrm{i}$ because the value is different when the branch cut is approached from the left or from the right side by the contour. Now, the logarithm can be studied explicitly. Rewriting

$$\begin{aligned}\ln(-y^2+\mu^2) &= \ln\left[(\mathrm{i}y+\mu)(\mathrm{i}y-\mu)\right] \\ &= \ln(\mathrm{i}y+\mu)+\ln(\mathrm{i}y-\mu),\end{aligned}$$

while $\mathrm{i}y \to \mathrm{i}(y+z_+) = \mathrm{i}y-\mu$ this is for the C_1 part

$$\begin{aligned}\ln(-y^2+\mu^2) &= \ln(\mathrm{i}y-\mu+\mu)+\ln(\mathrm{i}y-2\mu) \\ &= \ln(\mathrm{i}y+\delta)+\ln(\mathrm{i}y-2\mu) \\ &\underset{\delta\to 0_+}{=} \ln y-\frac{\pi}{2}\mathrm{i}+\ln(\mathrm{i}y-2\mu)\end{aligned}$$

as a result of the complex logarithm and because the branch cut is approached from the right side. For the C_2 part, the same substitution gives

$$\begin{aligned}\ln(-y^2+\mu^2) &= \ln(\mathrm{i}y-\mu+\mu)+\ln(\mathrm{i}y-2\mu) \\ &= \ln(\mathrm{i}y-\delta)+\ln(\mathrm{i}y-2\mu) \\ &\underset{\delta\to 0_-}{=} \ln y+\frac{3\pi}{2}\mathrm{i}+\ln(\mathrm{i}y-2\mu)\end{aligned}$$

so that

$$\ln(-y^2+\mu^2)-\ln(-y^2+\mu^2) = -\frac{\pi}{2}\mathrm{i}-\frac{3\pi}{2}\mathrm{i} = -2\pi\mathrm{i}.$$

Consequently, using the proposed substitution $\mathrm{i}y \to \mathrm{i}(y+z_+) = \mathrm{i}y-\mu$, the integrals over the contours C_1 and C_2 are

$$\begin{aligned}\int_{C_1}+\int_{C_2} &= -\mathrm{i}\int_0^\infty \mathrm{d}y \frac{\mathrm{e}^{-\pi(y+z_+)}}{2\sinh\left[\pi(y+z_+)\right]}(-2\pi\mathrm{i}) \\ &= -2\pi\int_0^\infty \mathrm{d}y \frac{\mathrm{e}^{-\pi(y+z_+)}}{2\sinh\left[\pi(y+z_+)\right]} \\ &= \ln\left[1-\mathrm{e}^{-2\pi z_+}\right].\end{aligned}$$

Finally, the integration over the L part leads to

$$\int_L = -\ln\left[1-\mathrm{e}^{-2\pi z_+}\right],$$

as the sum of integrals over the contours C_1 and C_2 is the negative integral over L (5.14). For the C_- contour, the same calculation applies using a contour Γ_- in the negative complex plane. The contribution will be

$$\int_{C_-} = -\ln\left[1-\mathrm{e}^{-2\pi z_-}\right],$$

ergo the derivative of I_2 leads with $z_+ = -\mathrm{i}n_1\tau_1 + \sqrt{n_1^2\tau_2^2 + \mu^2}$ to the following expression:

$$\begin{aligned}\lim_{\substack{s\to 0\\ \mu^2\to 0}} \frac{\mathrm{d}}{\mathrm{d}s} I_2(s) &= -2 \lim_{\mu^2\to 0} \sum_{n_1} \ln\left[1-\mathrm{e}^{-2\pi z_+}\right] \\ &= -2 \lim_{\mu^2\to 0} \ln\left[1-\mathrm{e}^{-2\pi\mu}\right] - 2 \sum_{\substack{n_1=-\infty\\ n_1\neq 0}}^{\infty} \ln\left[1-\mathrm{e}^{-2\pi(-\mathrm{i}n_1\tau_1+n_1\tau_2)}\right] \\ &= -2 \lim_{\mu^2\to 0} \ln\left[1-\mathrm{e}^{-2\pi\mu}\right] - 4 \sum_{n_1=1}^{\infty} \ln\left[1-\mathrm{e}^{-2\pi\mathrm{i}n_1\tau}\right], \end{aligned} \tag{5.15}$$

where again the the zero mode $n_1 = 0$ was taken out, so that in the second term, the limit $\mu^2 \to 0$ could be taken. The first expression can be expanded because the limit $\mu^2 \to 0$ will be taken later on

$$-2\ln\left[1-\mathrm{e}^{-2\pi\mu}\right] = -2\ln 2\pi\mu + 2\pi\mu + \mathcal{O}(\mu^2). \tag{5.16}$$

Conclusively,

$$\begin{aligned}\lim_{s\to 0}\frac{\mathrm{d}}{\mathrm{d}s}G(s)| = &\underbrace{2\ln\tau_2 - 2\ln(2\pi m)}_{(5.9)} + \underbrace{2\pi\mu}_{(5.12)} - \underbrace{\frac{\pi\tau_2}{3}}_{(5.13)} \\ &+ \underbrace{2\ln(2\pi\mu) - 2\pi\mu}_{(5.16)} + \underbrace{4\sum_{n_1=1}^{\infty}\ln\left[1-\mathrm{e}^{2\pi\mathrm{i}n_1\tau}\right]}_{(5.15)},\end{aligned}$$

so that the the zero mode cancels out and limit $\mu^2 \to 0$ can be taken. The expression

$$-\frac{\pi\tau_2}{3} + 4\sum_{n_1=1}^{\infty}\ln\left(1-\mathrm{e}^{2\pi\mathrm{i}n_1\tau_2}\right) = 2\ln|\eta(\tau)|^2$$

is just connected with the Dedekind eta function defined by

$$\eta(\tau) = q^{1/24}\prod_{k=1}^{\infty}\left(1-q^k\right), \qquad q = \mathrm{e}^{2\pi\mathrm{i}\tau},$$

whose properties will be investigated later on. Combining the calculations

$$G'(0) = 2\ln|\eta(\tau)|^2 + 2\ln\tau_2 = 2\ln\tau_2|\eta(\tau)|^2$$

and adding the prefactor (5.8),

$$\begin{aligned}\zeta_2'(0) &= \ln\frac{\tau_2}{A} - G'(0) \\ &= -\ln A + \ln\tau_2 - 2\ln\tau_2|\eta(\tau)|^2 \\ &= -\ln A - 2\ln\sqrt{\tau_2}|\eta(\tau)|^2\end{aligned}$$

is obtained. This can be transformed in

$$\begin{aligned}\left.\frac{\mathrm{d}}{\mathrm{d}z}\zeta_2(z)\right|_{z=0} &= -\ln\frac{A}{4\pi} - 2\ln\left(\sqrt{4\pi\tau_2}|\eta(\tau)|^2\right)\\ &= -\ln A - 2\ln\left(\sqrt{\tau_2}|\eta(\tau)|^2\right)\\ &= -2\ln\left(\sqrt{A\tau_2}|\eta(\tau)|^2\right).\end{aligned}$$

5.3. Massless Klein-Gordon field

In a new setup, a more 'physical' approach will be examined. This goes back to a blog entry of John Baez [Bae98a, Bae98b]. The main idea is to use the analogy, that the investigated field is analogous to field of a massless field theory, the massless Klein-Gordon field. As it has been seen before, the eigenvalues of the Laplacian are given by

$$\lambda_{n_1,n_2} = (2\pi)^2\left[\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2}\right], \qquad n_i \in \mathbb{Z}.$$

The determinant is 'ill-defined' by the product

$$\det{}'\Delta = \prod_{n_1,n_2}\lambda_{n_1,n_2},$$

which can be redefined via zeta function regularizing

$$\ln\det{}'\Delta = -\lim_{z\to 0}\frac{\mathrm{d}}{\mathrm{d}z}\zeta_\Delta(z),$$

where the spectral zeta function is

$$\zeta_\Delta(z) = \sum{}'\lambda_{n_1,n_2}^{-z}.$$

The partition function is given by a path integral, where the Euclidean action S is used instead of the Hamiltonian from the chapters before. Especially for a Euclidean free scalar field φ on $L_1 \times L_2$, the action functional is defined as [PS95]

$$S = \frac{1}{2}\int\limits_{L_1\times L_2}\mathrm{d}^2x\varphi(x)\Delta\varphi(x).$$

The partition function is given by the path integral

$$Z = \int\mathcal{D}\varphi\mathrm{e}^{-S} = (\det{}'\Delta)^{-1/2}.$$

For a scalar field with mass μ the Laplacian Δ can be replaced by

$$\Delta \to \Delta_\mu = \Delta + \mu^2,$$

which is needed later on.

In statistical physics, the partition function can as well be written in terms of the trace, as it has been used in the introductory chapters. In this section, the value L_2 is used as the Euclidean time. The value L_1 then represents one space dimension. The partition function is defined as

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\hat{H}L_2}, \tag{5.17}$$

where $\hat{H}$ is the Hamiltonian of the scalar field. The scalar field represents a free massless Klein-Gordon field, where the Hamiltonian is given by a collection of harmonic oscillators

$$\hat{H} = \sum_k \omega(k) \left[a^\dagger(k)a(k) + \frac{1}{2}\right].$$

Here $a^\dagger$ and a are the common creation and annihilation operators. The circular frequency is given by

$$\omega(k) = \sqrt{k^2 + \mu^2} \overset{\mu=0}{=} |k|, \quad k = \frac{2\pi}{L_1}n, \qquad n \in \mathbb{Z}. \tag{5.18}$$

To perform the trace, the energies for the massless case are needed, which are given by

$$E(\{l_n\}) = \sum_{n\in\mathbb{Z}} \frac{2\pi}{L_1}|n| \left(l_n + \frac{1}{2}\right).$$

This calculation is as well known from the quantum mechanic harmonic oscillator. Number l represents the different energy levels, which are possible for the collection of n harmonic oscillators given by the Hamiltonian $\hat{H}$. The Klein-Gordon field used here is given by all frequency modes. This means, that the sum over n is over all numbers in $\mathbb{Z}$. With the energies given, the trace can be evaluated, as the energies are the eigenvalues of the Hamiltonian. The partition function now reads

$$\begin{aligned} Z &= \prod_{n\in\mathbb{Z}} \sum_{l=0}^{\infty} \mathrm{e}^{-L_2 \frac{2\pi}{L_1}(l_n+1/2)|n|} \\ &= \prod_{n\in\mathbb{Z}} \frac{\mathrm{e}^{-\pi\frac{L_2}{L_1}|n|}}{1-\mathrm{e}^{-2\pi\frac{L_2}{L_1}|n|}} \\ &= \prod_{n\in\mathbb{Z}} q^{1/2|n|}(1-q^{|n|})^{-1} \end{aligned}$$

which is owing to the representation of the geometric series, q is given by $q(\tau) = \mathrm{e}^{2\pi i\tau} = \mathrm{e}^{-2\pi L_2/L_1}$. Omitting the zero mode for $n = 0$ in the partition function, a new partition function is given by

$$\begin{aligned} Z' &= \prod_{n\in\mathbb{Z}\setminus\{0\}} q^{1/2|n|}(1-q^{|n|})^{-1} \\ &= \prod_{n=1}^{\infty} q^n(1-q^n)^{-2} \\ &= q^{\sum_{n=1}^{\infty} n}\left[\prod_{n=1}^{\infty}(1-q^n)\right]^{-2}. \end{aligned} \tag{5.19}$$

Now, the surprising result of the zeta function regularization (see appendix B.3) is needed in order to handle the infinite sum in the exponent of the prefactor

$$1+2+3+\ldots = \sum_{n=1}^{\infty} n = \zeta(-1) = -\frac{1}{12}.$$

This leads to

$$\begin{aligned} Z' &= q^{-1/12}\left[\prod_{n=1}^{\infty}(1-q^n)\right]^{-2} \\ &= |\eta(\tau)|^{-2} \end{aligned}$$

with the Dedekind eta function

$$\eta(\tau) = q^{1/24}\left[\prod_{n=1}^{\infty}(1-q^n)\right].$$

From the path integral (5.17), it is known that

$$\begin{aligned} \det{}'\,\Delta &\sim |\eta(\tau)|^4, \\ \det{}'\,\Delta &= \mathcal{C}|\eta(\tau)|^4, \end{aligned}$$

where a constant $\mathcal{C}$ is needed as a consequence of the contribution of the zero mode. In the last steps, the divergency for $n = 0$ was excluded. To handle this factor in above equation, the case of a massive Klein Gordon field has to be analyzed

$$\det \Delta_\mu = \det{}'\,\Delta\lambda_{0,0},$$

where the zero mode is given by the constant solution $\lambda_{0,0} = \mu^2$, so that

$$\det{}'\,\Delta = \lim_{\mu\to 0}\frac{\det \Delta_\mu}{\mu^2}.$$

In this case, the circle frequency (5.18) is given by

$$\omega(k) = \sqrt{k^2+\mu^2} = \frac{2\pi}{L_1}\sqrt{n^2+\frac{L_1^2}{4\pi^2}\mu^2} =: \frac{2\pi}{L_1}n',$$

so that for $n = 0$, the value of n' is $n' = mL_1/(2\pi)$ and by a similar calculation as in (5.19), the partition function reads

$$\begin{aligned} Z &= \prod_{n\in\mathbb{Z}} \mathrm{e}^{-\pi\frac{L_2}{L_1}n'} \left(1 - \mathrm{e}^{-2\pi\frac{L_2}{L_1}n'}\right)^{-1} \\ &= \mathrm{e}^{-\mu L_2/2} \left(1 - \mathrm{e}^{\mu L_2}\right)^{-1} \cdot Z' \\ &= \frac{Z'}{\mathrm{e}^{\mu L_2/2} - \mathrm{e}^{-\mu L_2/2}} \\ &= \frac{Z'}{2\sinh(\mu L_2/2)} \end{aligned}$$

Ensuing, the limit $\mu \to 0$ can be taken

$$\mathcal{C} \det{}' \Delta = \lim_{\mu\to 0} \det{}' \Delta \frac{(2\sinh(\mu L_2/2))^2}{\mu^2} = L_2^2 \det{}' \Delta$$

because of

$$\lim_{x\to 0} \frac{4\sinh^2(\alpha x/2)}{x^2} = \alpha^2.$$

Finally, this gives

$$\det{}' \Delta = L_2^2 |\eta(\tau)|^4$$

or

$$\ln \det{}' \Delta = 2 \ln L_2 |\eta(\tau)|^2.$$

This solution only handles the case that L_2 was chosen as the Euclidean time before. Switching $L_1 \leftrightarrow L_2$ gives the solution

$$\ln \det{}' \Delta = 2 \ln L_1 |\eta(\tau')|^2,$$

where now $\tau' = 1/\tau$ from before. It is found out, that

$$\begin{aligned} \ln \det{}' \Delta &= 2 \ln(L_2 |\eta(\tau)|^2) \\ &= 2 \ln \left(\sqrt{L_1 L_2} \sqrt{\frac{L_2}{L_1}} |\eta(\tau)|^2 \right) \\ &= 2 \ln \left(\sqrt{L_1 L_2 \Im(\tau)} |\eta(\tau)|^2 \right) \end{aligned}$$

which ensures that the modular invariance $\tau \to 1/\tau$ is correct. Finally identifying $A = L_1 L_2$, it results in

$$\frac{\mathrm{d}}{\mathrm{d}z} \zeta_\Delta(z) = -\ln \det{}' \Delta = -2 \ln \left(\sqrt{A \Im(\tau)} |\eta(\tau)|^2 \right)$$

A more elegant but less intuitive way to gain the correct zero mode contribution would be to calculate the zero mode in the way it has been done before by the method of collective coordinates. A partition function here can be given by

$$\begin{aligned} Z &= \int \mathcal{D}\varphi \mathrm{e}^{-\frac{1}{2}(\varphi,\Delta\varphi)} \\ &= \int \mathrm{d}c_0 \int \prod_{n>0} \mathrm{d}c_n \mathrm{e}^{-\frac{1}{2}\sum_{n>0}\lambda_n c_n^2} \\ &= \sqrt{A} \int \prod_{n>0} \mathrm{d}c_n \mathrm{e}^{-\frac{1}{2}\sum_{n>0}\lambda_n c_n^2} \\ &= \sqrt{A} \prod_{n>0} \lambda_n^{-1/2}, \end{aligned}$$

where the collective coordinate c_0 was used as before.

5.4. Result

As the results in the above calculations gave the Dedekind eta function, the properties of this function will be studied in detail before giving the result for the geometric dependence of the factor $C(\tau)$.

5.4.1. Properties of the Dedekind Eta function

The resulting determinant of the Laplacian was always given through the Dedekind Eta function, which is defined by

$$\eta(\tau) = q^{1/24} \prod_{k=1}^{\infty} \left(1 - q^k\right), \qquad q = \mathrm{e}^{2\pi \mathrm{i}\tau}. \tag{5.20}$$

A plot of the eta function is shown in Figure 5.4. To compare the results to other results in literature, the value for $\tau = \mathrm{i}$ is needed. This can be derived from a special value of the Euler q-series $\Phi(q)$, which was given by Ramanujan in his 'Lost Notebook', [AB05]

$$\Phi(\mathrm{e}^{-2\pi}) = \frac{\mathrm{e}^{\pi/12}\Gamma(1/4)}{2\pi^{3/4}}, \tag{5.21}$$

which is related to the Dedekind eta function by

$$\Phi(q) = q^{-1/24}\eta(\tau), \qquad q = \mathrm{e}^{2\pi \mathrm{i}\tau}$$

so that

$$\eta(\mathrm{i}) = \mathrm{e}^{-\pi/12}\Phi(\mathrm{e}^{-2\pi}) = \frac{\Gamma(1/4)}{2\pi^{3/4}}. \tag{5.22}$$

This result is equivalently gained by using the Selberg-trace formula. But the result in [Sel56] is achieved by calculating the Laplacian on a symmetric setup, therefore, this

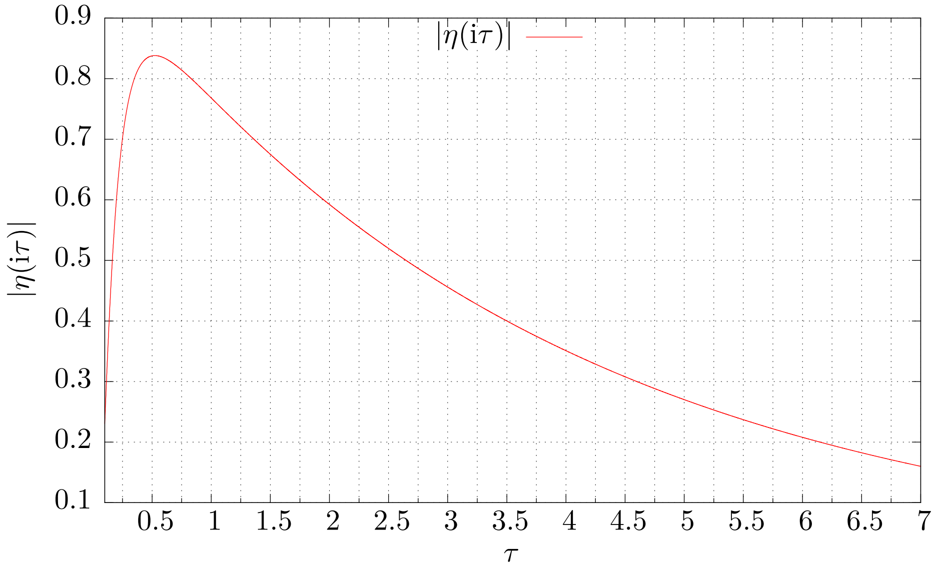

Figure 5.4.: Plot of the Dedekind eta function performed with numerical data from `Mathematica`.

result is gained with a similar calculation as before, setting $L_1 = L_2 = L$ (see for instance [Eli95]).

Another property is the symmetry, which was indicated in the following scheme

$$\eta(-1/\tau) = \sqrt{-i\tau}\eta(\tau), \tag{5.23}$$

implying

$$\sqrt{\tau}|\eta(\tau)|^2 = \sqrt{1/\tau}|\eta(1/\tau)|^2, \tag{5.24}$$

what is just the modular invariance imposed in the introduction $\tau \to 1/\tau$. This can also be observed in the plot of the right hand side of equation (5.24) in Figure 5.5.

5.4.2. Geometric dependence of critical fluctuations

After describing the properties of the Dedekind eta function, the result for the correlation length can now be given. As this result differs only in the prefactor $C(\tau)$ from the present results, this factor is evaluated now. The result is

$$C(\tau) = \frac{\sqrt{2}}{\sqrt{\pi \Im(\tau)}|\eta(\tau)|^2}. \tag{5.25}$$

At first, this result can be compared to the results of the symmetric system. For $L_1 = L_2$ the ratio is $\tau = i$, so that

$$C = C(i) = \sqrt{\frac{2}{\pi} \frac{4\pi^3/2}{\Gamma^2(1/4)}} = 1.351956\ldots, \tag{5.26}$$

which is the same result obtained analytically in [Mün90]. Furthermore, the solution provides the modular invariance $\tau \to 1/\tau$, as this result is not changed qualitatively the behaviour gained from the Dedekind eta function. The interface tension will not chang, because there is no factor τ included in the exponential that contributes to the interface tension in (4.1). Therefore the only change with geometric dependence is included in $C(\tau)$. A comparison of the static factor $C = C(\mathrm{i})$ with the geometric depending factor $C(\tau)$ is given in Figure 5.6. It can be seen, that there is a dramatic change in this factor. This means, the correlation length increases with the deviation of aspect ratio from the value 1.

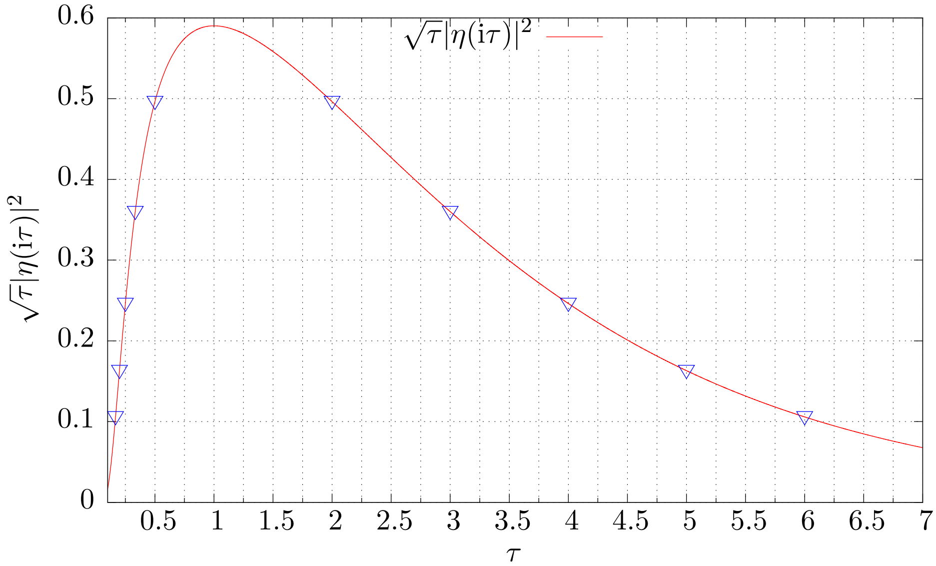

Figure 5.5.: Plot of $\sqrt{\tau}|\eta(\tau)|^2$ with triangles denoting the values at integer values and their inverse.

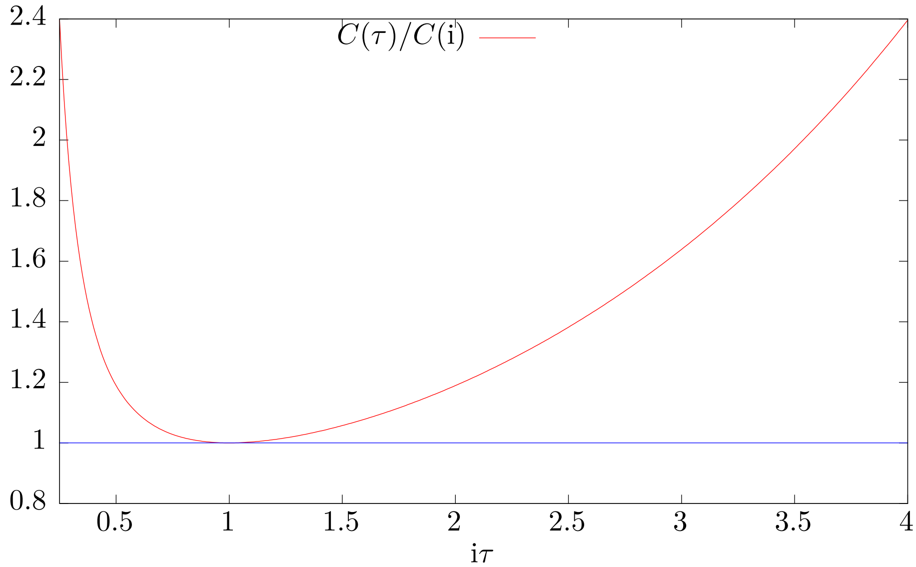

Figure 5.6.: The factor $C(\tau)$ depending on the aspect ratio of L_1 and L_2 compared to the constant factor C (blue line).

6

Conclusion and outlook

As proposed in the introduction, field theoretical methods have presented a fruitful universal method for analysing interface fluctuations in three dimensions. This thesis extended the examination of interface fluctuations on new structures with a genuine attention on the geometric dependences. As underlying geometrical structure, a cuboid was investigated and the suggested solution has been calculated by different methods.

In 2, it could be shown that the derivative raised for fluctuations, is responsible for the geometric dependence of the correlation length in the Ginzburg-Landau theory. Referring to [Mün89], field theoretical methods, reaching from path integral formalism over the methods of collective coordinates and the instanton pseudo-particles, have been prolific to develop this theory in chapter 3. The reasons using these methods were gathered in detail in the last part of the first chapter, where the correlation length was identified by the energy spitting of a massless particle in field theories. In chapter 4, it was shown by zeta regularization and heat kernel methods that only the transversal modes depend on the geometrical setup of the system. Therefore, for new geometries only these modes, corresponding to the two-dimensional Laplacian, need to be recalculated. Especially the zeta regularization techniques have shown universal applications in these fields, since they are applied in almost every calculation in chapter 4 and 5.

In chapter 5, the geometry was focussed on a rectangular setup. Before calculating the determinant explicitly, the geometrical structure with the imposed boundary conditions was transformed into a torus by considerations from conformal field theory. Then, three different methods were used. The first method has shown to be quite direct, getting along without a deep understanding in complex analysis. The second method, due to the Sommerfeld-Watson transformation, turned out to be rather complicated but also quite elegant – it can be reduced on a few steps, when the reader is used to complex analysis. Whereas the existing literature on this method is presented fairly abbreviated, this thesis made a contrast and exposed this calculation most precisely. Both calculations delivered an expression involving the Dedekind eta function insuring that the solution is invariant under the transformation $L_1 \to L_2$ as proposed in the introduction. In a third method, the calculation was redone and the analogy between the Laplacian and a massless Klein-Gordon field was used in order to write the partition function, obtained from statistical mechanical considerations, in terms of harmonic oscillators. This method highlighted to be a very intuitive approach for physicists, delivering the same solution. However, this calculation is not as elegant as the two others, as the solution needs to be modified by an argument in order to cover the proposed invariance. It could be shown then, that for a strict solution, the method of collective coordinates needs to be applied again.

As there is a deeper connection to conformal field theory in this rectangular setup with periodic boundary conditions, another method, involving Virasoro algebra could be possible.

A further calculation on a similar problem could be to impose other geometries as basal area. As the calculation of the normal mode is invariant under the imposed geometric structure, only the geometry of the Laplacian needs to be recalculated. For instance, there are solutions for the circular Laplacian [Wei87], eventually there is an approach solving elliptic problems, thus where it should also be a factor depending on the geometrical structure.

In the future, it should be researched, if there is a proper limit law for the Dedekind eta function, which would make a reduction on two dimensions possible, where the correlation length can be compared to a direct two dimensional calculation, e.g. in [PF83].

Because of the structure of the problem, which was motivated by the Ising model in this thesis, there should also be an approach solving the geometric dependence of the correlation length numerically by a Monte-Carlo calculation in order to test the presented solution, as presented in the work of other papers [Mün89, Mün90]. It shows, that a quantitative experimental analysis of the interface fluctuations is difficult to reach, but it should be possible to test the geometrical dependence qualitatively in experiments.

A similar calculation applies for an effective string theory in quantum chromo dynamics. In the confining regime, the quark anti-quark pair $q\bar{q}$ is described by Wilson Loops [LW02] where the partition function can be written as

$$Z \sim \mathrm{e}^{-V(R)T},$$

where $V(R)$ is the potential and T is the time-line of the world sheet. As confining regime of quantum chromo dynamics contains in general two phases: the strong coupling phase and the rough phase. The two are separated by the so-called roughening transition which is the point in which the strong coupling expansion in the Wilson loop ceases to converge. These two phases are related to two different behaviours of the quantum fluctuations. In the strong coupling phase, these fluctuations are massive, while in the rough phase they become massless. This fact can be used in order to describe this transition by the massless theory in two dimensions. Calculating this transition by setting the time-line direction L_2 and $R = L_1$ ends up in the same calculations as before, leading to the Dedekind eta function. Therefore, this so called Lüscher term [LSW80] can be calculated this way. As there are too many expressions that have to be defined to reach the effective string theory, this has been omitted in this work, but it is an interesting fact, applying these calculations in other fields of physics.

A

Form and energy of the kink-profile

A.1. Form of the kink

The variation of the Hamiltonian near the classical solution provides

$$\left.\frac{\delta H}{\delta\phi}\right|_{\phi=\phi_0} = \frac{1}{2}(-2\nabla^2\phi_0) + \frac{g}{4!}4\phi_0^3 - \frac{m^2}{4}2\phi_0 = 0, \tag{A.1}$$

or to be more general

$$-\nabla^2\phi_0(\mathbf{x}) + V'(\phi(\mathbf{x})) = 0,$$

where $V'(\phi)$ means the derivative of the potential V with respect to the function ϕ. As it was proposed, the boundary conditions in z-direction were defined anti-periodic, so that

$$\bar{\phi} = \lim_{z\to\pm\infty}\phi_0(z) = \pm v.$$

In this direction, the variation of the Hamiltonian (A.1) provides

$$-\frac{\partial^2}{\partial z^2}\phi_0(z) + \frac{g}{6}\phi_0^3(z) - \frac{m^2}{2}\phi_0(z) = 0. \tag{A.2}$$

This equation maintains for all $z \in [-\infty, \infty]$. Therefore, the constant values of ϕ_0 in the limits cancel out the second derivative, so that the vacuum expectation is

$$\frac{g}{6}v^3 = \frac{m^2}{2}v \quad \Rightarrow \quad v = \sqrt{\frac{3m^2}{g}} \tag{A.3}$$

besides the trivial solution $v = 0$. In equation (A.2), the z-direction was observed and can be rewritten more generally performing a saddle point evaluation

$$\frac{\partial^2}{\partial z^2}\phi_0 = V'(\phi_0) \tag{A.4}$$

Now a solution of (A.4) is searched, which gives a minimum of the Euler-Lagrange equation. It is a non-linear differential equation of second order that can be solved by using the substitution

$$\frac{\partial}{\partial z}\left(\phi'(z)\right)^2 = 2\frac{\partial}{\partial z}V'(\phi). \tag{A.5}$$

From integration, it follows

$$\begin{aligned} \int_a^z \mathrm{d}z &= \pm \int_0^\phi \frac{\mathrm{d}\tilde{\phi}}{\sqrt{2V[\tilde{\phi}]}} \\ &= \pm \int_0^\phi \frac{\mathrm{d}\tilde{\phi}}{\sqrt{\frac{g}{12}}(\tilde{\phi}^2 - v^2)} \\ \Leftrightarrow \quad z - a &\mp \sqrt{\frac{g}{12}}\frac{\operatorname{arctanh}\left(\frac{\phi}{v}\right)}{v}. \end{aligned}$$

Therefore, the solution

$$\phi_0(z) = \mp v \tanh\left[\frac{m}{2}(z-a)\right] \tag{A.6}$$

is obtained with (A.3). It shows, that from (A.5), two solutions follow, where the sign can be chosen.

A.2. Energy of the kink

The energy integral is given by the spatial integration over the Hamiltonian density

$$\mathcal{H}[\phi_0] = \frac{1}{2}(\nabla\phi_0)^2 + V[\phi_0].$$

The first derivative of the kink solution (A.6) is

$$\frac{\partial}{\partial z}\phi_0 = \frac{mv}{2}\operatorname{sech}^2\left[\frac{m}{2}(z-a)\right]. \tag{A.7}$$

Substituting this into the z-component of the energy integral ,

$$\begin{aligned} \int \mathrm{d}z \frac{1}{2}\left(\frac{\partial}{\partial z}\phi_0\right)^2 &= \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}u\, v^2\frac{m^2}{4}\operatorname{sech}^4\left(\frac{m}{2}u\right) \\ &= \frac{m^2}{8}\left[\frac{2\tanh\left(\frac{m}{2}u\right)\left[\operatorname{sech}^2\left(\frac{m}{2}u\right)+2\right]}{3m}\right]_{-\infty}^{\infty} \\ &= \frac{mv^2}{3} \end{aligned}$$

is obtained and with (A.3), it follows

$$\int \mathrm{d}z \frac{1}{2}\left(\frac{\partial}{\partial z}\phi_0\right)^2 = \frac{m^3}{g}.$$

The other spatial directions with the dilations L_1 and L_2 with periodic boundary conditions then lead to

$$\int \mathrm{d}^3x \frac{1}{2}\left(\nabla\phi_0\right)^2 = L_1 L_2 \frac{m^3}{g}.$$

The same result follows for the potential $V(\phi_0)$

$$\begin{aligned}
\int \mathrm{d}^3x V[\phi_0] &= \int \mathrm{d}^3x \left\{\frac{g}{4!}\phi_0^4 - \frac{m^2}{4}\phi_0^2 + \frac{3}{8}\frac{m^4}{g}\right\} \\
&= L_1 L_2 \int \mathrm{d}u \left\{\frac{g}{4!}v^4 \tanh^4(u) - \frac{m^2}{4}v^2 \tanh^2(u) + \frac{3}{8}\frac{m^4}{g}\right\} \\
&= L_1 L_2 \Bigg[\frac{g}{4!}v^4 \left\{u - \frac{8}{3m}\tanh(u) + \frac{2}{3m}\tanh(u)\,\mathrm{sech}^2(u)\right\} \\
&\qquad\qquad - \frac{m^2}{4}v^2(u - \tanh(u)) + \frac{3}{8}\frac{m^4}{g}u\Bigg]_{-\infty}^{\infty}.
\end{aligned}$$

Now v can be substituted with (A.3) and the linear terms, each individually leading to divergence, cancel out, whereas the $\tanh(x)$ as an odd function cancels out too by symmetric limits

$$\begin{aligned}
\int \mathrm{d}^3x V(\phi_0) &= L_1 L_2 \left[\frac{g}{24}\frac{9m^4}{g^2}z - \frac{m^2}{4}\frac{3m^2}{g}z + \frac{3}{8}\frac{m^4}{g}z\right]_{-\infty}^{\infty} + L_1 L_2 \frac{m^3}{g} \\
&= L_1 L_2 \left[\left\{\frac{9}{24} - \frac{3}{4} + \frac{3}{8}\right\}\frac{m^4}{g}z\right]_{-\infty}^{\infty} = L_1 L_2 \frac{m^3}{g}
\end{aligned}$$

Therefore, the solution of the energy integral

$$H\left[\phi_0(\mathbf{x})\right] = 2L_1 L_2 \frac{m^3}{g}$$

is the energy of a kink.

B

Properties of special functions

B.1. The Gamma function

A generalization of the factorial $n!$, $n \in \mathbb{N}$ for real or complex numbers leads to the representation

$$\Gamma(n) = (n-1)!,$$

where the gamma function is defined as

$$\Gamma(z) = \int_0^\infty \mathrm{d}t t^{z-1} \mathrm{e}^{-t}$$

for all $z > 0$. For the factorial the following equation

$$(n+1)! = (n+1)n!$$

is valid for all $n \in \mathbb{N}$. This property can be transferred to the gamma function using integration by parts and the L'Hôpital rule

$$\Gamma(z+1) = z\Gamma(z) \quad \Rightarrow \quad \Gamma(z) = (z-1)\Gamma(z-1). \tag{B.1}$$

This recursive property can be used to define the gamma function on all real numbers z, except for nonpositive integers. A specific value of the Gamma function is

$$\Gamma(1/2) = \sqrt{\pi}, \tag{B.2}$$

which results by a substitution $t \to \sqrt{t}$ in the above integral giving a Gaussian integral. With this value, all values of half integer numbers can be achieved by (B.1).

Another important result is the reflection formula for $0 < z < 1$ due to L. Euler [AAR99] that reads

$$\Gamma(1-z)\Gamma(z) = \frac{\pi}{\sin(\pi z)}, \tag{B.3}$$

which can be used to calculate the products

$$\Gamma(1/2)\Gamma(1/2) = \pi \tag{B.4}$$
$$\Gamma(-1/2)\Gamma(1/2) = \Gamma(-1/2+1-1)\Gamma(1/2) = -2\Gamma(1/2)\Gamma(1/2) = -2\pi, \tag{B.5}$$

where (B.1) was used in the second relation. The following relations are obtained from the result $\Gamma(1) = 1$ and (B.1) or obtained from the derivatives of the gamma function given in [AAR99] and [BMMS13]

$$\frac{1}{\Gamma(0)} = 0 \tag{B.6}$$
$$\Gamma'(1) = -\gamma \tag{B.7}$$
$$\Gamma'(0) \to \infty \tag{B.8}$$
$$\Gamma'(1/2) = -\sqrt{\pi}(\gamma + \ln 4), \tag{B.9}$$
$$\lim_{z\to 0} \frac{\mathrm{d}}{\mathrm{d}z} \frac{1}{\Gamma(z)} = 1 \tag{B.10}$$
$$\lim_{z\to 0} \frac{\mathrm{d}}{\mathrm{d}z} \frac{1}{\Gamma(1-z)} = \gamma, \tag{B.11}$$

where γ is the Euler-Mascheroni constant.

B.2. The Euler beta function

The beta function is closely related to the gamma function. It is defined by

$$B(x,y) = \int_0^\infty \frac{t^{x-1}}{(1+t)^{x+y}}\,\mathrm{d}t$$

for $\Re(x) > 0$ and $\Re(y) > 0$. By the following representation

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)},$$

the analytic continuation of the gamma function applies. The beta function is used in this thesis to evaluate expressions like

$$\lim_{z\to 0} \frac{\mathrm{d}}{\mathrm{d}z} I(z) = \lim_{z\to 0} \frac{\mathrm{d}}{\mathrm{d}z} \int_{-\infty}^{\infty} \mathrm{d}x (a^2 + x^2)^{-z} \tag{B.12}$$
$$= 2 \lim_{z\to 0} \frac{\mathrm{d}}{\mathrm{d}z} \int_0^\infty \mathrm{d}x (a^2 + x^2)^{-z} \tag{B.13}$$

for any a and by the substitution $t = x^2/a^2$, $\mathrm{d}t = 2x/a^2\mathrm{d}x$, the integral becomes

$$\begin{aligned} I(z) &= \int_0^\infty \mathrm{d}t \frac{a^2\sqrt{t}}{(a^2+a^2t)^z} \\ &= a^{1-2z}\int_0^\infty \mathrm{d}t \frac{t^{1/2}}{(1+t)^z} \\ &= a^{1-2z}B(1/2, z-1/2). \end{aligned}$$

And the derivative with respect to z is

$$I'(z) = -2\ln(a)a^{1-2z}B(1/2, z-1/2) + a^{1-2z}B'(1/2, z-1/2), \tag{B.14}$$

where in the limit $z \to 0$, the first term vanishes according to $B(1/2, z-1/2) \to 0$. Because of (B.6) the derivative of the beta function is given by the derivatives of the gamma function which give here

$$\begin{aligned} \lim_{z\to 0} B'(1/2, z-1/2) &= \lim_{z\to 0} \Gamma(1/2)\frac{\Gamma'(z-1/2)\Gamma(z) - \Gamma(z-1/2)\Gamma'(z)}{\Gamma^2(z)} \\ &= -\sqrt{\pi}\lim_{z\to 0}\frac{-2\sqrt{\pi}\Gamma'(z)}{\Gamma^2(z)}. \end{aligned}$$

This expression gives

$$\lim_{z\to 0}\frac{\Gamma'(z)}{\Gamma^2(z)} = -\lim_{z\to 0}\frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\Gamma(z)} = -1$$

from (B.10). Conclusively for (B.12)

$$\lim_{z\to 0}\frac{\mathrm{d}}{\mathrm{d}z}I(z) = -2\pi a. \tag{B.15}$$

Instead of the limit $z \to 0$, in another calculation the limit $z \to 1$ is needed. Beginning with (B.14), it follows

$$\lim_{z\to 1}\frac{\mathrm{d}}{\mathrm{d}z}I(z) = -2\ln(a)a^{-1}\pi + a^{-1}(-\pi\ln 4), \tag{B.16}$$

where in the first term, the value of the gamma function at 1/2 was used and in the second term, the values of the derivative of the gamma function (B.7) and (B.9) were used.

B.3. The Riemann zeta function

The Riemann zeta function gives a connection between series and integrals. The famous series

$$\zeta(z) = \sum_{n=1}^{\infty} n^{-z}, \tag{B.17}$$

which converges for $\Re(z) > 1$, can also be defined as the integral

$$\zeta(z) = \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t \frac{t^{z-1}}{\mathrm{e}^t - 1}. \tag{B.18}$$

The zeta function can be continued analytically by the so called reflection formula (using the reflection property of the gamma function)

$$\pi^{-s/2}\Gamma(s/2)\zeta(s) = \pi^{1/2-s/2}\Gamma(1/2 - s/2)\zeta(1-s) \tag{B.19}$$

$$\zeta(s) = 2^s \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(1-s)\zeta(1-s) \tag{B.20}$$

so that the zeta function is defined for any $z \in \mathbb{C}\backslash\{1\}$. The reflection formula provides the surprising solution

$$\zeta(-1) = \sum_n n = -\frac{1}{12}. \tag{B.21}$$

The value at $s = 0$ is the sum

$$\zeta(0) = \sum_n 1 = -\frac{1}{2}. \tag{B.22}$$

Another important value is

$$\zeta(2) = \sum_n n^{-2} = \frac{\pi^2}{6}. \tag{B.23}$$

The derivative of the zeta function provides [AAR99]

$$\zeta'(0) = -\frac{1}{2} \ln(2\pi). \tag{B.24}$$

C

THE ERROR FUNCTION INTEGRAL

The integral

$$\int_{-\infty}^{\infty} f(x)\mathrm{d}x = \int_{-\infty}^{\infty} \mathrm{d}x \frac{\mathrm{e}^{-t(x^2+a^2)}}{x^2+a^2} \tag{C.1}$$

for $a > 0$ needs to be solved. For this the following expression can be achieved

$$\int_{-\infty}^{\infty} \mathrm{d}x \frac{\mathrm{e}^{-t(x^2+a^2)}}{x^2+a^2} = \int_{-\infty}^{\infty} \mathrm{d}x \left(\frac{1}{x^2+a^2} - \int_{0}^{t} \mathrm{d}\alpha \mathrm{e}^{-\alpha(x^2+a^2)} \right), \tag{C.2}$$

because the function $f(x)$ can be rewritten by the following integral

$$\int_{0}^{t} \mathrm{d}\alpha \mathrm{e}^{-\alpha(x^2+a^2)} = -\frac{\mathrm{e}^{-t(x^2+a^2)}}{x^2+a^2} + \frac{1}{x^2+a^2},$$

using the derivative. This has been used in (C.2) to replace $\eta(x)$ in (C.1).

The integral over the first term in (C.2) is easy to perform by using the arctan. The result is for $a > 0$

$$\int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{x^2+a^2} = \frac{\pi}{a}. \tag{C.3}$$

Succeeding, the second term has to be solved. From the theorem of Fubini follows

$$\int_{-\infty}^{\infty} \mathrm{d}x \int_{0}^{t} \mathrm{d}\alpha \mathrm{e}^{-\alpha(x^2+a^2)} = \int_{0}^{t} \mathrm{d}\alpha \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-\alpha(x^2+a^2)}.$$

By substituting $z = \sqrt{\alpha}x$, this integral separates into two parts which can be solved independently

$$\int_0^t \mathrm{d}\alpha \frac{\mathrm{e}^{-a^2\alpha}}{\sqrt{\alpha}} \int_{-\infty}^{\infty} \mathrm{d}z \mathrm{e}^{-z^2}.$$

The inner integral here is the Gaussian integral. The solution can be obtained by going over to polar coordinates

$$\int_{-\infty}^{\infty} \mathrm{d}z \mathrm{e}^{-z^2} = \sqrt{\pi}. \tag{C.4}$$

Finally, the integral

$$I = \sqrt{\pi} \int_0^t \mathrm{d}\alpha \frac{\mathrm{e}^{-a^2\alpha}}{\sqrt{\alpha}} \tag{C.5}$$

needs to be solved. Here, the lower boundary of the integral is zero, so that the improper integral has to be solved, taking the limit

$$\lim_{\beta \to 0} \int_\beta^t \mathrm{d}\alpha \frac{\mathrm{e}^{-a^2\alpha}}{\sqrt{\alpha}}.$$

By substituting $u = a\sqrt{\alpha}$, the limit $\beta \to 0$ can be taken

$$\begin{aligned} \lim_{\beta \to 0} \int_{a\sqrt{\beta}}^{a\sqrt{t}} \frac{2\sqrt{\alpha}}{a} \mathrm{d}u \frac{\mathrm{e}^{-u^2}}{\sqrt{\alpha}} &= \lim_{\beta \to 0} \frac{2}{a} \int_{a\sqrt{\beta}}^{a\sqrt{t}} \mathrm{d}u \mathrm{e}^{-u^2} \\ &= \lim_{\beta \to 0} \frac{2}{a} \left(\int_{-\infty}^{a\sqrt{t}} \mathrm{d}u \mathrm{e}^{-u^2} - \int_{-\infty}^{a\sqrt{\beta}} \mathrm{d}u \mathrm{e}^{-u^2} \right) \\ &= \frac{2}{a} \int_{-\infty}^{a\sqrt{t}} \mathrm{d}u \mathrm{e}^{-u^2} - \frac{\sqrt{\pi}}{a}. \end{aligned}$$

The Gaussian integral is symmetric and its value is $\sqrt{\pi}$. We can use this property to rewrite the integral above because the upper boundary is $a\sqrt{t} > 0$. Thus, the integration from $-\infty$ to 0 can be taken out and the integral can be rewritten in terms of the error function $\mathrm{erf}(x)$

$$\begin{aligned} \int_{-\infty}^{a\sqrt{t}} \mathrm{d}u \mathrm{e}^{-u^2} &= \frac{\sqrt{\pi}}{2} + \int_0^{a\sqrt{t}} \mathrm{d}u \mathrm{e}^{-u^2} \\ &= \frac{\sqrt{\pi}}{2} + \frac{\sqrt{\pi}}{2} \mathrm{erf}(a\sqrt{t}). \end{aligned}$$

Finally, the integral (C.5) reads

$$I = \frac{\pi}{a} + \frac{\pi}{a}\operatorname{erf}(a\sqrt{t}) - \frac{\pi}{a} = \frac{\pi}{a}\operatorname{erf}(a\sqrt{t}),$$

which can together with the solution of the first part (C.3) be used in (C.2) to solve the problem

$$\begin{aligned}\int\limits_{-\infty}^{\infty} \mathrm{d}x \frac{\mathrm{e}^{-t(x^2+a^2)}}{x^2+a^2} &= \frac{\pi}{a} - \frac{\pi}{a}\operatorname{erf}(a\sqrt{t}) \\ &= \frac{\pi}{a}\left(1 - \operatorname{erf}(a\sqrt{t})\right).\end{aligned}$$

D

Calculation of ζ_1

The following integral is going to be evaluated

$$\begin{aligned} \zeta_1(z) &= \frac{1}{\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-1} L_1 L_2 (4\pi t)^{-1} \left[\tilde{K}_t(Q) - 1\right] \\ &= \frac{L_1 L_2}{4\pi\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-2} \mathrm{e}^{-3m^2 t/4} + \frac{L_1 L_2}{4\pi\Gamma(z)} \int_0^\infty \mathrm{d}t t^{z-2} \int_{-\infty}^\infty \mathrm{d}p g(p) \mathrm{e}^{-t(m^2+p^2)}, \end{aligned} \tag{D.1}$$

where the derivative with respect to z is going to be taken in the limit $z \to 0$. Substituting $x = 3/4m^2 t$ and $y = (m^2 + p^2)t$ in (D.1) leads to the following integral, replacing $L_1 L_2 / 4\pi =: C$ by a constant C

$$\zeta_1(z) = \frac{C}{\Gamma(z)} \left[\int_0^\infty \mathrm{d}x \left(\frac{4}{3m^2}\right)^{z-1} x^{z-2} \mathrm{e}^{-x} + \int_{-\infty}^\infty \mathrm{d}p g(p) \int_0^\infty \mathrm{d}y \frac{y^{z-2}\mathrm{e}^{-y}}{(m^2+p^2)^{z-1}} \right].$$

The first integral here is a representation of the Γ function and gives $\Gamma(z-1)$. The second integral evaluated with respect to y gives the same contribution $\Gamma(z-1)$. Then the integral reads

$$\zeta_1(z) = C \left[\frac{\Gamma(z-1)}{\Gamma(z)} \left(\frac{4}{3m^2}\right)^{z-1} + \frac{\Gamma(z-1)}{\Gamma(z)} \int_{-\infty}^\infty \mathrm{d}p g(p) (m^2+p^2)^{1-z} \right]$$

The first contribution is

$$\begin{aligned} F_0(z) &= \frac{1}{z-1} \left(\frac{3m^2}{4}\right)^{1-z} \\ \Rightarrow \quad F_0'(0) &= -\frac{3m^2}{4} + \frac{3}{4} \ln\frac{3}{4} + \frac{3}{2} \ln m \end{aligned}$$

This leaves the integral

$$I = \frac{\Gamma(z-1)}{\Gamma(z)} \int\limits_{-\infty}^{\infty} \mathrm{d}p g(p)(m^2+p^2)^{1-z} \tag{D.2}$$

to be evaluated. The spectral density (4.30)

$$g(p) = -\frac{m}{2\pi}\left(\frac{2}{p^2+m^2} + \frac{1}{p^2+\frac{m^2}{4}}\right)$$

can be transformed into

$$g(p) = -\frac{m}{2\pi}\left(\frac{3}{p^2+m^2} + \frac{\frac{3m^2}{4}}{(p^2+m^2)^2} + \frac{\left(\frac{3m^2}{4}\right)^2}{(p^2+m^2)^2(p^2+\frac{m^2}{4})}\right).$$

The following three integrals are gained for (D.2) using this spectral density

$$\begin{aligned}
F_1(z) &= -\frac{1}{z-1}\frac{3m}{2\pi}\int\limits_{-\infty}^{\infty}\mathrm{d}p(p^2+m^2)^{-z} \\
&= -\frac{1}{z-1}\frac{3}{2\pi}m^{2-2z}\int\limits_{-\infty}^{\infty}\mathrm{d}p(p^2+1)^{-z} \\
F_2(z) &= -\frac{1}{z-1}\frac{3m^3}{8\pi}\int\limits_{-\infty}^{\infty}\mathrm{d}p(p^2+m^2)^{-1-z} \\
&= -\frac{1}{z-1}\frac{3}{8\pi}m^{2-2z}\int\limits_{-\infty}^{\infty}\mathrm{d}p(p^2+1)^{-1-z} \\
F_3(z) &= -\frac{1}{z-1}\frac{m}{2\pi}\left(\frac{3m^2}{4}\right)^2\int\limits_{-\infty}^{\infty}\mathrm{d}p\frac{1}{(p^2+m^2)^{1+z}(p^2+\frac{m^2}{4})} \\
&= -\frac{1}{z-1}\frac{m^{1-2z}}{2\pi}\left(\frac{3}{4}\right)^2\int\limits_{-\infty}^{\infty}\mathrm{d}p\frac{1}{(p^2+1)^{1+z}(p^2+\frac{1}{4})},
\end{aligned}$$

Here, all transformations can be achieved by a substitution of $p \to pm$. The solution for F_1 can be found be the beta function

$$\begin{aligned}
F_1(z) &= -\frac{1}{z-1}\frac{3m^{2-2z}}{2\pi}B(1/2, z-1/2) \\
\Rightarrow \quad F_1'(0) &= \frac{3}{2\pi}m^2(-2\pi) = -3m^2,
\end{aligned}$$

where the derivative of the beta function and $B(1/2,-1/2)=0$ has been used. The second integral F_2 is found in the same manner

$$F_2'(z) = -\left(-\frac{1}{(z^2-1)}\frac{3}{8\pi}m^{2-2z} - \frac{2}{z-1}\frac{3}{8\pi}m^{2-2z}\ln m\right)\int_{-\infty}^{\infty} \mathrm{d}p(p^2+1)^{-1-z}$$

$$- \frac{1}{z-1}\frac{3}{8\pi}m^{2-2z}\frac{\mathrm{d}}{\mathrm{d}z}\int_{-\infty}^{\infty} \mathrm{d}p(p^2+1)^{-1-z}$$

$$\Rightarrow \quad F_2'(0) = m^2\left(\frac{3}{8\pi} - \frac{3}{4\pi}\ln m\right)\int_{-\infty}^{\infty} \mathrm{d}p(p^2+1)^{-1}$$

$$- \lim_{z\to 0}\frac{1}{z-1}\frac{3}{8\pi}m^{2-2z}\frac{\mathrm{d}}{\mathrm{d}z}\int_{-\infty}^{\infty} \mathrm{d}p(p^2+1)^{-1-z}$$

The first integral gives

$$\int \mathrm{d}p(p^2+1)^{-1} = B(1/2,1/2) = \pi,$$

by the transformation of the integral into a beta function (see B.2). The second integral can solved with beta function ($s = z+1$) as well

$$\frac{\mathrm{d}}{\mathrm{d}s}\int_{-\infty}^{\infty} \mathrm{d}p(p^2+1)^{-s} = B'(1/2, s-1/2) \to -2\pi\ln 2$$

and the expression becomes

$$-\frac{3}{4}m^2\ln 2.$$

Therefore, in the limit $z\to 0$ the expression is

$$F_2'(0) = \frac{3m^2}{4}\left(\frac{1}{2} - \ln m\right) - \frac{3}{4}m^2\ln 2.$$

For F_3 the following applies

$$F_3'(z) = -\frac{9m}{32\pi}\left(-\frac{1}{(z-1)^2}m^{-2z} + \frac{2}{z-1}m^{-2z}\ln m\right)\int_{-\infty}^{\infty} \mathrm{d}p\frac{1}{(p^2+1)^{1+z}(p^2+\frac{1}{4})}$$

$$- \frac{9m}{32\pi}\frac{1}{z-1}m^{-2z}\frac{\mathrm{d}}{\mathrm{d}z}\int_{-\infty}^{\infty} \mathrm{d}p\frac{1}{(p^2+1)^{1+z}(p^2+\frac{1}{4})}$$

$$\Rightarrow \quad F_3'(0) = \frac{9m}{32\pi}(1-2\ln m)\int_{-\infty}^{\infty} \mathrm{d}p\frac{1}{(p^2+1)(p^2+\frac{1}{4})}$$

$$+ \lim_{z\to 0}\frac{9m}{32\pi}\frac{\mathrm{d}}{\mathrm{d}z}\int_{-\infty}^{\infty} \mathrm{d}p\frac{1}{(p^2+1)^{1+z}(p^2+\frac{1}{4})}.$$

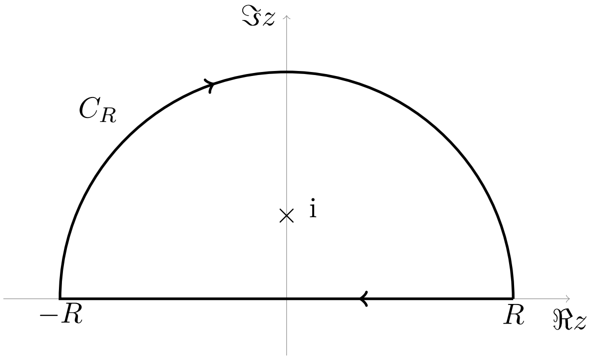

Figure D.1.: Contour Γ_R in order to integrate the integral (D.5).

As the second integral converges, the following expression is achieved

$$\lim_{z\to 0}\frac{\mathrm{d}}{\mathrm{d}z}\int_{-\infty}^{\infty}\mathrm{d}p\frac{1}{(1+p^2)^{1+z}(p^2+\frac{1}{4})}=-\int_{-\infty}^{\infty}\mathrm{d}p\frac{\ln(p^2+1)}{(1+p^2)(p^2+\frac{1}{4})}. \tag{D.3}$$

For both integrals in (D.3), a fraction decomposition can be applied, leaving for the first integral

$$\frac{4}{3}\int_{-\infty}^{\infty}\mathrm{d}p\left[\frac{1}{p^2+\frac{1}{4}}-\frac{1}{p^2+1}\right]=\frac{4}{3}\pi,$$

because of the arcus tangens again. For the second integral, the following is achieved

$$\frac{4}{3}\int_{-\infty}^{\infty}\mathrm{d}p\left[\frac{\ln(p^2+1)}{p^2+1/4}-\frac{\ln(p^2+1)}{p^2+1}\right], \tag{D.4}$$

which can be evaluated in the complex plane (see figure D.1) considering the integral

$$\oint_{\Gamma_R}\mathrm{d}z\frac{\ln(z+i)}{z^2+1}. \tag{D.5}$$

This integral can be evaluated due to the residue theorem because of the the residue at $z=i$

$$\oint_{\Gamma_R}\mathrm{d}z\frac{\ln(z+i)}{z^2+1}=\mathrm{Res}_{z=i}\left(\frac{\ln(z+i)}{z^2+1}\right)=2\pi\mathrm{i}\frac{\ln(2\mathrm{i})}{2\mathrm{i}}=\pi\left(\ln 2+\frac{\mathrm{i}\pi}{2}\right), \tag{D.6}$$

where the last expression follows because of the complex logarithm. The integral

$$\begin{aligned}\int_{-R}^{R}\mathrm{d}x\frac{\ln(x+\mathrm{i})}{x^2+1}&=\int_{0}^{R}\mathrm{d}x\frac{\ln(-x+\mathrm{i})}{x^2+1}+\int_{0}^{R}\mathrm{d}x\frac{\ln(x+\mathrm{i})}{x^2+1}\\&=\int_{0}^{R}\mathrm{d}x\frac{\ln(x^2+1)+\mathrm{i}\pi}{x^2+1}\end{aligned}$$

then follows by equaling the real parts, because the integral over the contour C_R goes to zero as $R \to \infty$. The solution (D.6) the limit $R \to \infty$ is given by

$$\pi \left(\ln 2 + \frac{\mathrm{i}\pi}{2} \right) = \int_0^\infty \mathrm{d}x \frac{\ln(x^2+1) + \mathrm{i}\pi}{x^2+1}.$$

Therefore, equaling the real parts, the solution of the second term in (D.4) is

$$\int \mathrm{d}p \frac{\ln(p^2+1)}{p^2+1} = 2\pi \ln 2,$$

while for the first term the same procedure applies, resulting in

$$\int \mathrm{d}p \frac{\ln(p^2+1)}{p^2+\frac{1}{4}} = 2\pi \ln \frac{9}{4}.$$

And together the expression (D.4) results in

$$\frac{8\pi}{3} \left(\ln \frac{9}{4} - \ln 2 \right) = \frac{8\pi}{3} \ln \frac{9}{8},$$

giving

$$F_3'(0) = \frac{3m^2}{8} (1 - 2 \ln m) - \frac{3m^2}{4} \ln \frac{9}{8}.$$

Conclusively, the contribution of $\zeta_1(z)$ is given by

$$\begin{aligned}
\zeta_1'(0) = C\Big(& -\frac{3m^2}{4} + \frac{3m^2}{4} \ln \frac{3}{4} + \frac{3m^2}{2} \ln m \\
& - 3m^2 \\
& + \frac{3m^2}{8} - \frac{3m^2}{4} \ln m - \frac{3m^2}{4} \ln 2 \\
& + \frac{3m^2}{8} - \frac{3m^2}{4} \ln m - \frac{3m^2}{4} \ln \frac{9}{8} \Big) \\
= Cm^2 & \left(-3 + \frac{3}{4} (2 \ln m - \ln m - \ln m) + \frac{3}{4} \left(\ln \frac{3}{4} - \ln 2 - \ln \frac{9}{8} \right) \right) \\
= -Cm^2 & \left(3 + \frac{3}{4} \ln 3 \right).
\end{aligned}$$

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Erklärung zur Masterarbeit

Hiermit versichere ich, dass die vorliegende Arbeit über "Geometric dependence of interface fluctuations" selbstständig verfasst worden ist, dass keine anderen Quellen und Hilfsmittel als die angegebenen benutzt worden sind und dass die Stellen der Arbeit, die anderen Werken – auch elektronischen Medien – dem Wortlaut oder Sinn nach entnommen wurden, auf jeden Fall unter Angabe der Quelle als Entlehnung kenntlich gemacht worden sind.

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