Gaussian Model and Additivity

Gaußsches Modell und Additivität

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Abstract

Additivity is one possible generalisation of the concept of extensivity of thermodynamic quantities for **finite** physical systems in thermal equilibrium. This thesis concerns itself with the additivity of the Gaussian model of a ferromagnet, originally introduced by Berlin and Kac in 1952. The main focus of the thesis lies on the treatment of the next-neighbour Gaussian model on finite lattice domains in two dimensions. Given a lattice domain $\mathcal{D} \subset \mathbb{Z}^d$, the free energy βF of an additive system at inverse temperature β can be written as

$$\beta F(\mathcal{D};\beta) = \sum_{n=0}^{d} f_n(\beta)\, M_n^{(d)}(\mathcal{D}) + R(\mathcal{D};\beta), \tag{1}$$

where $M_n^{(d)}(\mathcal{D})$ are the $d+1$ basic geometric measures of $\mathcal{D}$, the so-called Minkowski functionals. In two dimensions $M_0^{(2)}(\mathcal{D})$, $M_1^{(2)}(\mathcal{D})$ and $M_2^{(2)}(\mathcal{D})$ are the volume, the surface area and the Euler number of $\mathcal{D}$, respectively. The geometric quantities $M_n^{(d)}(\mathcal{D})$ for $n \geq 1$ stem from the boundary $\partial\mathcal{D}$ of the system and are negligible compared to the volume $M_0^{(d)}(\mathcal{D})$ for infinitely large systems. The coefficients f_i correspond to thermodynamic quantities like pressure, surface tension, bending rigidities, etc. and only depend on the dimension d, the temperature and the spin interaction parameters. The remaining term R decays exponentially with the system size $|\mathcal{D}|$ in the thermodynamic limit for non-critical temperatures. The main result of this thesis is that the additivity of the Gaussian model, i.e. Eq. (1), holds

- for convex domains $\mathcal{D}$ in arbitrary dimensions, see Chap. II.2. The coefficients f_i are calculated explicitly analytically and discussed for $d \leq 3$. For $d > 3$, the tools for a straight-forward calculation of the coefficients f_i are laid out.
- for convex domains with an applied homogeneous magnetic field in one and two dimensions and a homogeneous boundary field in two dimensions, see Chap. II.3. The corresponding modifications of the coefficients f_i are calculated. The magnetic field breaks the symmetry between the ferromagnetic and antiferromagnetic spin-spin coupling.

On the other hand, the additivity breaks down

- at the critical temperature and/or spin coupling strength in arbitrary dimensions, where the correlation length of the system diverges. In this case, the remaining term R in Eq. (1) is $\mathcal{O}(\log|\mathcal{D}|)$ instead of exponentially decaying with the system size, see Chap. II.2.
- for non-convex domains $\mathcal{D}$ in two dimensions. In this case, the Euler number $M_2^{(2)}(\mathcal{D})$ in Eq. (1) has to be replaced with the number of convex corners of $\mathcal{D}$ multiplied with the coefficient $f_2/4$ plus the number of concave corners of $\mathcal{D}$ multiplied with the coefficient $\tilde{f}_2/4$. The coefficient f_2 is calculated analytically, the coefficient $\tilde{f}_2$ is determined numerically in Part. III. $\tilde{f}_2$ is linearly

independent of $f_0,\ f_1,\ f_2$. All additional contributions still decay exponentially in the thermodynamic limit for non-critical temperatures and spin coupling parameters.

- for long-range spin-spin interactions. The free energy of a Gaussian spin chain with quadratically decaying spin-spin interactions features a remaining term R which decays as $|\mathcal{D}|^{-2}$ instead of exponentially, see Chap. IV.2. In general, the additivity breaks down in the presence of long-range interactions.

Furthermore the partition sum of the next-neighbour Gaussian model on triangular and hexagonal lattice types is calculated. Corresponding mathematical properties and arising difficulties are discussed in Chap. IV.1.

Concluding, this thesis shows that the free energy of the next-neighbour Gaussian model in two dimensions obeys a decomposition similar to Eq. (1), although the extensive thermodynamic quantities of the model are in general not strictly additive.

Zusammenfassung

Additivität ist eine Verallgemeinerung des Konzepts der Extensivität für **endliche** physikalische Systeme im thermischen Gleichgewicht. Diese Arbeit untersucht die Additivität des Gauß'schen Modells eines Ferromagneten, welches 1952 von Berlin und Kac eingeführt wurde. Der Schwerpunkt der Arbeit liegt auf der Untersuchung des zweidimensionalen Gauß'schen Modells mit nächste-Nachbar Wechselwirkungen auf endlichen Gitterdomänen. Sei $\mathcal{D} \subset \mathbb{Z}^d$ eine endliche Gitterdomäne. Die freie Energie βF eines additiven physikalischen Systems bei inverser Temperatur β hat die Form

$$\beta F(\mathcal{D};\beta) = \sum_{n=0}^{d} f_n(\beta)\, M_n^{(d)}(\mathcal{D}) + R(\mathcal{D};\beta). \tag{1}$$

$M_n^{(d)}(\mathcal{D})$ sind die $d+1$ geometrischen Maße der Domäne $\mathcal{D}$, die sogenannten Minkowski-Funktionale. In zwei Dimensionen sind $M_0^{(2)}(\mathcal{D})$, $M_1^{(2)}(\mathcal{D})$ und $M_2^{(2)}(\mathcal{D})$ das Volumen, die Oberfläche und die Euler-Zahl von $\mathcal{D}$. Die Größen $M_n^{(d)}(\mathcal{D})$ mit $n \geq 1$ sind geometrische Maße der Oberfläche $\partial\mathcal{D}$ von $\mathcal{D}$ und sind im Grenzwert unendlich großer Systeme verschwindend gering verglichen mit dem Volumen $M_0^{(d)}(\mathcal{D})$. Die Koeffizienten f_i entsprechen thermodynamischen Größen wie Druck, Oberflächenspannung und Biegesteifigkeit und hängen nur von der Dimension d des Systems, der Temperatur und der Art der Spin-Spin Wechselwirkung ab. Der Restterm R verschwindet exponentiell mit der Systemgröße $|\mathcal{D}| \equiv M_0^{(d)}(\mathcal{D})$ im thermodynamischen Limes. Ein wesentliches Ergebnis dieser Arbeit ist der Nachweis, dass das Gauß'sche Modell unter folgenden Bedingungen additiv ist, d.h. Eq. (1) erfüllt:

- Für konvexe Domänen $\mathcal{D}$ in beliebiger Dimension für nicht-kritische Temperaturen. Die Koeffizienten f_i werden in Chap. II.2 explizit analytisch berechnet und diskutiert für ein-, zwei- und dreiminesionale Systeme. In höheren Dimensionen werden die relevanten mathematischen Größen des Gauß'schen Modells weitgehend bestimmt, sodass die Berechnung der Koeffizienten f_i einfach erfolgen kann.

- Für konvexe Domänen mit einem räumlich konstanten magnetischen Feld in einer und zwei Dimensionen, sowie mit einem konstanten Randfeld in zwei Dimensionen. Die entprechenden Korrekturen der Koeffizienten f_i werden in Chap. II.3 explizit analytisch berechnet. Das Magnetfeld zerstört die Symmetrie zwischen ferromagnetischer und antiferromagnetischer Spin-Spin Kopplung.

Es weiteres Ergebnis dieser Arbeit ist, dass die Additivität des Gauß'schen Modells unter folgenden Bedingungen nicht mehr erfüllt ist:

- Bei kritischer Temperatur, bei der die Korrelationslänge des Systems divergiert. In diesem Fall ist der Restterm R in Eq. (1) von der Ordnung $\mathcal{O}(\log|\mathcal{D}|)$ und nicht mehr exponentiell verschwindend, siehe Chap. II.2.

- Für nichtkonvexe Domänen $\mathcal{D}$ in zwei Dimensionen. In diesem Fall muss die Euler-Zahl $M_2^{(2)}(\mathcal{D})$ in Eq. (1) durch die Anzahl der konvexen Ecken von $\mathcal{D}$, multipliziert mit $f_2/4$, plus die Anzahl der konkaven Ecken von $\mathcal{D}$, multpliziert mit einem Koeffizienten $\tilde{f}_2/4$ ersetzt werden. Der Koeffizient f_2 wird analytisch bestimmt. Der Koeffzient $\tilde{f}_2$ wird in Part. III numerisch bestimmt. $\tilde{f}_2$ ist linear unabhängig von $f_0,\ f_1,\ f_2$. Alle zusätzlichen Beiträge zur freien Energie verschwinden exponentiell mit der Systemgröße bei nichtkritischer Temperatur.

- Bei langreichweitigen Spin-Spin Wechselwirkungen. Die freie Energie des eindimensionalen Gauß'schen Systems mit quadratisch abfallenden Wechselwirkungen weist einen Restterm R auf, der quadratisch – und nicht exponentiell – mit der Systemgröße abfällt, siehe Chap. IV.2. Im Allgemeinen kann man bei langreichweitigen Wechselwirkungen keine Additivität annehmen.

Darüber hinaus wird in Chap. IV.1 die Zustandssumme des Gauß'schen Modells auf dem hexagonalen und dem Dreicks-Gitter berechnet. Es werden die entsprechenden mathematischen Eigenschaften diskutiert.

Zusammenfassend wird im Rahmen dieser Arbeit gezeigt, dass, obwohl das zweidimensionale Gauß'sche Modells mit nächste-Nachbar Wechselwirkung nicht strikt additiv ist, die freie Energie als eine Linearkombination der geometrischen Maße der grundlegenden Gitterdomäne geschrieben werden kann, ähnlich zu Eq. (1).

Contents

Part I.

Additivity in thermodynamics

This thesis concerns itself with the notion of *additivity* of physical systems in thermodynamic equilibrium. In order to illustrate the basic ideas, we consider the grand potential $\Omega[\mathcal{D};\beta,\mu]$ of a fluid at inverse temperature β and chemical potential μ, confined in the domain $\mathcal{D} \subseteq \mathbb{R}^3$, which is a closed subset of the three-dimensional space. One generally assumes that Ω is extensive, i.e. proportional to the volume $V(\mathcal{D}) \equiv |\mathcal{D}|$ of the system, with the proportionality constant equal to the negative pressure p of the fluid:

$$\Omega(\mathcal{D};\beta,\mu) = -p(\beta,\mu)\,|\mathcal{D}|. \tag{I.0.1}$$

In general, this is only true for the thermodynamic limit, i.e. for infinitely large systems without boundaries. If we consider a finite system, the grand potential, as a function of the container $\mathcal{D}$, depends on the shape of the boundary $\partial\mathcal{D}$ of $\mathcal{D}$ in a complex way. However, in 1957 Hadwiger [5] developed a mathematical theorem, which states that any *motion invariant, continuous* and *additive* function of a closed subset $\mathcal{D}$ of $\mathbb{R}^3$ is a linear combination of the four basic geometric measures of $\mathcal{D}$: its volume, surface area, integrated mean and integrated Gaussian curvature of the boundary $\partial\mathcal{D}$, see [25], [21], [19] and [5] for details on Hadwiger theorem and integral geometry. We state the theorem and its prerequisites in a more rigorous way: Consider a real mapping Ω,

$$\Omega : K \to \mathbb{R},\ \mathcal{D} \mapsto \Omega(\mathcal{D}) \tag{I.0.2}$$

from the set K of finite unions of closed convex subsets of $\mathbb{R}$. We say that Ω is

(i) Motion invariant: if rotating and/or translating the body $\mathcal{D}$ does not change the value of Ω, i.e. for any combination g of rotations and translations

$$\Omega(g\,\mathcal{D}) = \Omega(\mathcal{D}).$$

(ii) Continuous: if for any sequence $(\mathcal{D}_n)_{n\in\mathbb{N}}$, $\mathcal{D}_n \in K$ converging[1] to $\mathcal{D}$, the values of the mapping converge, i.e.

$$\lim_{n\to\infty} \Omega(\mathcal{D}_n) = \Omega(\mathcal{D}).$$

(iii) Additive: if for any two bodies $\mathcal{D}_1,\ \mathcal{D}_2 \in K$ the function of the union $\mathcal{D}_1 \cup \mathcal{D}_2$ can be written as

$$\Omega(\mathcal{D}_1 \cup \mathcal{D}_2) = \Omega(\mathcal{D}_1) + \Omega(\mathcal{D}_2) - \Omega(\mathcal{D}_1 \cap \mathcal{D}_2).$$

Hadwiger's Theorem states, that for any mapping Ω, which fulfills the conditions $(i)...(iii)$ there exist unique real coefficients $f_0, ..., f_d$, such that

$$\Omega(\cdot) = \sum_{n=0}^{d} f_n\, M_n^{(d)}(\cdot). \tag{I.0.3}$$

Here, $M_n^{(d)}$ are the d so called Minkowski functionals, which in

[1] Convergence on the set K of convex subsets of $\mathbb{R}^d$ is defined in [5].

- $d = 1$ correspond to the volume, i.e. the length, and the Euler number (number of components of $\mathcal{D}$, if $\mathcal{D}$ non-convex),
- $d = 2$ correspond to the surface area, the circumference length and the Euler number of the body $\mathcal{D}$,
- $d = 3$ correspond to the volume, the surface area, the integrated mean curvature of $\partial\mathcal{D}$ and the integrated Gaussian curvature of $\partial\mathcal{D}$,
- higher dimensions correspond to well-defined geometrical measures of $\mathcal{D}$, see [25], [21], [19] and [5] for details.

If we, for the time-being, assume that the grand potential Ω of a gas confined to a container $\mathcal{D}$ fulfills $(i), ..., (iii)$, we straight-forwardly obtain a geometric decomposition of Ω as a linear combination of d geometric measures. The coefficients f_n of the linear combination correspond to thermodynamic functions like pressure, surface tension and bending rigidities. This would allow for a potent description of thermodynamics of confined systems. One can ask: For which physical systems does an extensive thermodynamic potential fulfill the prerequisites $(i)...(iii)$? It is reasonable to expect that for sufficiently smooth interaction potentials (ii) is fulfilled, i.e. the grand potential is continuous as a function of shape of the container $\mathcal{D}$. Also, in absence of external fields like gravitation, one can easily prove that Ω is motion-invariant, such that (i) is also fulfilled. However, the condition of additivity turns out to be more complicated. Let us consider a real gas confined in the container $\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2$, where $\mathcal{D}_1$, $\mathcal{D}_2$ are two separate containers: $\mathcal{D}_1 \cap \mathcal{D}_2 = \emptyset$, $\Omega(\mathcal{D}_1 \cap \mathcal{D}_2; \beta, \mu) = 0$. The grand potential can be written as

$$\Omega(\mathcal{D}_1 \cup \mathcal{D}_2; \beta, \mu) = \Omega(\mathcal{D}_1; \beta, \mu) + \Omega(\mathcal{D}_2; \beta, \mu) + \Delta\Omega,$$

Where $\Delta\Omega$ stems from the interaction of the particles in $\mathcal{D}_1$ with the ones in $\mathcal{D}_2$ and, in general, does not vanish, meaning that Ω is non-additive. However, motivated by the elegance and simplicity of Hadwiger's theorem, we formulate a more general version of the decomposition Eq. (I.0.3): Assume $\mathcal{D} \subset \mathbb{R}^d$ is the container, t, $\lambda \in \mathbb{R}$, $t > 0$, Ω the relevant extensive thermodynamic potential (for instance, we neglect all variables except $\mathcal{D}$). With $\lambda\mathcal{D} \subset \mathbb{R}$ we denote the container $\mathcal{D}$, scaled by the factor λ.

$$\Omega(\lambda\mathcal{D}) = \sum_{n=0}^{d} f_d \, M_n^{(d)}(\mathcal{D}) \, \lambda^n + \mathcal{O}\left(\mathrm{e}^{-t\,\lambda}\right), \quad \text{as } \lambda \to \infty. \tag{I.0.4}$$

The equality sign here refers to asymptotic equality in the limit of large scaling parameter λ. The first sum on the right-hand side corresponds to Eq. (I.0.3) from Hadwiger's theorem, the additional contribution accounts for any corrections to Hadwiger's theorem, which we assume to *decay exponentially* with the size λ of the system. Our *central question* now is: Which physical systems obey the decomposition Eq. (I.0.4), i.e. are "almost additive"? The validity of this description has been tested

in [13], it has been applied, among other fields, to protein folding in [22] and solvation of complex molecules in [18]. The main focus of this thesis lies on the question of additivity of the Gaussian model of ferromagnetism, which is tightly related to the spherical and the Ising models. To illustrate the underlying concepts, we treat real diluted gases and the Ising model within the framework of the decomposition Eq. (I.0.4). However, we start by discussing different possibilities to define geometrical measures of lattice containers.

I.1. Lattice containers and their geometrical measures

The main focus of this thesis lies on the treatment of the two-dimensional Gaussian model within the geometrical interpretation of its partition sum which goes hand in hand with the decomposition Eq. (I.0.4). The purpose of this section is to present and discuss different possibilities to define geometrical measures like volume, surface area and integrated curvatures of lattice domains. Furthermore, we briefly discuss the impact of different definitions of geometric measures on the decomposition Eq. (I.0.4). Let us consider a simple rectangular $N \times M$ lattice, e.g. the one depicted in Fig. I.0.1. Throughout this thesis, when talking about geometrical properties of this lattice, we refer to it as the "lattice container" or "lattice domain". Within the framework of a typical lattice model a spin is attached to each lattice site, spins being any real numbers in the case of a Gaussian system and from the set $\{-1, +1\}$ in the case of an Ising system. When talking about the geometrical properties of

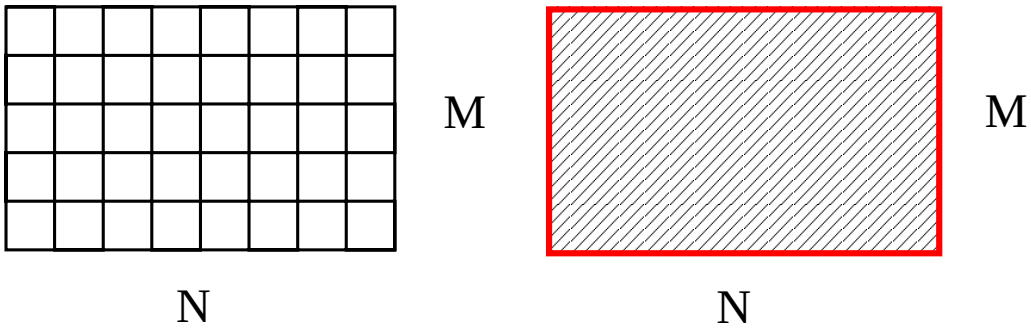

Figure I.0.1.: Left side: $N \times M$ lattice container. A spin is attached to each lattice site. Right side: illustration of the geometrical measures of the container – the shaded area corresponds to the volume of the system. The red thick line is the boundary of the system, its length corresponds to the surface area of the container.

the container in Fig. I.0.1, the intuitive approach would suggest that the volume of the container grows with the particle number, i.e. the number of lattice sites – and thus would correspond to the shaded area. On the other hand, one would expect the surface area to grow linearly with the circumference length – the length of the

thick red line in Fig. I.0.1. The third basic geometric measure of two-dimensional domains is the Euler number which can be calculated as the number of components of the domain minus the number of holes of the domain. The Euler number is illustrated in Fig. I.0.2. It is important to point out that, once the lattice domain is chosen, the Euler number stays constant when the domain is scaled up in the thermodynamic limit, e.g. the Euler number of the $N \times M$ rectangular lattice domain is 1, independent of $N,\ M$. Since the goal of this thesis is to obtain a decomposition of

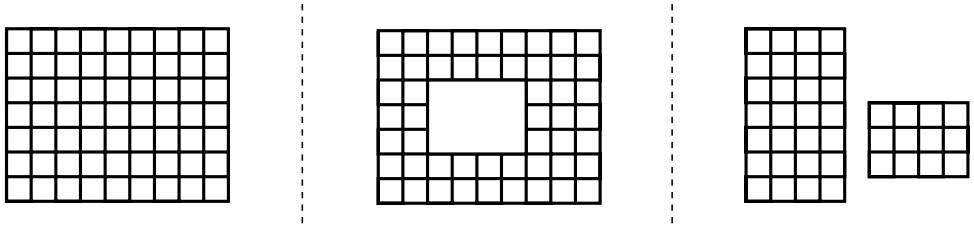

Figure I.0.2.: Illustration of the Euler number of a lattice container. The Euler number is the number of components of the domain minus the number of holes of the domain. The lattice on the left side has one component and zero holes. The lattice in the middle features one component and one hole – and thus the Euler number of zero. To raise the Euler number above 1, one has to introduce additional components to the lattice domains – the lattice domain on the right hand side consists of two components and zero holes and has the Euler number 2.

the free energy of the Gaussian system as a linear combination of the basic geometric measures of the underlying lattice domain, it is important to point out that there is a certain freedom in the choice of the exact definition of these geometric measures: Considering the $N \times M$ lattice, one could define the volume of the system as NM and the surface area as $2(N + M)$. The Euler number is constant, independent of $N,\ M$ and is always equal 1. Assuming Eq. (I.0.4) holds, one would obtain the free energy F (omitting all arguments except the geometrical measures)

$$\begin{aligned} F &= (\text{volume}) f_0 + (\text{surface area}) f_1 + (\text{euler number}) f_2 \\ &= NM\, f_0 + 2(N + M)\, f_1 + f_2, \end{aligned} \tag{I.0.5}$$

with the volume, surface, and corner coefficients $f_0,\ f_1,\ f_2$ respectively. These coefficients do not depend on the shape and the size of the lattice domain. Alternatively, one could define the geometric measures, as suggested in Fig. I.0.1: the volume would be $(N - 1)(M - 1)$ and the surface area $2(N + M - 2)$. This would merely lead to a redefinition of the thermodynamic coefficients f_i:

$$\begin{aligned} F &= (\text{volume}) \tilde{f}_0 + (\text{surface area}) \tilde{f}_1 + (\text{euler number}) \tilde{f}_2 \\ &= (N - 1)(M - 1)\, \tilde{f}_0 + 2(N + M - 2)\, \tilde{f}_1 + \tilde{f}_2. \end{aligned} \tag{I.0.6}$$

The new coefficients $\tilde{f}_i$ read

$$\begin{aligned}\tilde{f}_0 &= f_0,\\ \tilde{f}_1 &= \frac{2f_1 + f_0}{2},\\ \tilde{f}_2 &= f_2 + f_0 + 4f_1.\end{aligned}$$

This freedom in the definition of the geometrical measures is universal and can be applied to other systems than lattice systems, see [13], [10] for examples. One should point out that this freedom of definition is facilitated by considering all geometric contributions to the free energy: Neglecting the surface and/or the curvature contributions from Eq. (I.0.4) would lead to ambiguities in the definition of the volume of the container. For the purpose of this thesis, all definitions of the geometric measures which fulfill the following rules for a $N \times M$ lattice are equivalent:

- The volume is a quadratic and positive function of the variable (N, M).
- The surface area is a linear positive function of (N, M)
- The Euler number is 1.

The definition of geometric measures of more complicated lattice domains should follow from the definition of these measures for the $N \times M$ lattice. Concluding, one can say that the choice of the definition of geometric measures of the underlying domain has no impact on the physical properties of the system. Any redefinitions of the geometric measures should lead to redefinitions of the thermodynamic coefficients f_i as linear combinations of each other. The geometric measures of lattice domains in higher dimensions (and in one dimension) can be defined in a similar matter and obey similar rules.

I.2. Virial expansion of real gases

Consider a d-dimensional gas consisting of identical particles of mass m confined in the container $\mathcal{D}$. The particles interact via a spherically symmetric two-particle potential U. We choose the grand-canonical approach to describe the problem. Our starting point is the grand-canonical partition sum $Z_{\text{G.C.}}(\mathcal{D}; \beta; \mu)$ with the inverse temperature β and the chemical potential μ as native variables:

$$Z_{\text{G.C.}}(\mathcal{D}; \beta, \mu) = \sum_{N=0}^{\infty} \frac{z^N}{N!} \frac{Q_N}{\lambda_T^{dN}}, \tag{I.0.7}$$

where we use the following conventions:

$$
\begin{aligned}
f &= \exp\left(-\beta\, U\right) - 1, \ \text{ is the Mayer-}f\text{-function,}\\
\lambda_T &= \sqrt{\frac{2\,\pi\,\hbar^2}{m\,k_B T}}, \ \text{ is the thermal wavelength,}\\
z &= \exp(\beta\,\mu), \ \text{ is the fugacity,}\\
Q_N &= \int_{\mathcal{D}} \mathrm{d}^d r_1 ... \int_{\mathcal{D}} \mathrm{d}^d r_N \prod_{i<j}^{N} \left(1 + f_{i,j}\right) \ \text{ is the } N\text{-particle configuration integral.}
\end{aligned}
$$

Since evaluating $Z_{\text{G.C.}}$ for arbitrary interactions is a difficult task, we consider the limit of small z using a virial expansion, see [6], [8], which for bulk fluids corresponds to the low-density limit. For the expansion up to the order z^2, we need the first three configuration integrals:

$$
\begin{aligned}
Q_0 &= 1,\\
Q_1 &= |\mathcal{D}|,\\
Q_2 &= |\mathcal{D}|^2 + \int_{\mathcal{D}} \mathrm{d}^d r_1 \int_{\mathcal{D}} \mathrm{d}^d r_2\, f_{1,2} = |\mathcal{D}|^2 + b_2,
\end{aligned}
$$

with the second virial coefficient b_2. The grand potential Ω reads

$$
\beta\,\Omega(\mathcal{D};\beta,\mu) = -\log Z_{\text{G.C.}}(\mathcal{D};\beta;\mu) = \beta\,\Omega^{\text{ideal}}(\mathcal{D};\beta,\mu) - \frac{1}{2}\,z^2\,b_2(\mathcal{D};\beta) + \mathcal{O}(z^3),
$$

where $\beta\,\Omega^{\text{ideal}} = -z\,|\mathcal{D}|$ is the ideal-gas contribution. The fact that the system is finite is mirrored in the coefficient b_2. In [2], b_2 was examined for finite-range interactions U (meaning $U(r) = 0$ for distances larger than a finite $r \in \mathbb{R}_+$) via a curvature expansion of $\partial\mathcal{D}$. Using the definition

$$
f_i := \int_{\mathbb{R}^d} \mathrm{d}^d r\, f(r)\, |r|^{i+1-d}, \tag{I.0.8}
$$

one can summarise the results for $d = 3$ as following: let $\lambda \in \mathbb{R}$, we omit all arguments of b_2, except $\mathcal{D}$. For $\lambda \to \infty$, we obtain

$$
\begin{aligned}
b_2(\lambda\,\mathcal{D}) &= |\mathcal{D}|\,f_2\,\lambda^3 - \frac{|\partial\mathcal{D}|}{4}\,f_3\,\lambda^2 + \frac{K(\mathcal{D})}{48}\,f_5, \ \text{ if } \mathcal{D} \text{ is a ball,}\\
b_2(\lambda\,\mathcal{D}) &= |\mathcal{D}|\,f_2\,\lambda^3 - \frac{|\partial\mathcal{D}|}{4}\,f_3\,\lambda^2 + \mathcal{O}\left(\lambda^0\right), \ \text{ if } \partial\mathcal{D} \text{ is smooth,}\\
b_2(\lambda\,\mathcal{D}) &= |\mathcal{D}|\,f_2\,\lambda^3 - \frac{|\partial\mathcal{D}|}{4}\,f_3\,\lambda^2 + \frac{4\,H(\mathcal{D})}{3\pi^2}\,f_4\,\lambda - \frac{K(\mathcal{D})}{8\pi^2}\,f_5, \ \text{ if } \mathcal{D} \text{ is a cuboid.}
\end{aligned}
$$

Here we assume that the two-particle potential U is such that all appearing coefficients f_i are finite. $K(\mathcal{D})$, $H(\mathcal{D})$ denote the Euler number and the integrated mean curvature of $\partial\mathcal{D}$, which equals $\pi/4 \times$ (total edge length of $\mathcal{D}$) for cuboids . Remarkably, the series in λ terminates at λ^0 for spherical and cuboid containers. While the

first both results are in agreement (the first result being a special case of the second one), they are both in conflict with the third result – of course only if we assume the universal validity of the decomposition Eq. (I.0.4). Nevertheless, these results yield a geometric decomposition, consistent with Eq. (I.0.4), of the grand potential Ω in the low fugacity limit.

Additionally, in [13] König, Roth and Mecke considered a three-dimensional hard spheres gas. Using density functional theory they have shown that the grand potential $\Omega(\mathcal{D}; \beta, \mu)$ of a hard spheres gas confined in a container $\mathcal{D}$ at temperature β and chemical potential μ is a linear combination of the four Minkowski functionals of $\mathcal{D}$, i.e. the volume, the surface area, the integrated mean and the integrated Gaussian curvature (which is the Euler number). The calculations were carried out for planar, cylindric and spherical confining geometries $\mathcal{D}$. The main result states that higher powers of local curvatures beyond the Gaussian curvature, integrated over the surface $\partial\mathcal{D}$ of $\mathcal{D}$ do not contribute to the grand potential and thus the decomposition Eq. (I.0.3) is complete and not a truncated power series.

I.3. Spin Ising model

Consider a one-dimensional spin Ising model with next-neighbour interactions consisting of N spins $s_1, ..., s_N$ and the boundary spins s_0, s_{N+1} which are not part of the system. The spin interactions are characterised by the ferromagnetic interaction constant $J < 0$ with $K := -\beta J$. One can calculate the partition sum Z and the free energy βF in a straight forward way for any choice of boundary conditions and any temperature $0 < \beta < \infty$:

$$\beta F(N, \beta) = N f_0(\beta) + f_1(\beta) + \mathcal{O}\left(\mathrm{e}^{-\lambda N}\right). \tag{I.0.9}$$

The coefficients f_0, f_1 and the correlation length λ are independent of the system size N and read

$$\lambda = -\log\tanh(K), \tag{I.0.10}$$

$$f_0 = -\log 2\cosh K, \tag{I.0.11}$$

$$f_1 = \begin{cases} 0 & , \text{ for periodic b.c.} \\ \log\cosh K - \sum_{s\in\{s_0, s_{N+1}\}} \log\cosh Ks & , \text{ for } s_0,\ s_{N+1} \in \mathbb{R}. \end{cases} \tag{I.0.12}$$

We interpret N as the volume of the system. The surface area is either zero in the case of periodic boundary conditions or 1 for fixed boundary spins. This result mirrors the decomposition Eq. (I.0.4): All contributions to the free energy beyond the geometric contributions vanish exponentially in the thermodynamic limit.

As another example, consider the two-dimensional Ising model with next-neighbour interactions on a $N \times M$ rectangular lattice. Let the interaction constant in both directions be $K = -\beta J > 0$. We start with toroidal boundary conditions, i.e. the N-th

spin column is interacting with the first spin column and the M-th spin row is interacting with the first spin row. The exact partition sum of this system was calculated by Onsager, [16], a detailed calculation can be found in [9]. The free energy reads:

$$\beta F(M,N,\beta) = MN\, f_0(\beta) + R(M,N,\beta). \tag{I.0.13}$$

The coefficient f_0 reads

$$f_0 = -\frac{1}{2\pi^2}\int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta\, \log\left[4\cosh^2 2K - 4\sinh 2K\,(\cos\varphi + \cos\Theta)\right]. \tag{I.0.14}$$

The system features a magnetisation phase transition at the critical temperature T_c given by $2K_c = \sinh^{-1}(1)$. For non-critical temperatures, the following identity holds for the remaining term R_N, as the system grows in the thermodynamic limit $M, N \to \infty,\ \ M/N = const.$:

$$R_N(\beta) = \begin{cases} \mathcal{O}\left(\mathrm{e}^{-\lambda N}\right) & ,\ T > T_c \\ \log 2 + \mathcal{O}\left(\mathrm{e}^{-\lambda N}\right) & ,\ T < T_c. \end{cases} \tag{I.0.15}$$

The inverse correlation length λ reads

$$\lambda = \log 2 + \frac{1}{\pi}\int_0^\pi \mathrm{d}\varphi\, \log\left(\frac{\cosh^2 2K}{\sinh 2K} - \cos\varphi\right). \tag{I.0.16}$$

We interpret MN as the volume of the system and say that the surface area of the system and the Euler number vanish due to toroidal boundaries. Then this result is in agreement with the decomposition Eq. (I.0.4): The free energy is given by the volume contribution, the remaining term R decays exponentially in the thermodynamic limit and features the additional contribution $\log 2$ for sub-critical temperatures due to the phase transition.

In the next example we consider a $N \times M$ Spin Ising system with following boundary conditions: periodically connected in the horizontal direction, i.e. N-direction, $(+-)$ boundary spins along the upper border (so N has to be even), $(+)$ boundary spins along the lower border. The partition sum Z of this system was calculated in [12]:

$$Z = (4\sinh 2K)^{\frac{MN}{2}} \prod_{j=1}^{\frac{N}{2}} \prod_{k=1}^{M} \exp\left[f\left(\pi\frac{2j-1}{N}, \pi\frac{k}{M+1}\right)\right], \tag{I.0.17}$$

$$f(x,y) = \log\left[\frac{\cosh^2 2K}{\sinh 2K} - \cos x - \cos y\right]. \tag{I.0.18}$$

The free energy can be evaluated using the Euler-Maclaurin summation formula, see Sec. A.4:

$$\beta F = MN\, f_0 + N\, f_1 + R(N,M), \tag{I.0.19}$$

where the volume coefficient f_0 is the same as in Eq. (I.0.14). The coefficient f_1 reads

$$f_1 = -\frac{1}{2\pi^2}\int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta \, \log \frac{\frac{\cosh^2 2K}{\sinh 2K} - \cos\varphi - \cos\Theta}{\sqrt{\left(\frac{\cosh^2 2K}{\sinh 2K} - \cos\varphi\right)^2 - 1}}. \tag{I.0.20}$$

We interpret the coefficient f_1 as the surface coefficient and the contribution Nf_1 as the surface contribution to the free energy. The Euler-Maclaurin summation formula states that the remaining term $R(N, M)$ decays exponentially with the system size in the thermodynamic limit, see Sec. A.4.

I.4. Outline

The main goal of this thesis is to analyse the Gaussian model with respect to its additivity and the question whether this model obeys a geometric decomposition like Eq. (I.0.4). The layout of this thesis is as following: We start with the general definition of the Gaussian model and its relation to the spherical and the Ising models in Chap. II.1. In Chap. II.2, we study the basic solution of the Gaussian model with different boundary conditions in arbitrary dimensions for convex containers and the underlying mathematical properties. We introduce a magnetic field in Chap. II.3 and analyse its contribution to the partition sum of the one and two-dimensional Gaussian model. In Part. III we consider the two-dimensional Gaussian model on non-convex lattice domains, starting with developing and presenting analytic tools suitable for this task in Chap. III.1. We reduce the evaluation of the partition sum of the Gaussian model on a large class of non-convex lattice containers – the "properly scaling" containers – to the partition sum of the most simple non-convex container. Furthermore, we give examples of non-convex containers which can not be treated with the developed methods and lay out alternative ways to approach the calculation of the corresponding partition sums. Finally, we evaluate the partition sum of the Gaussian model on "properly scaling" domains numerically. In Part. IV, the last part of this thesis, we study generalisations and extensions of the basic Gaussian model: We examine the impact of different lattice types and different interaction types on additivity and the vanishing remainder terms in Eq. (I.0.4).

Abbreviations, symbols and notations

Given a function $f : M \to \mathbb{R},\ x \mapsto f(x)$, with $M = \mathbb{R}$ or $M = \mathbb{N}$, the Landau symbol $\mathcal{O}$ is defined as

$$f(x) = \mathcal{O}\left(g(x)\right) \quad \text{for} \quad x \to x_0 :\Leftrightarrow \quad \limsup_{x \to x_0} \frac{f(x)}{g(x)} < \infty. \tag{I.0.21}$$

Convention: We say the function f is **exponentially** decaying for $x \to \infty$ if a real positive number $\lambda > 0$ exists such that

$$f(x) = \mathcal{O}\left(\mathrm{e}^{-\lambda x}\right), \text{ as } x \to \infty, \text{ or if} \tag{I.0.22}$$

$$f(x) = \mathcal{O}\left(x^{-k}\right), \ \forall k \in \mathbb{N}, \text{ as } x \to \infty. \tag{I.0.23}$$

Additionally, the notation

$$f(x) = g(x) + \mathcal{O}\left(h(x)\right), \text{ for } x \to x_0 \tag{I.0.24}$$

refers to asymptotic equality, i.e.

$$\begin{aligned} f(x) &= g(x) + \mathcal{O}\left(h(x)\right), \text{ for } x \to x_0 \\ :\Leftrightarrow f(x) - g(x) &= \mathcal{O}\left(h(x)\right), \text{ for } x \to x_0. \end{aligned} \tag{I.0.25}$$

We denote the set of $N \times M$ matrices with matrix entries from the set A with

$$\mathrm{Mat}(N \times M, A). \tag{I.0.26}$$

For a matrix $M \in \mathrm{Mat}(N \times N, \mathbb{R})$ we denote the determinant with

$$|M| := \mathrm{det} M. \tag{I.0.27}$$

The notations

$$\begin{aligned} &\mathrm{diag}(a_1, ..., a_N) \ \text{ and} \\ &\mathrm{diag}(a_n)_{n=1,...,N} \ \text{ and} \\ &\mathrm{diag}(a_n). \end{aligned}$$

denote a $N \times N$ matrix with the diagonal entries $a_1, ..., a_N$, starting with a_1 in the upper left corner. All other entries are zero. The notation $\mathrm{diag}(a)$ denotes a diagonal matrix with a in its diagonal entries.

Part II.

Gaussian model of magnetism

II.1. Introduction and relation to the spherical and the Ising models

In this section, we introduce the next-neighbour Gaussian model of ferromagnetism, define the partition sum and outline the main mathematical problems occurring during its evaluation. The Gaussian and the spherical model were originally introduced in [7].

We consider $|\mathcal{D}|$ lattice sites, confined to the domain $\mathcal{D}$, which is a subset of $\mathcal{Z}^d$. Here, d refers to the space dimension we are considering. At each lattice site we assign a spin $s \in \mathbb{R}$. We denote the entity of all spins with the vector $(s_1, ..., s_{|\mathcal{D}|}) \equiv \boldsymbol{s}$. The Hamiltonian $-\beta H$ of the Gaussian model in units of $k_B T$ reads

$$-\beta H := \begin{cases} \mathbb{R}^{|\mathcal{D}|} \longrightarrow \mathbb{R} \\ \boldsymbol{s} \mapsto -\sum_{i=1}^{N} s_i^2 + K \sum_{\langle i,j \rangle} s_i s_j. \end{cases}$$

The summation $\langle i, j \rangle$ runs over all pairs $s_i,\ s_j$ of next neighbours and takes the boundary conditions into account. The Hamiltonian is quadratic as function of the spin $\boldsymbol{s}$ and thus can be written using a symmetric matrix $M \in \mathrm{Mat}\left(|\mathcal{D}| \times |\mathcal{D}|, \mathbb{R}\right)$:

$$-\beta H = \boldsymbol{s}^t M \boldsymbol{s}. \tag{II.1.1}$$

The dimension of the system, the boundary conditions and the geometry of the container are from now on encoded in the matrix M. Since M is symmetric, an orthonormal Matrix T and and a $|\mathcal{D}|$-tuple of eigenvalues $(\lambda_1, ..., \lambda_{|\mathcal{D}|}) \in \mathbb{R}^{|\mathcal{D}|}$ exist, such that

$$T^t M T = \mathrm{diag}(\lambda_1, ..., \lambda_{|\mathcal{D}|}). \tag{II.1.2}$$

We define the partition sum Z of the system as

$$Z := \pi^{-\frac{|\mathcal{D}|}{2}} \int_{\mathbb{R}^{|\mathcal{D}|}} \mathrm{d}^{|\mathcal{D}|}\boldsymbol{s} \, \exp\left(\boldsymbol{s}^t M \boldsymbol{s}\right). \tag{II.1.3}$$

It should be noted that the factor $\pi^{-|\mathcal{D}|/2}$ is merely a convenient normalisation and does not bear a physical meaning. To evaluate the integral, we carry out the coordinate transformation $\boldsymbol{x} = T^t \boldsymbol{s}$:

$$Z = \pi^{-\frac{|\mathcal{D}|}{2}} \int_{\mathbb{R}^{|\mathcal{D}|}} \mathrm{d}^{|\mathcal{D}|}\boldsymbol{x} \, \exp\left(\sum_{i=1}^{|\mathcal{D}|} \lambda_i x_i^2\right). \tag{II.1.4}$$

Obviously, for the partition sum to stay well-defined and finite, the matrix M has to be negative definite, i.e. all eigenvalues λ_i have to be negative. With this assumption, we obtain the partition sum and the free energy F:

$$Z = \pi^{-\frac{|\mathcal{D}|}{2}} \prod_{i=1}^{|\mathcal{D}|} \sqrt{\frac{\pi}{|\lambda_i|}} = \frac{1}{\sqrt{|\det M|}}, \tag{II.1.5}$$

$$\beta F = -\log Z = \tfrac{1}{2} \log |\det M| = \tfrac{1}{2} \sum_{i=1}^{|\mathcal{D}|} \log |\lambda_i|. \tag{II.1.6}$$

The partition sum of the system is given by the determinant of the interaction matrix M.

Relation to the Ising and the spherical models

Apparently, the Gaussian model is similar to the Ising model. While the Ising model features discreet degrees of freedom $s_i \in \{-1, 1\}$, the Gaussian model relaxes this constraint to continuous degrees of freedom $s_i \in \mathbb{R}$. This turns the partition sum from the trace of a $2^{|\mathcal{D}|} \times 2^{|\mathcal{D}|}$ transfer matrix (see, for example [9]) to the determinant of a $|\mathcal{D}| \times |\mathcal{D}|$ interaction matrix, making the model much more accessible for analytic calculations. One apparent difference between the Hamiltonians of both models, the self-interaction

$$-\sum_{i=1}^{N} s_i^2 \tag{II.1.7}$$

between the degrees of freedom in the Gaussian model has to be introduced, as it turns out, to assure that the interaction matrix M is negative definite and the partition sum well defined. While being easier to calculate, the Gaussian model lacks one of the most important features of the Ising model: a phase transition. However by slightly modifying the Gaussian model, we arrive at the spherical model, which has a mean-field phase transition. Instead of integrating the spins over the whole space $\mathbb{R}^{|\mathcal{D}|}$, we restrict the integration to the sphere $\sum_i s_i^2 = |\mathcal{D}|$. The partition sum Z_s of the spherical model reads, up to a normalisation factor,

$$Z_\mathrm{s} = \int_{\sum_i s_i^2 = |\mathcal{D}|} \mathrm{d}^{|\mathcal{D}|}\boldsymbol{s} \; \exp\left[\boldsymbol{s}^t \; (M + \mathbb{1}) \; \boldsymbol{s}\right]. \tag{II.1.8}$$

It should be noted that this restriction naturally leads to the fact, that

$$\sum_i s_i^2 = |\mathcal{D}|, \tag{II.1.9}$$

which is also a property of the Ising model. To make the connection between the Gaussian and the spherical model obvious, we rewrite the condition $\sum_i s_i^2 = |\mathcal{D}|$

using a δ-function:

$$
\begin{aligned}
Z_{\mathrm{s}} &= \int_{\mathbb{R}^{|\mathcal{D}|}} \mathrm{d}^{|\mathcal{D}|}\boldsymbol{s}\ \exp\left[\boldsymbol{s}^{\,t}\ (M+\mathbb{1})\ \boldsymbol{s}\right]\ \delta\left(\sum_i s_i^2 - |\mathcal{D}|\right) \\
&= \int_{\mathbb{R}^{|\mathcal{D}|}} \mathrm{d}^{|\mathcal{D}|}\boldsymbol{s}\ \exp\left[\boldsymbol{s}^{\,t}\ (M+\mathbb{1})\ \boldsymbol{s}\right]\ \int_{\mathbb{R}} \mathrm{d}\alpha\ \exp\left[-i\,\alpha\ \left(\sum_i s_i^2 - |\mathcal{D}|\right)\right]. \qquad \text{(II.1.10)}
\end{aligned}
$$

One can interchange the order of integration and evaluate the partition sum, see [7] for detailed calculation. From the above expression, one can already recognise that all important features of the spherical model are encoded in the underlying Gaussian model. Thus, to study a possible geometric decomposition of the free energy of the finite-size spherical model, one has to closely examine the corresponding Gaussian model.

II.2. Basic solution for convex lattice domains in arbitrary dimensions

In this section we discuss the free energy of the Gaussian model for convex, i.e. rectangular, domains $\mathcal{D}$ in arbitrary dimensions. To study boundary contributions (like surface tension) and corner contributions to the partition sum and the free energy, we consider different boundary conditions. In particular, we consider free boundary conditions and boundary conditions with different types of periodicity in $d = 1$ and $d = 2$. For $d = 3$ we only outline the solution for arbitrary boundary conditions, since the detailed solution turns out to be straight forward after studying $d = 1$ and $d = 2$. For higher dimensions, we present the eigenvalues of the interaction matrix for free boundary conditions, which allow for the calculation of the free energy. Furthermore, we carry out a virial expansion of the Gaussian model in $d = 1$. The mathematical tools required for this section, e.g. the eigenvalues, eigenvectors and the inverse of the interaction matrices are derived and discussed in detail in Sec. A.2.

II.2.1. One dimension

We consider a string of N spins $s_i \in \mathbb{R}$, $i = 1, .., N$. The goal is to calculate the free energy for periodic and free boundary conditions.

II.2.1.1. Periodic boundary conditions

We apply periodic boundary conditions: The N-th spin is interacting with the first spin, see Fig. II.2.1. The Hamiltonian reads

$$-\beta H = -\sum_{i=1}^{N} s_i^2 + K \sum_{i=1}^{N} s_i s_{i+1}, \quad s_{N+1} \equiv s_1. \tag{II.2.1}$$

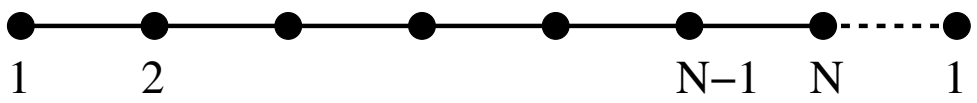

Figure II.2.1.: Periodic Gaussian chain consisting of N spins. Black dots correspond to spins. Every two neighbour spins interact with each other. Additionally, the first spin interacts with the N-th spin.

Interaction matrix and its eigenvalues

The interaction matrix $M_{\mathrm{p}} \in \mathrm{Mat}\,(N \times N, \mathbb{R})$ of the system reads.

$$M_{\mathrm{p}} = \begin{bmatrix} -1 & \frac{K}{2} & 0 & \cdots & 0 & 0 & \frac{K}{2} \\ \frac{K}{2} & -1 & \frac{K}{2} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2} & -1 & \frac{K}{2} \\ \frac{K}{2} & 0 & 0 & \cdots & 0 & \frac{K}{2} & -1 \end{bmatrix} \tag{II.2.2}$$

According to Sec. A.2, the eigenvalues λ_n read:

$$\lambda_n = -1 + K\cos\left(2\pi\tfrac{n}{N}\right),\ n \in \{1, ..., N\}. \tag{II.2.3}$$

In order for the partition sum to be well defined, all eigenvalues have to be negative. We have to choose $|K| < 1$ to guarantee this for all system sizes $N \in \mathbb{N}$. Thus, we obtain all eigenvalues of M_{p} with the physical condition of negative eigenvalues

$$\begin{aligned} &\lambda_n = -1 + K\cos\varphi_n,\ \ \varphi_n = 2\pi\tfrac{n}{N},\ \ n \in \{1, ..., N\}, \\ &|K| < 1. \end{aligned} \tag{II.2.4}$$

Calculating the free energy

The free energy F_{p} of the system reads

$$\beta F_{\mathrm{p}} = \tfrac{1}{2}\sum_{n=1}^{N} \log|\lambda_n| = \tfrac{1}{2}\sum_{n=1}^{N} \log\left(1 - K\,\cos\varphi_n\right). \tag{II.2.5}$$

We apply the trapezoidal rule for periodic functions, see Sec. A.4

$$\beta F_{\mathrm{p}} = \tfrac{N}{4\pi}\int_0^{2\pi} \mathrm{d}\varphi\ \log\left(1 - K\cos\varphi\right) + R(N, K). \tag{II.2.6}$$

The remaining term R vanishes faster than any integer power of N:

$$R(N, K) = \mathcal{O}\left(N^{-k}\right),\ \ \forall k \in \mathbb{N},\ \text{as}\ N \to \infty. \tag{II.2.7}$$

Rewriting the free energy, we obtain

$$\begin{aligned} \beta F_{\mathrm{p}} =& \tfrac{N}{2\pi}\int_0^{\pi} \mathrm{d}\varphi\ \log\left(1 - K\cos\varphi\right) + R(N, K) \\ =& \tfrac{N}{2}\log\frac{1 + \sqrt{1 - K^2}}{2} + R(N, K). \end{aligned} \tag{II.2.8}$$

II.2.1.2. Free boundaries

In the next step, we consider a Gaussian spin chain with free boundary conditions. The Hamiltonian reads

$$-\beta H = -\sum_{i=1}^{N} s_i^2 + K \sum_{i=1}^{N-1} s_i s_{i+1}. \tag{II.2.9}$$

Interaction matrix

The interaction matrix $M_\mathrm{f} \in \mathrm{Mat}\left(\mathbb{R}^N \times \mathbb{R}^N\right)$ is Toeplitz and has the form

$$M_\mathrm{f} = \begin{bmatrix} -1 & \frac{K}{2} & 0 & \cdots & 0 & 0 & 0 \\ \frac{K}{2} & -1 & \frac{K}{2} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2} & -1 & \frac{K}{2} \\ 0 & 0 & 0 & \cdots & 0 & \frac{K}{2} & -1 \end{bmatrix}. \tag{II.2.10}$$

The properties of Toeplitz matrices are discussed in Sec. A.2. The eigenvalues of the interaction matrix for free boundary conditions read:

$$\begin{aligned} &\lambda_n = -1 + K\cos\Theta_n, \;\; \Theta_n = \pi\tfrac{n}{N+1}, \;\; n \in \{1, ..., N\}, \\ &|K| \leq 1. \end{aligned} \tag{II.2.11}$$

Here, the second condition results from the requirement that the interaction matrix has to be negative definite. One should note the similarity to the eigenvalues of the periodic system, see Eq. (II.2.4). In contrast to the periodic system, free boundary conditions allow for the choice $K = \pm 1$: if $K = \pm 1$ all eigenvalues stay negative for any finite system size N. In the thermodynamic limit $N \to \infty$, the largest eigenvalue converges to zero, which leads to a logarithmic divergence of the free energy, see Sec. II.2.1.4.

Estimating the free energy

We can estimate the free energy in two different ways: Either we use the determinant, calculated in Sec. A.2, or we apply the trapezoidal rule to the eigenvalues Eq. (II.2.11). We keep the notation from Sec. A.2 in mind,

$$\tau_\pm = \frac{-1 \pm \sqrt{1 - K^2}}{2}, \tag{II.2.12}$$

and start with the determinant:

$$\begin{aligned}\beta F_{\mathrm{f}} &= \tfrac{1}{2}\log|\det M| = \tfrac{1}{2}\log\left(\left|\tau_-^N\right|\frac{1-\left(\frac{\tau_+}{\tau_-}\right)^{N+1}}{1-\frac{\tau_+}{\tau_-}}\right)\\ &= \tfrac{1}{2}\left\{N\log|\tau_-| - \log\left(1-\tfrac{\tau_+}{\tau_-}\right) + \log\left[1-\left(\tfrac{\tau_+}{\tau_-}\right)^{N+1}\right]\right\}\\ &= \tfrac{N}{2}\log\tfrac{1+\sqrt{1-K^2}}{2} - \tfrac{1}{2}\log\left(1-\tfrac{-1+\sqrt{1-K^2}}{-1-\sqrt{1-K^2}}\right) + \mathcal{O}\left(\mathrm{e}^{-\frac{\tau_+}{\tau_-}N}\right).\end{aligned} \tag{II.2.13}$$

Alternatively, using the eigenvalues we obtain

$$\beta F_{\mathrm{f}} = \tfrac{1}{2}\sum_{n=1}^{N}\log|\lambda_i| = \tfrac{1}{2}\sum_{n=1}^{N}\log\left(1-K\cos\pi\tfrac{n}{N+1}\right). \tag{II.2.14}$$

Applying the trapezoidal rule yields

$$\begin{aligned}\sum_{n=1}^{N}\log\left(1-K\cos\pi\tfrac{n}{N+1}\right) =& \tfrac{N+1}{\pi}\int_0^\pi \mathrm{d}\varphi\,\log\left(1-K\cos\varphi\right)\\ &- \tfrac{1}{2}\log\left(1-K^2\right) + R(N,K).\end{aligned} \tag{II.2.15}$$

Evaluating the integral,

$$\tfrac{1}{\pi}\int_0^\pi \mathrm{d}\varphi\,\log\left(1-K\cos\varphi\right) = \log\tfrac{1+\sqrt{1-K^2}}{2}, \tag{II.2.16}$$

we confirm, that both methods yield the same result. Summarising:

$$\begin{aligned}\beta F_{\mathrm{f}} &= \tfrac{N}{2}\log\tfrac{1+\sqrt{1-K^2}}{2} + \tfrac{1}{2}\log\tfrac{1+\sqrt{1-K^2}}{2\sqrt{1-K^2}} + R(N,K)\\ &= \beta F_{\mathrm{p}} + \tfrac{1}{2}\log\tfrac{1+\sqrt{1-K^2}}{2\sqrt{1-K^2}} + R(N,K).\end{aligned} \tag{II.2.17}$$

In addition to the volume contribution

$$\tfrac{N}{2}\log\tfrac{1+\sqrt{1-K^2}}{2}, \tag{II.2.18}$$

which also appears in the free energy of the periodic system, the Gaussian chain with free boundary conditions features the constant contribution

$$\tfrac{1}{2}\log\tfrac{1+\sqrt{1-K^2}}{2\sqrt{1-K^2}}, \tag{II.2.19}$$

which we interpret as the boundary contribution, in accordance to the geometric decomposition Eq. (I.0.4).

Exponential decay of the remaining term

According to the geometric decomposition Eq. (I.0.4), we expect all additional terms in the free energy, which go beyond the geometric contributions, to decay exponentially with the size N of the system. Using Eq. (A.33), we recognise

$$|\det M_f| = \frac{\left(1+\sqrt{1-K^2}\right)^{N+1}}{2\sqrt{1-K^2}} \left[1 - \left(\frac{1-\sqrt{1-K^2}}{1+\sqrt{1-K^2}}\right)^{N+1}\right], \tag{II.2.20}$$

$$\beta F_{\mathrm{f}} = \frac{N}{2}\log\frac{1+\sqrt{1-K^2}}{2} + \frac{1}{2}\log\frac{1+\sqrt{1-K^2}}{2\sqrt{1-K^2}} - \log\left[1 - \left(\frac{1-\sqrt{1-K^2}}{1+\sqrt{1-K^2}}\right)^{N+1}\right]. \tag{II.2.21}$$

Thus, the remaining term R decays exponentially with N/λ, where λ is the correlation length of the system:

$$R(N,K) = \log\left[1 - \left(\frac{1-\sqrt{1-K^2}}{1+\sqrt{1-K^2}}\right)^{N+1}\right] = \mathcal{O}\left(\mathrm{e}^{-(N+1)/\lambda(K)}\right), \text{ for } N \to \infty \tag{II.2.22}$$

$$\lambda(K) = \left[\log\left(1+\sqrt{1-K^2}\right) - \log\left(1-\sqrt{1-K^2}\right)\right]^{-1}. \tag{II.2.23}$$

The correlation length is symmetric under the transformation $K \mapsto -K$. In Fig. II.2.2,

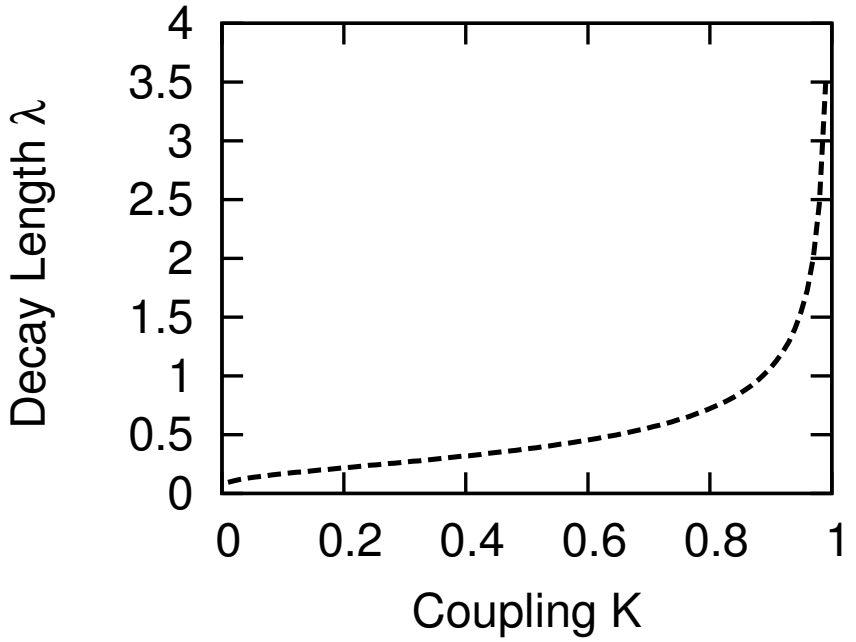

Figure II.2.2.: Correlation length λ as a function of the coupling K, see Eq. (II.2.23). As can be expected from the partition sum, the correlation length at vanishing coupling vanishes, $\lambda(0) = 0$ and $\lim_{K\to\pm1}\lambda(K) = \infty$.

the correlation length is plotted against the coupling strength K.

II.2.1.3. Virial expansion

In this section we carry out a virial expansion of the system, i.e. an expansion of the free energy in the parameter K which corresponds to the interaction strength between two neighbouring spins. Starting from given boundary conditions and the corresponding interaction matrix M, we write the partition sum as usual:

$$Z = \frac{1}{\sqrt{|\det M|}}. \tag{II.2.24}$$

We rewrite the determinant:

$$\det M = \det\left(\mathrm{diag}(-1) + \delta M\right) = \left[\det \mathrm{diag}(-1)\right]\left[\det\left(1_N - K\,A\right)\right], \tag{II.2.25}$$

where the matrix A can be obtained from the interaction matrix M and does not depend on K:

$$A := \frac{M - \mathrm{diag}(-1)}{K}. \tag{II.2.26}$$

The second determinant can be expressed as

$$\det\left(1_N - K\,A\right) = \exp\left\{-\sum_{j=1}^{\infty} \frac{K^j}{j} \mathrm{tr}\left(A^j\right)\right\}. \tag{II.2.27}$$

Thus, we immediately obtain a power series expansion of the free energy F:

$$\beta F = -\log Z = -\frac{1}{2}\sum_{j=1}^{\infty} \frac{K^j}{j} \mathrm{tr}\left(A^j\right). \tag{II.2.28}$$

Now, the only remaining task is to calculate the trace of A^j. We consider both periodic and free boundary conditions.

Periodic boundary conditions

For periodic boundary conditions we denote the matrix A as A_p and it has the following form:

$$A_\mathrm{p} := \frac{M_\mathrm{p} - \mathrm{diag}(-1)}{K} = \begin{bmatrix} 0 & \frac{1}{2} & 0 & \cdots & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \cdots & 0 & \frac{1}{2} & 0 \end{bmatrix}. \tag{II.2.29}$$

The trace of A_{p}^j can be calculated directly from its eigenvalues a_n. We obtain the eigenvalues using the same methods as in Sec. A.2, since A_n is a circulant.

$$a_n = \cos\left(2\pi\frac{n}{N}\right), \quad n = 1, ..., N. \tag{II.2.30}$$

We denote the corresponding free energy as F_{p}. Terminating the series expansion after the contribution K^n, we obtain:

$$\beta F_{\mathrm{p}} = -\frac{1}{2}\sum_{j=1}^{n}\frac{K^j}{j}\sum_{k=1}^{N}\cos^j\left(2\pi\frac{k}{N}\right) + \mathcal{O}\left(K^{n+1}\right). \tag{II.2.31}$$

Our goal is to study the expansion coefficients W_{p} of the power series expansion:

$$W_{\mathrm{p}}(j, N) := \sum_{k=1}^{N}\cos^j\left(2\pi\frac{k}{N}\right). \tag{II.2.32}$$

In the next step we show that these coefficients consist of a term linear in the system size N and otherwise only have a contribution which vanishes for systems larger than a certain finite system size (which, of course, depends on j). We reformulate this claim:

Proposition: Let $j \in \mathbb{N}$. We write

$$W_{\mathrm{p}}(j, N) = N\, w_0(j) + r(j, N). \tag{II.2.33}$$

The contribution r obeys: $r(j, N) = 0 \;\; \forall N > j$.

Proof: We start with the expansion coefficients which correspond to **odd** powers of K. In order to evaluate the sums, we use the Fourier decomposition of cos^j, see Sec. A.1:

$$\begin{aligned} W_{\mathrm{p}}(2j-1, N) =& \frac{1}{2^{2j-2}}\sum_{i=0}^{j-1}\binom{2j-1}{i}\sum_{k=1}^{N}\cos\left[(2j-1-2i)2\pi\frac{k}{N}\right] \\ =& \frac{1}{2^{2j-2}}\sum_{i=1}^{j}\binom{2j-1}{j-i}\sum_{k=1}^{N}\cos\left[(2i-1)2\pi\frac{k}{N}\right]. \end{aligned} \tag{II.2.34}$$

Using the addition theorems from Sec. A.1, we obtain

$$\begin{aligned} \sum_{k=1}^{N}\cos\left[(2i-1)2\pi\frac{k}{N}\right] &= \cos\left(\frac{N+1}{N}\pi(2i-1)\right)\frac{\sin\left(\pi\left(2i-1\right)\right)}{\sin\left(\frac{\pi(2i-1)}{N}\right)} \\ &= \begin{cases} N, & \text{if } 2i-1 \bmod N = 0, \\ 0, & \text{else.} \end{cases} \end{aligned} \tag{II.2.35}$$

From the summation over i we know, that $1 \leq i \leq j$ and thus $1 \leq 2i-1 \leq 2j-1$. Consequently,

$$(N > 2j-1) \;\Rightarrow\; W_{\mathrm{p}}(2j-1, N) = 0. \tag{II.2.36}$$

So far, we have proven the proposition for odd j. Now we look at **even** powers of K:

$$W_{\mathrm{p}}(2j, N) = \frac{N}{2^{2j}}\binom{2j}{j} + 2\sum_{i=0}^{j-1}\binom{2j}{i}\sum_{k=1}^{N}\cos\left[2(j-i)2\pi\frac{k}{N}\right]. \tag{II.2.37}$$

Applying the addition theorem again:

$$\begin{aligned}\sum_{k=1}^{N}\cos\left[2(j-i)2\pi\frac{k}{N}\right] &= \cos\left(\frac{N+1}{N}2\pi(j-i)\right)\frac{\sin\left(2\pi\left(j-i\right)\right)}{\sin\left(2\pi\frac{j-i}{N}\right)} \\ &= \begin{cases} N, & \text{if } 2(j-i) \bmod N = 0, \\ 0, & \text{else.}\end{cases}\end{aligned} \tag{II.2.38}$$

Thus, we have shown

$$N > 2j \;\Rightarrow\; W_{\mathrm{p}}(2j, N) - \frac{N}{2^{2j}}\binom{2j}{j} = 0. \tag{II.2.39}$$

We have proven the proposition. The coefficient $w_0(j)$ reads

$$w_0(j) = \begin{cases}\frac{1}{2^j}\binom{j}{j/2}, & \text{even } j, \\ 0, & \text{else.}\end{cases} \tag{II.2.40}$$

We summarise the virial expansion of the periodic system:

$$\begin{aligned}\beta F_{\mathrm{p}} &= -\frac{1}{4}\sum_{j=1}^{n}\frac{K^{2j}}{j}\,N\,w_0(2j) + r_n(N) + \mathcal{O}\left(K^{2n+1}\right), \\ r_n(N) &= 0,\ \forall N > 2n.\end{aligned} \tag{II.2.41}$$

One should note that the power series converges, as expected, to the volume coefficient of the one-dimensional Gaussian chain, see Eq. (II.2.8):

$$-\frac{1}{4}\sum_{j=1}^{\infty}\frac{K^{2j}}{j}\,w_0(2j) = \frac{1}{4\pi}\int_0^{2\pi}\mathrm{d}\varphi\,\log\left(1-K\cos\varphi\right). \tag{II.2.42}$$

Free boundary conditions

The eigenvalues a_n of the matrix A_{f} of the virial expansion for free boundary conditions read

$$a_n = \cos\left(\pi\frac{n}{N+1}\right), \quad n = 1, ..., N. \tag{II.2.43}$$

Carrying out the power series expansion of βF_{f}:

$$\beta F_{\mathrm{f}} = -\frac{1}{2}\sum_{j=1}^{n}\frac{K^j}{j}\sum_{k=1}^{N}\cos^j\left(\pi\frac{k}{N+1}\right)+\mathcal{O}\left(K^{n+1}\right), \tag{II.2.44}$$

we define the expansion coefficients W_{f}:

$$W_{\mathrm{f}}(j,N) := \sum_{k=1}^{N}\cos^j\left(\pi\frac{k}{N+1}\right). \tag{II.2.45}$$

Our next step is similar to the case of periodic boundary conditions: We prove that W_{f}, for a fixed first argument, is a sum of a contribution linear in N and a constant term, all other contributions vanishing for large enough system size.

Proposition: Let $j \in \mathbb{N}$. We write

$$W_{\mathrm{f}}(j,N) = N\,w_0(j) + w_1(j) + r(j,N). \tag{II.2.46}$$

The contribution r obeys $r(j,N) = 0 \;\; \forall N > j$.

Proof: We start with odd powers:

$$\cos^{2j-1}\left(\pi\frac{k}{N+1}\right) = \frac{1}{2^{2j-2}}\sum_{i=1}^{j}\binom{2j-1}{j-i}\cos\left[(2i-1)\pi\frac{k}{N+1}\right]. \tag{II.2.47}$$

Applying the addition theorem yields

$$\begin{aligned}\sum_{k=1}^{N}\cos\left[(2i-1)\pi\frac{k}{N+1}\right] &= \cos\left(\frac{2i-1}{2}\pi\right)\frac{\sin\left(\frac{2i-1}{2}\frac{N}{N+1}\pi\right)}{\sin\left(\frac{2i-1}{2(N+1)}\pi\right)} \\ &= \begin{cases} N, & \text{if } \frac{2i-1}{2} \bmod (N+1) = 0, \\ 0, & \text{else.}\end{cases}\end{aligned} \tag{II.2.48}$$

We know that $2j-1 > 2i-1$ and thus:

$$\begin{aligned} N > 2j-1 \;&\Rightarrow\; N > 2i-1 \;\Rightarrow N > \frac{2i-1}{2} \\ &\Rightarrow\; \frac{2i-1}{2} \bmod (N+1) \neq 0 \;\Rightarrow\; W_{\mathrm{f}}(2j-1,N) = 0. \end{aligned} \tag{II.2.49}$$

Now let us address even powers of K:

$$\sum_{k=1}^{N}\cos^{2j}\left(k\frac{\pi}{N+1}\right) = \frac{N}{2^{2j}}\binom{2j}{j} + 2\sum_{k=1}^{N}\sum_{i=1}^{j}\binom{2j}{j-i}\cos\left(2\pi i\frac{k}{N+1}\right). \tag{II.2.50}$$

We evaluate the k-sum, assuming $N > j$:

$$\sum_{k=1}^{N} \cos\left(2\pi i \frac{k}{N+1}\right) = \cos(\pi i)\, \frac{\sin\left(\pi \frac{N}{N+1} i\right)}{\sin \frac{\pi i}{N+1}}. \tag{II.2.51}$$

The addition theorem for $sin(x+y)$ gives us

$$\begin{aligned} \frac{\sin\left(\pi \frac{N}{N+1} i\right)}{\sin \frac{\pi i}{N+1}} = \frac{\sin \pi i \left(1 - \frac{1}{N+1}\right)}{\sin \frac{\pi i}{N+1}} &= \frac{\sin \pi i \cos \frac{\pi i}{N+1} - \sin \frac{\pi i}{N+1} \cos \pi i}{\sin \frac{\pi i}{N+1}} \\ &= -\cos \pi i, \end{aligned} \tag{II.2.52}$$

and

$$2 \sum_{k=1}^{N} \sum_{i=1}^{j} \binom{2j}{j-i} \cos\left(2\pi i \frac{k}{N+1}\right) = -2 \sum_{i=1}^{j} \binom{2j}{j-i} \cos^2 \pi i = -2 \sum_{i=1}^{j} \binom{2j}{j-i}. \tag{II.2.53}$$

We define the coefficient w_1 as follows:

$$w_1(2j) := \sum_{i=1}^{j} \binom{2j}{j-i}. \tag{II.2.54}$$

Thus, we have carried out the virial expansion of the one-dimensional Gaussian system with free boundary conditions:

$$\begin{aligned} &\beta F_{\mathrm{f}} = -\frac{1}{4} \sum_{j=1}^{n} \frac{K^{2j}}{j} \left[N\, w_0(2j) - 2\, w_1(2j)\right] + r_n(N) + \mathcal{O}\left(K^{2n+1}\right), \\ &r_n(N) = 0,\ \forall N > 2n. \end{aligned} \tag{II.2.55}$$

Again, the summation over w_1 converges to the surface contribution of the free energy with free boundary conditions, see Eq. (II.2.17).

Conluding, we can say that the virial expansion of the next-neighbour Gaussian model in one dimension obeys a geometric decomposition similar to Eq. (I.0.4) with the remaining term vanishing at a finite system size.

II.2.1.4. Summary and results

In this section we summarise the results of the one-dimensional Gaussian model and discuss the asymptotic behaviour of the canonical partition sum in the limit of critical coupling.

Free energy and its geometric decomposition

For general boundary conditions the partition sum is defined for coupling parameters $|K| < 1$. The free energy F of the system reads

$$\beta F = f_0^{1\mathrm{d}} |\mathcal{D}| + f_1^{1\mathrm{d}} |\partial\mathcal{D}| + R(N, K), \tag{II.2.56}$$

where $|\mathcal{D}| = N$ is the number of spins in the system and is interpreted as the volume of the system, according to Sec. I.1. The quantity $|\partial\mathcal{D}|$ is the surface area of the system. The surface area of n separated Gaussian chains with **free** boundary conditions equals n, while the surface area of a Gaussian chain with periodic boundaries vanishes. R is the remaining term which vanishes faster than any power of N as N grows to infinity. The coefficients $f_0^{1\mathrm{d}}$, $f_1^{1\mathrm{d}}$ correspond to the decomposition Eq. (I.0.4) and read

$$f_0^{1\mathrm{d}} = \frac{1}{2} \log \frac{1 + \sqrt{1 - K^2}}{2}, \tag{II.2.57}$$

$$f_1^{1\mathrm{d}} = \frac{1}{2} \log \frac{1 + \sqrt{1 - K^2}}{2\sqrt{1 - K^2}}. \tag{II.2.58}$$

Both coefficients are depicted on the left-hand side of Fig. II.2.3

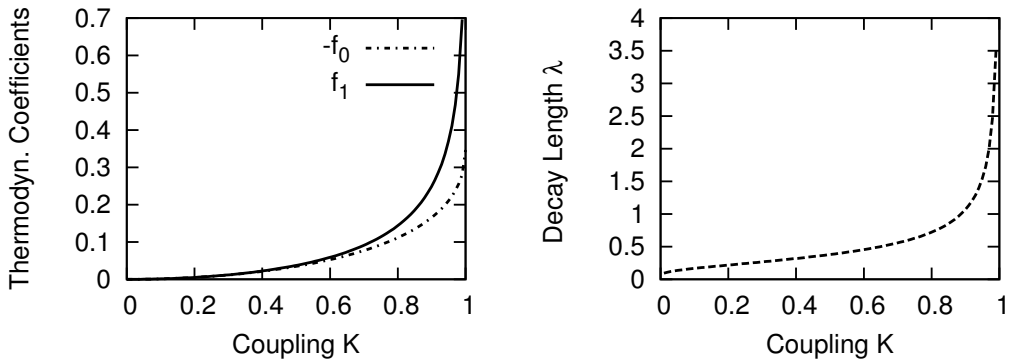

Figure II.2.3.: Left: the volume coefficient $f_0^{1\mathrm{d}}$ and the surface coefficient $f_1^{1\mathrm{d}}$ as functions of the spin-spin coupling K. Both coefficients are symmetric around $K = 0$. Right: correlation length λ as a function of the coupling K. In Eq. (II.2.23) one can see that $\lambda(0) = 0$ and $\lim_{K \to \pm 1} \lambda(K) = \infty$.

Critical coupling

This section addresses the behaviour of the thermodynamic coefficients $f_0^{1\mathrm{d}}$, $f_1^{1\mathrm{d}}$ and the convergence of the partition sum in the limit of critical coupling strength. The

volume coefficient $f_0^{1\mathrm{d}}$ is bounded and has the following properties:

$$\left|f_0^{1\mathrm{d}}(K)\right| < \infty, \quad \forall\, K \in [-1,1], \tag{II.2.59}$$

$$\lim_{K\to\pm1}\left|\frac{\mathrm{d}}{\mathrm{d}K} f_0^{1\mathrm{d}}(K)\right| = \infty. \tag{II.2.60}$$

The surface coefficient reflects the fact that the partition sum diverges for $|K| = 1$ and $N \to \infty$:

$$\lim_{K\to\pm1}\left|f_1^{1\mathrm{d}}(K)\right| = \infty. \tag{II.2.61}$$

One should point out that the thermodynamic limit $N \to \infty$ and the limit of critical coupling $K \to \pm 1$ can not be interchanged freely: In the case of **periodic** boundary conditions the partition sum is only defined for $|K| < 1$. Then the following statement holds for the free energy:

$$\beta F = N f_0^{1\mathrm{d}} + R(N,K), \tag{II.2.62}$$

$$R(N,K) = \mathcal{O}\left(N^{-k}\right), \quad \forall\, k \in \mathbb{N}, \text{ for } N \to \infty. \tag{II.2.63}$$

Interchanging the limits leads to

$$\left|\lim_{K\to\pm1}\lim_{N\to\infty}\frac{1}{N}\beta F\right| = \left|\lim_{K\to\pm1} f_0^{1\mathrm{d}}\right| < \infty, \tag{II.2.64}$$

$$\left|\lim_{K\to\pm1}\frac{1}{N}\beta F\right| = \infty, \quad \forall\, N \in \mathbb{N}. \tag{II.2.65}$$

On the other hand in the case of **free** boundary conditions the partition sum is defined for all couplings $K \in [-1,1]$, in particular for $K \in \{\pm1\}$. However, for the critical coupling $K = \pm 1$, the free energy features additional terms as $N \to \infty$:

$$\beta F = \begin{cases} N f_0^{1\mathrm{d}} + f_1^{1\mathrm{d}} + \mathcal{O}\left(\mathrm{e}^{-(N+1)/\lambda(K)}\right), & \text{if } |K| < 1, \\ N f_0^{1\mathrm{d}} + \log(N+1) + \mathcal{O}(1), & \text{if } |K| = 1. \end{cases} \tag{II.2.66}$$

This results from the evaluation of the Euler-Maclaurin formula for integrands with singularities, see [23], [11] for details. The correlation length λ is derived and discussed in Sec. II.2.1.2 and illustrated on the right-hand side of Fig. II.2.3.

II.2.2. Two dimensions

In this section we discuss the partition sum of the two-dimensional Gaussian model for toroidal, cylindric, Moebius strip and free boundary conditions. The calculation of the eigenvalues, the eigenvectors and the inverse of the interaction matrices is performed in Sec. A.2. We start by considering a rectangular lattice consisting of $M \times$

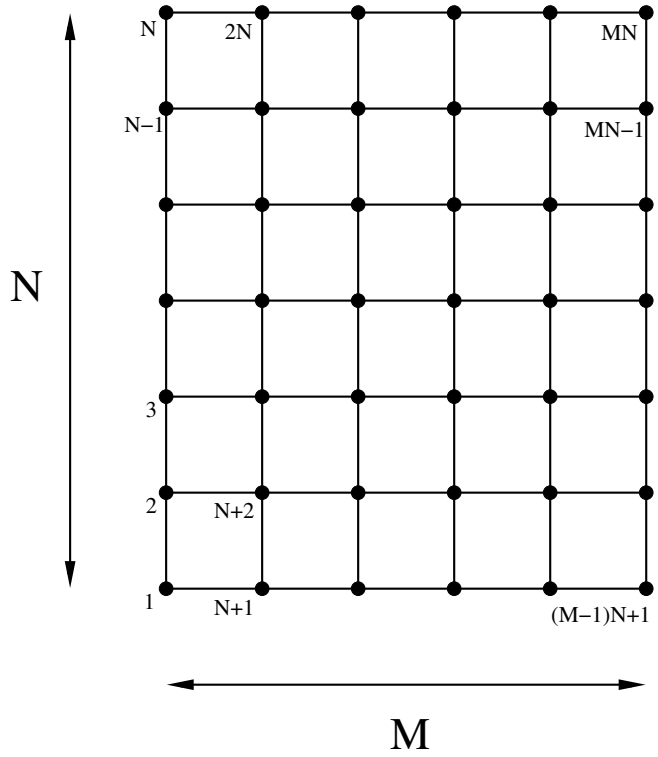

Figure II.2.4.: A two-dimensional Gaussian lattice consisting of $M \times N$ sites. Each site is symbolised with a circular dot and corresponds to a spin. Every two neighbouring spins which are connected by black lines interact with each other. The numeration of the spins is chosen such that the first column corresponds to the spins $1, ..., N$, the second column corresponds to the spins $N + 1, ..., 2N$ etc.

N sites. A spin is attached to each lattice site, two neighbouring spins interacting with each other, see Fig. II.2.4 The shape of the interaction matrix of the system depends on the numeration of the spins. Unless mentioned otherwise, we choose the numeration which is illustrated in Fig. II.2.4. After that, the interaction matrix is fully determined by the choice of boundary conditions.

II.2.2.1. Toroidal boundaries

We start with toroidal boundary conditions: The spins of the M-th column and N-th row interact with the spins of the first column and the first row respectively. To simplify the notation of the Hamiltonian, we denote the spin in the m-th row and n-th column as $s_{m,n}$. Thus, the Hamiltonian reads:

$$-\beta H = -\sum_{n,m} s_{m,n}^2 + K \sum_{m=1}^{M} \sum_{n=1}^{N} s_{m,n} s_{m,n+1} + K \sum_{m=1}^{M} \sum_{n=1}^{N} s_{m,n} s_{m+1,n} \ , \qquad \text{(II.2.67)}$$

where $s_{m,N+1} \equiv s_{m,1}$, $s_{M+1,n} \equiv s_{1,n}$, mirroring the boundary conditions. The system is fully translational invariant and, from the geometric point of view, does not possess a boundary.

Interaction matrix, eigenvalues

We denote the interaction matrix as $M_{\mathrm{t}}^{2\mathrm{d}}$. The system size dictates that $M_{\mathrm{t}}^{2\mathrm{d}} \in \mathrm{Mat}\,(NM \times NM, \mathbb{R})$ and

$$M_{\mathrm{t}}^{2\mathrm{d}} = \begin{bmatrix} M_{\mathrm{p}} & \frac{K}{2}1_N & 0 & \cdots & 0 & 0 & \frac{K}{2}1_N \\ \frac{K}{2}1_N & M_{\mathrm{p}} & \frac{K}{2}1_N & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2}1_N & M_{\mathrm{p}} & \frac{K}{2}1_N \\ \frac{K}{2}1_N & 0 & 0 & \cdots & 0 & \frac{K}{2}1_N & M_{\mathrm{p}} \end{bmatrix}. \tag{II.2.68}$$

Here, $M_{\mathrm{p}} \in \mathrm{Mat}\,(N \times N, \mathbb{R})$ is the interaction matrix of the one-dimensional Gaussian model with periodic boundary conditions. The eigenvalues α_{nm}^{t} of the interaction matrix $M_{\mathrm{t}}^{2\mathrm{d}}$ are:

$$\alpha_{nm}^{\mathrm{t}} = -1 + K\cos\varphi_n + K\cos\varphi_m = -1 + K\cos 2\pi\frac{n}{N} + K\cos 2\pi\frac{m}{M}, \tag{II.2.69}$$
$$2|K| < 1.$$

The condition $2|K| < 1$ results from the requirement that all eigenvalues have to be negative. One should point out the similarity with the eigenvalues of the one-dimensional system, see Eq. (II.2.4).

Free energy

In this section, we calculate the free energy of the two-dimensional Gaussian lattice with toroidal boundary conditions. We start with the eigenvalues:

$$\beta F_{\mathrm{t}}^{2\mathrm{d}} = \tfrac{1}{2}\log\left|\det M_{\mathrm{t}}^{2\mathrm{d}}\right| = \tfrac{1}{2}\sum_{n,m=1}^{N,M}\log|\alpha_{nm}|. \tag{II.2.70}$$

Similar to $d = 1$, we use the trapezoidal rule:

$$\beta F_{\mathrm{t}}^{2\mathrm{d}} = \tfrac{NM}{2\pi^2}\int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\theta \log\left(1 - K\cos\varphi - K\cos\theta\right) + R(N,M,K). \tag{II.2.71}$$

We evaluate one of the integrals

$$\beta F_{\mathrm{t}}^{2\mathrm{d}} = \tfrac{NM}{2\pi}\int_0^\pi \mathrm{d}\varphi \log\tfrac{1+K\cos\varphi+\sqrt{(1+K\cos\varphi)^2-K^2}}{2} + R(N,M,K). \tag{II.2.72}$$

One should note that, since the system has no boundary and no surface (due to the toroidal boundary conditions), we expect this expression to be the volume contribution to free energy, in correspondence to the decomposition Eq. (I.0.4). The remaining term R vanishes faster than any power of N, M, according to the Euler-Maclaurin formula for periodic functions, see Sec. A.4:

$$R(N,M,K) = \mathcal{O}\left(N^{-k}\right), \quad \forall M \in \mathbb{N},\ K \in \left(-\tfrac{1}{2},\tfrac{1}{2}\right), \text{ as } N \to \infty, \tag{II.2.73}$$

$$R(N,M,K) = \mathcal{O}\left(M^{-k}\right), \quad \forall N \in \mathbb{N},\ K \in \left(-\tfrac{1}{2},\tfrac{1}{2}\right), \text{ as } M \to \infty. \tag{II.2.74}$$

II.2.2.2. Cylindric boundaries

To estimate the boundary contribution to the free energy, i.e. the surface tension of the system, we consider a two-dimensional Gaussian strip with cylindric boundary conditions: The first row interacts with the N-th row, but, in contrast to toroidal boundaries, the first column and the M-th column are subject to free boundary conditions and do not interact with each other. In this way, the system has a boundary with the length $2N$. To write down the Hamiltonian, we denote the spin in the m-th row and n-th column with $s_{m,n}$:

$$-\beta H = -\sum_{n,m} s_{m,n}^2 + K \sum_{m=1}^{M} \sum_{n=1}^{N} s_{m,n} s_{m,n+1} + K \sum_{m=1}^{M-1} \sum_{n=1}^{N} s_{m,n} s_{m+1,n}, \tag{II.2.75}$$

here, $s_{m,N+1} \equiv s_{m,1}$ mirrors the cylindric boundaries.

Interaction matrix

To write down the interaction matrix in a more convenient way, we numerate the spins consequently, as in Fig. II.2.4. The interaction matrix $M_{\mathrm{c}}^{2\mathrm{d}}$ reads.

$$M_{\mathrm{c}}^{2\mathrm{d}} = \begin{bmatrix} M_{\mathrm{p}} & \frac{K}{2}1_N & 0 & \cdots & 0 & 0 & 0 \\ \frac{K}{2}1_N & M_{\mathrm{p}} & \frac{K}{2}1_N & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2}1_N & M_{\mathrm{p}} & \frac{K}{2}1_N \\ 0 & 0 & 0 & \cdots & 0 & \frac{K}{2}1_N & M_{\mathrm{p}} \end{bmatrix}. \tag{II.2.76}$$

Again, $M_{\mathrm{p}} \in \mathrm{Mat}\left(\mathbb{R}^N \times \mathbb{R}^N\right)$ is the interaction matrix of the one-dimensional periodic system. We obtain the eigenvalues of the interaction matrix from Sec. A.2.

$$\alpha_{nm}^{\mathrm{c}} = -1 + K\cos\varphi_n + K\cos\theta_m = -1 + K\cos 2\pi\tfrac{n}{N} + K\cos\pi\tfrac{m}{M+1}, \tag{II.2.77}$$
$$2|K| \leq 1.$$

The index c refers to cylindric boundary conditions and will be omitted whenever it is obvious which type of boundary conditions is under consideration. One should point out the similarity to the eigenvalues of the toroidal system, see Eq. (II.2.69), as well as the one-dimensional systems, see Eq. (II.2.4) and Eq. (II.2.11).

Free energy

The free energy $\beta F_{\mathrm{c}}^{2\mathrm{d}}$ of the system reads

$$\beta F_{\mathrm{c}}^{2\mathrm{d}} = \tfrac{1}{2} \log \left| \det M_{\mathrm{c}}^{2\mathrm{d}} \right| = \tfrac{1}{2} \sum_{n,m=1}^{N,M} \log |\alpha_{nm}^{\mathrm{c}}|. \tag{II.2.78}$$

Applying the trapezoidal rule transforms the sum over n into an integral (up to exponentially decaying contributions). However, the sum over m additionally features a constant contribution:

$$\begin{aligned}
\sum_{n,m=1}^{N,M} \log |\alpha_{nm}^{\mathrm{c}}| &= \sum_{n,m=1}^{N,M} \log \left(1 - K\cos 2\pi \tfrac{n}{N} - K \cos \pi \tfrac{m}{M+1}\right) \\
&= \tfrac{N}{\pi} \int_0^\pi \mathrm{d}\varphi \Bigg\{ \tfrac{M+1}{\pi} \int_0^\pi \mathrm{d}\theta \, \log\left(1 - K\cos\varphi - K\cos\theta\right) \\
&\quad - \tfrac{1}{2} \log\left[(1 - K\cos\varphi)^2 - K^2\right] \Bigg\} + R(N,M,K) \\
&= \tfrac{NM}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\theta \log\left(1 - K\cos\varphi - K\cos\theta\right) \\
&\quad + \tfrac{N}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\theta \log \tfrac{1 - K\cos\varphi - K\cos\theta}{\sqrt{(1-K\cos\varphi)^2 - K^2}} + R(N,M,K).
\end{aligned} \tag{II.2.79}$$

Finally, we obtain the free energy:

$$\begin{aligned}
\beta F_{\mathrm{c}}^{2\mathrm{d}} &= \tfrac{NM}{2\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\theta \log\left(1 - K\cos\varphi - K\cos\theta\right) \\
&\quad + \tfrac{N}{2\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\theta \log \tfrac{1 - K\cos\varphi - K\cos\theta}{\sqrt{(1-K\cos\varphi)^2 - K^2}} + R(N,M,K).
\end{aligned} \tag{II.2.80}$$

We rewrite this result and compare it to the free energy $F_{\mathrm{t}}^{2\mathrm{d}}$ of the toroidal system, see Eq. (II.2.72):

$$\beta F_{\mathrm{c}}^{2\mathrm{d}} = \beta F_{\mathrm{t}}^{2\mathrm{d}} + \tfrac{N}{2\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\theta \log \tfrac{1 + K\cos\varphi + K\cos\theta}{\sqrt{(1+K\cos\varphi)^2 - K^2}} + R(N,M,K). \tag{II.2.81}$$

The remaining term R decays faster than any power of N, M. As expected, this expression features a contribution proportional to the length $2N$ of the free boundary of the system. We interpret it as the surface contribution according to Eq. (I.0.4).

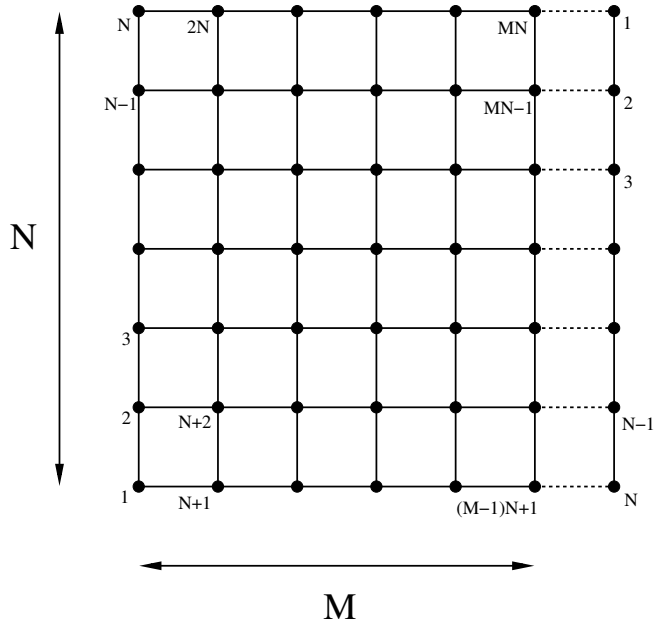

Figure II.2.5.: A two-dimensional Gaussian system, consisting of $M = 6$ columns, $N = 7$ spins each. In contrast to the cylindric boundary conditions, with Moebius boundary conditions the last column interacts with the first column "in reversed order".

II.2.2.3. Moebius strip

To determine the influence of topology on the partition sum, we consider a Gaussian system with Moebius strip boundary conditions, see Fig. II.2.5. We denote the interaction matrix as $M_{\mathrm{m}}^{\mathrm{2d}}$:

$$M_{\mathrm{m}}^{\mathrm{2d}} = \begin{bmatrix} M_{\mathrm{f}} & \frac{K}{2}1_N & 0 & \cdots & 0 & 0 & \frac{K}{2}J_N \\ \frac{K}{2}1_N & M_{\mathrm{f}} & \frac{K}{2}1_N & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2}1_N & M_{\mathrm{f}} & \frac{K}{2}1_N \\ \frac{K}{2}J_N & 0 & 0 & \cdots & 0 & \frac{K}{2}1_N & M_{\mathrm{f}} \end{bmatrix}. \tag{II.2.82}$$

Here, the matrix J_N connects the first and the last column and reads:

$$(J_N)_{i,j} = \delta_{i+j,N+1}. \tag{II.2.83}$$

As discussed in Sec. A.2, the eigenvalues with odd indices $\lambda_{2j-1,k}$ read

$$\lambda_{2j-1,k} = -1 + K\cos\left(\pi\tfrac{2j-1}{N+1}\right) + K\cos\left(2\pi\tfrac{k}{M}\right), \tag{II.2.84}$$

while the eigenvalues with even indices $\lambda_{2j,k}$ read

$$\lambda_{2j,k} = -1 + K\cos\left(\pi\tfrac{2j}{N+1}\right) + K\cos\left(\pi\tfrac{2k-1}{M}\right). \tag{II.2.85}$$

The introduction of "twisted" boundary conditions shifts half of the spectrum. Nevertheless, the partition sum and the free energy in the thermodynamic limit remain unchanged up to exponentially decaying contributions, which is a direct result of the Euler-Maclaurin formula.

$$\log\det M_{\mathrm{m}}^{2\mathrm{d}} = \log\det M_{\mathrm{c}}^{2\mathrm{d}}. \tag{II.2.86}$$

II.2.2.4. Free boundary conditions

After having estimated the volume contribution to the free energy in Sec. II.2.2.1 and the surface contribution in Sec. II.2.2.2, we determine the corner contribution in this section. In order to do this, we introduce and discuss a Gaussian strip with free boundary conditions. We calculate the eigenvalues and write down the inverse and the eigenvectors of the interaction matrix in Sec. A.2. The Hamiltonian reads

$$-\beta H = -\sum_{n,m} s_{m,n}^2 + K\sum_{m=1}^{M}\sum_{n=1}^{N-1} s_{m,n}s_{m,n+1} + K\sum_{m=1}^{M-1}\sum_{n=1}^{N} s_{m,n}s_{m+1,n}. \tag{II.2.87}$$

Interaction matrix

The interaction matrix $M_{\mathrm{f}}^{2\mathrm{d}}$ results from removing all entries, which correspond to periodic interactions from the interaction matrix of cylindric boundaries $M_{\mathrm{c}}^{2\mathrm{d}}$:

$$M_{\mathrm{f}}^{2\mathrm{d}} = \begin{bmatrix} M_{\mathrm{f}} & \frac{K}{2}1_N & 0 & \cdots & 0 & 0 & 0 \\ \frac{K}{2}1_N & M_{\mathrm{f}} & \frac{K}{2}1_N & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2}1_N & M_{\mathrm{f}} & \frac{K}{2}1_N \\ 0 & 0 & 0 & \cdots & 0 & \frac{K}{2}1_N & M_{\mathrm{f}} \end{bmatrix}. \tag{II.2.88}$$

Instead of the circulant matrix M_{p} on the main block diagonal, we use the matrix M_{f} of the one-dimensional system with free boundary conditions. The calculations of the eigenvalues α_{nm}^{f} in Sec. A.1 yield:

$$\alpha_{nm}^{\mathrm{f}} = -1 + K\cos\theta_n + K\cos\theta_m = -1 + K\cos\pi\tfrac{n}{N+1} + K\cos\pi\tfrac{m}{M+1}, \tag{II.2.89}$$
$$2|K| \leq 1.$$

Again, one should note the similarity to the toroidal and the cylindric eigenvalues, see Eq. (II.2.69), Eq. (II.2.69).

Free energy

The calculation of the free energy occurs in the same way as for other boundary conditions:

$$\beta F_{\mathrm{c}}^{2\mathrm{d}} = \tfrac{1}{2}\log\left|\det M_{\mathrm{f}}^{2\mathrm{d}}\right| = \tfrac{1}{2}\sum_{n,m=1}^{N,M}\log|\alpha_{nm}^{\mathrm{f}}|. \tag{II.2.90}$$

Applying the trapezoidal rule yields

$$\begin{aligned}\sum_{n,m=1}^{N,M}\log|\alpha_{nm}^{\mathrm{f}}| = \sum_{m=1}^{M}\Bigg[&\tfrac{N+1}{\pi}\int_0^\pi \mathrm{d}\varphi\log\left(1-K\cos\varphi-K\cos\pi\tfrac{m}{M+1}\right)\\ &-\log\sqrt{\left(1-K\cos\pi\tfrac{m}{M+1}\right)^2-K^2}+R(N,K)\Bigg]\\ =&\tfrac{N+1}{\pi}\int_0^\pi \mathrm{d}\varphi\left[\tfrac{M+1}{\pi}\int_0^\pi \mathrm{d}\theta\log\left(1-K\cos\varphi-K\cos\theta\right)\right.\\ &\left.-\log\sqrt{\left(1-K\cos\varphi\right)^2-K^2}\right]\\ &-\tfrac{M+1}{\pi}\int_0^\pi \mathrm{d}\theta\,\log\sqrt{1-K\cos\theta)^2-K^2}\\ &+\tfrac{1}{2}\left[\log\sqrt{(1-K)^2-K^2}+\log\sqrt{(1+K)^2-K^2}\right]+R(N,M,K).\end{aligned} \tag{II.2.91}$$

And finally,

$$\begin{aligned}\beta F_{\mathrm{f}}^{2\mathrm{d}} =&\beta F_{\mathrm{t}}^{2\mathrm{d}}+\tfrac{N+M}{2\pi^2}\int_0^\pi \mathrm{d}\varphi\int_0^\pi \mathrm{d}\theta\log\tfrac{1+K\cos\varphi+K\cos\theta}{\sqrt{(1+K\cos\varphi)^2-K^2}}\\ &+\tfrac{1}{2\pi^2}\int_0^\pi \mathrm{d}\varphi\int_0^\pi \mathrm{d}\theta\log\tfrac{(1+K\cos\varphi+K\cos\theta)(1-4K^2)^{\frac{1}{4}}}{(1+K\cos\varphi)^2-K^2}+R(N,M,K).\end{aligned}$$

$\beta F_{\mathrm{t}}^{2\mathrm{d}}$ is the free energy of the $M\times N$ Gaussian strip with toroidal boundaries. One should note that compared with the cylindric system, this expression features an additional boundary term, proportional to the length $2M$ of the new free boundary. Furthermore we observe a constant contribution independent of the system size,

$$\tfrac{1}{2\pi^2}\int_0^\pi \mathrm{d}\varphi\int_0^\pi \mathrm{d}\theta\log\tfrac{(1+K\cos\varphi+K\cos\theta)(1-4K^2)^{\frac{1}{4}}}{(1+K\cos\varphi)^2-K^2}, \tag{II.2.92}$$

which we interpret as the corner contribution, in accordance to Eq. (I.0.4).

II.2.2.5. Summary and results

In this section we summarise the results of the calculations of the partition sum of a **convex**, i.e. rectangular, Gaussian domain in two dimensions. For toroidal

boundary conditions the partition sum is defined for couplings $|K| < 1/2$. For cylindric and free boundary conditions the partition sum is additionally defined for $K \in \{-0.5, 0.5\}$ for all finite system sizes. The asymptotic form of the free energy in the thermodynamic limit reads

$$\beta F = f_0^{2\mathrm{d}} |\mathcal{D}| + f_1^{2\mathrm{d}} |\partial\mathcal{D}| + f_2^{2\mathrm{d}} K(\mathcal{D}) + R(N, M, K), \quad |K| < \frac{1}{2}. \tag{II.2.93}$$

According to Sec. I.1, $|\mathcal{D}|$ is the number of spins in the system which corresponds to the volume of the system. $|\partial\mathcal{D}|$ is the surface area of the system and $K(\mathcal{D})$ is the corner contribution and equals one. The surface area of a $M \times N$ Gaussian stripe is defined as:

- zero, for toroidal boundary conditions,
- $2M$ for cylindric boundary conditions (where M is the length of each of the two free boundaries),
- $2(M + N)$ for free boundary conditions.

The remaining term R vanishes faster than any power of N, M as N, $M \to \infty$. The coefficients $f_i^{2\mathrm{d}}$ read

$$\begin{aligned} f_0^{2\mathrm{d}} &= \frac{1}{2\pi} \int_0^\pi \mathrm{d}\varphi \, \log \frac{1 + K\cos\varphi + \sqrt{(1 + K\cos\varphi)^2 - K^2}}{2}, \\ f_1^{2\mathrm{d}} &= \frac{1}{2} f_0^{2\mathrm{d}} - \frac{1}{8} \log \frac{\left(1 - K + \sqrt{1 - 2K}\right)\left(1 + K + \sqrt{1 + 2K}\right)}{4}, \\ f_2^{2\mathrm{d}} &= f_0^{2\mathrm{d}} - \frac{1}{2} \log \frac{\left(1 - K + \sqrt{1 - 2K}\right)\left(1 + K + \sqrt{1 + 2K}\right)}{4} + \frac{1}{8} \log\left(1 - 4K^2\right). \end{aligned} \tag{II.2.94}$$

These coefficients have the following properties: Both $f_{0/1}^{2\mathrm{d}}$ are bounded but not their derivatives:

$$\left| f_{0/1}^{2\mathrm{d}}(K) \right| < \infty \quad \forall\, K \in [-0.5, 0.5], \tag{II.2.95}$$

$$\lim_{K \to \pm 0.5} \left| \frac{\mathrm{d}}{\mathrm{d}K} f_{0/1}^{2\mathrm{d}}(K) \right| = \infty. \tag{II.2.96}$$

The divergence of the free energy is reflected in the corner coefficient $f_2^{2\mathrm{d}}$:

$$\lim_{K \to \pm 0.5} \left| f_2^{2\mathrm{d}}(K) \right| = \infty. \tag{II.2.97}$$

All three coefficients are depicted in Fig. II.2.6

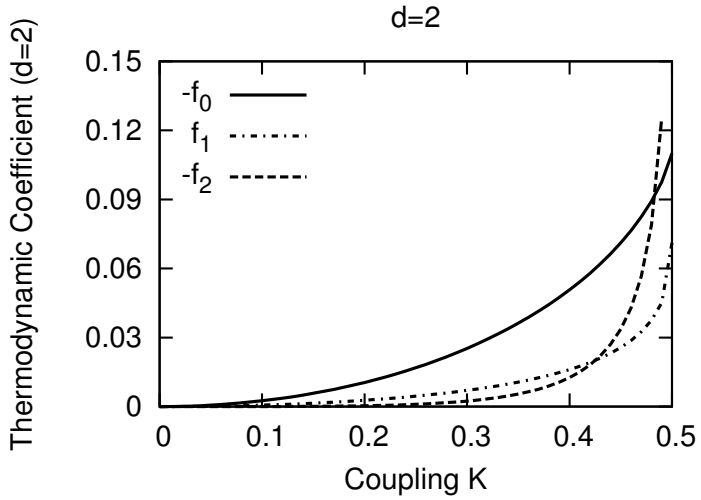

Figure II.2.6.: Volume coefficient f_0^{2d}, surface coefficient f_1^{2d} and corner coefficient f_2^{2d} as functions of the coupling K. All coefficients are symmetric around $K = 0$.

Asymptotic behaviour at critical coupling

The behaviour of the free energy under interchanging of the thermodynamic limit and the limit of critical coupling is similar to the one-dimensional case. Let $n_1, n_2 \in \mathbb{N}$. For a $n_1 N \times n_2 N$, Gaussian stripe with **toroidal** boundaries (defined only for $|K| < 0.5$) one obtains

$$\beta F = n_1 n_2 N^2 f_0^{2d} + R(N, K), \tag{II.2.98}$$

$$R(N, K) = \mathcal{O}\left(N^{-k}\right), \ \forall\, k \in \mathbb{N}, \ \text{ for } N \to \infty. \tag{II.2.99}$$

The following relations holds:

$$\lim_{K \to \pm 0.5} \left| \lim_{N \to \infty} \frac{1}{N^2} \beta F \right| = \left| n_1 n_2 \lim_{K \to \pm 0.5} f_0^{2d} \right| < \infty, \tag{II.2.100}$$

$$\lim_{K \to \pm 0.5} \left| \frac{1}{N^2} \beta F \right| = \infty, \ \ \forall N \in \mathbb{N}. \tag{II.2.101}$$

In the case of **cylindric** and **free** boundary conditions the partition sum is additionally defined for $|K| = 0.5$. Again, we have to consider two different cases: Let $n_1, n_2 \in \mathbb{N}$. We consider the free energy of a $n_1 N \times n_2 N$ Gaussian stripe with free edges of the length $n_1 N$ and periodically connected edges of the length $n_2 N$. Alternatively, we consider a Gaussian stripe where all edges are subject to free boundary conditions:

$$\beta F = n_1 n_2 N^2 f_0^{2d} + 2 n_1 N f_1^{2d} + R(N, K), \text{ cylindric b.c.} \tag{II.2.102}$$

$$\beta F = n_1 n_2 N^2 f_0^{2d} + 2N\left(n_1 + n_2\right) f_1^{2d} + f_2^{2d} + R(N, K), \text{ free b.c.} \tag{II.2.103}$$

The asymptotic behaviour of the remaining term R as a function of system size N depends on the coupling strength:

$$R(N,K) = \begin{cases} \mathcal{O}\left(N^{-k}\right), & \forall\, k \in \mathbb{N},\ \text{for } N \to \infty,\ \text{if } |K| < 0.5 \\ \mathcal{O}\left(\log N\right), & \text{for } N \to \infty,\ \text{if } |K| = 0.5. \end{cases} \tag{II.2.104}$$

II.2.3. Three and higher dimensions

In this section we briefly outline the solution of the Gaussian model in general dimensions. As already seen in the case $d = 2$ the key to the solution lies in studying the interaction matrices of the one-dimensional system. We start by discussing the three-dimensional system with different boundary conditions to illustrate the general case. Finally, we present the eigenvalues of the d-dimensional system with free boundary conditions. This allows us to calculate all contributions to the free energy up to contributions which decay faster than any power of the system size in the thermodynamic limit.

II.2.3.1. Interaction matrix, eigenvectors, eigenvalues

We consider a $N_1 \times N_2 \times N_3$ Gaussian cuboid. For each two opposite of its six faces, we can either choose free or periodic boundary conditions. Thus, we are looking at four possible types of boundary conditions (not counting permutations):

- periodic, i.e. each two opposite faces are interacting with each other,
- free at the "left" and the "right" faces and periodic else,
- free at the "left", "right", "upper", "lower" faces and periodically closed at the remaining two faces and
- the fully free boundary conditions.

Depending on the boundary conditions, the interaction matrix has the following form:

$$M^{3\mathrm{d}} = \begin{bmatrix} M_i^{2\mathrm{d}} & \frac{K}{2}1_{N_1N_2} & 0 & \cdots & 0 & 0 & \delta M \\ \frac{K}{2}1_{N_1N_2} & M_i^{2\mathrm{d}} & \frac{K}{2}1_{N_1N_2} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2}1_{N_1N_2} & M_i^{2\mathrm{d}} & \frac{K}{2}1_{N_1N_2} \\ \delta M & 0 & 0 & \cdots & 0 & \frac{K}{2}1_{N_1N_2} & M_i^{2\mathrm{d}} \end{bmatrix}. \tag{II.2.105}$$

Where $\delta M,\ M_i^{2\mathrm{d}} \in \mathrm{Mat}\left(N_1N_2 \times N_1N_2, \mathbb{R}\right)$ and

$$\delta M = \begin{cases} \mathrm{diag}\left(\frac{K}{2}, ..., \frac{K}{2}\right) & \text{, for fully periodic boundaries,} \\ 0 & \text{, else.} \end{cases} \tag{II.2.106}$$

The main-diagonal matrix M_i^{2d} describes the interactions within a two-dimensional layer of spins and depends on the boundary conditions within the layer:

$$M_i^{\mathrm{2d}} = \begin{cases} M_{\mathrm{t}}^{\mathrm{2d}}, & \text{if fully periodic,} \\ M_{\mathrm{t}}^{\mathrm{2d}}, & \text{if free at two faces,} \\ M_{\mathrm{c}}^{\mathrm{2d}}, & \text{if free at four faces,} \\ M_{\mathrm{f}}^{\mathrm{2d}}, & \text{if fully free.} \end{cases} \tag{II.2.107}$$

In the next step we calculate the eigenvalues of the interaction matrix. For the $N_1N_2N_3$ eigenvectors, which we denote with Ψ_{lmn}, we make the same ansatz as in $d = 2$, see Sec. A.2

$$\Psi_{lmn} = \left(z_1^{(n)}\Psi_{lm}, z_2^{(n)}\Psi_{lm}, ..., z_{N_3}^{(n)}\Psi_{lm}\right), \tag{II.2.108}$$

where $\left(z_1^{(n)}, ..., z_{N_3}^{(n)}\right)$ is the N_3-tuple of complex numbers which has to be determined and Ψ_{lm} is the lm-th eigenvector of M_i^{2d}. We denote the lm-th eigenvalue of M_i^{2d} with α_{lm}^i and the lmn-th eigenvalue of M_i^{3d} with λ_{lmn}^i. Explicitly evaluating the eigenvalue equation (in analogy to the two-dimensional case) yields the eigenvalues λ:

$$\lambda_{lmn}^i = \alpha_{lm}^i + K\cos\beta_n, \tag{II.2.109}$$

where $\beta_n = 2\pi\frac{n}{N}$, $n = 1, ..., N_3$ if we have fully periodic boundaries and $\beta_n = \pi\frac{n}{N_3+1}$ else. Thus, depending on the boundary conditions, we obtain four sets of eigenvalues of M^{3d}:

$$\lambda_{lmn}^{\mathrm{p}} = -1 + K\cos\varphi_l + K\cos\varphi_m + K\cos\varphi_n, \quad \text{fully periodic BC,} \tag{II.2.110}$$

$$\lambda_{lmn}^{\mathrm{1f}} = -1 + K\cos\varphi_l + K\cos\varphi_m + K\cos\theta_n, \quad \text{two free faces,} \tag{II.2.111}$$

$$\lambda_{lmn}^{\mathrm{2f}} = -1 + K\cos\varphi_l + K\cos\theta_m + K\cos\theta_n, \quad \text{four free faces,} \tag{II.2.112}$$

$$\lambda_{lmn}^{\mathrm{f}} = -1 + K\cos\theta_l + K\cos\theta_m + K\cos\theta_n, \quad \text{fully free BC.} \tag{II.2.113}$$

Here we use the convention for the angles φ_i, θ_j, as introduced in Sec. II.2.1:

$$\begin{aligned} \varphi_n &= 2\pi\frac{n}{N_i}, \quad n = 1, ..., N_i, \\ \theta_m &= \pi\frac{m}{N_j+1}, \quad m = 1, ..., N_j, \end{aligned} \tag{II.2.114}$$

N_i, N_j being the corresponding side lengths of the cuboid container.

II.2.3.2. Free energy

In the next step we calculate the free energy F of the system

$$\beta F = \tfrac{1}{2}\sum \log|\lambda_{lmn}|. \tag{II.2.115}$$

To evaluate the sum we use the Euler-Maclaurin summation formula which also tells us that all remaining contributions vanish exponentially with the size of the system. On the basis of the decomposition Eq. (I.0.4), we introduce the thermodynamic coefficients f_i

$$
\begin{aligned}
f_0^{3\mathrm{d}} &:= \tfrac{1}{2\pi^3}\int_{[0,\pi]^3} \mathrm{d}^3\varphi\, \log\left(1-K\sum_{i=1}^{3}\cos\varphi_i\right),\\
f_1^{3\mathrm{d}} &:= \tfrac{1}{4\pi^3}\int_{[0,\pi]^3} \mathrm{d}^3\varphi\, \log\frac{1-K\sum_{i=1}^{3}\cos\varphi_i}{\sqrt{\left(1-K\cos\varphi_1-K\cos\varphi_2\right)^2-K^2}},\\
f_2^{3\mathrm{d}} &:= \tfrac{1}{8\pi^3}\int_{[0,\pi]^3} \mathrm{d}^3\varphi\, \log\frac{\left(1-K\sum_{i=1}^{3}\cos\varphi_i\right)\left[\left(1-K\cos\varphi_1\right)^4-4K^2\left(1-K\cos\varphi_1\right)^2\right]^{\frac{1}{4}}}{\left(1-K\cos\varphi_1-K\cos\varphi_2\right)^2-K^2},\\
f_3^{3\mathrm{d}} &:= \tfrac{1}{2\pi^3}\int_{[0,\pi]^3} \mathrm{d}^3\varphi\, \log\frac{\left(1-K\sum_{i=1}^{3}\cos\varphi_i\right)\left[\left(1-K\cos\varphi_1\right)^4-4K^2\left(1-K\cos\varphi_1\right)^2\right]^{\frac{3}{4}}}{\left[\left(1-K\sum_{i=1}^{2}\cos\varphi_i\right)^2-K^2\right]^{\frac{3}{2}}\left[\left(1+3K^2\right)^2-16K^2\right]^{\frac{1}{8}}\left(1-K^2\right)^{\frac{1}{4}}}.
\end{aligned}
\tag{II.2.116}
$$

Furthermore, we denote the total number of spins, i.e. the volume, $N_1N_2N_3$ with N. Omitting all contributions which decay exponentially with the system size, we obtain the following expressions for the free energy of the system at different boundary conditions:

$$
\begin{aligned}
\beta F_{\mathrm{p}}^{3\mathrm{d}} &= N f_0^{3\mathrm{d}},\ \text{fully periodic BC},\\
\beta F_{1\mathrm{f}}^{3\mathrm{d}} &= N f_0^{3\mathrm{d}} + 2N_1N_2 f_1^{3\mathrm{d}},\ \text{one free pair of faces},\\
\beta F_{2\mathrm{f}}^{3\mathrm{d}} &= N f_0^{3\mathrm{d}} + 2\left(N_1N_2+N_1N_3\right) f_1^{3\mathrm{d}} + 4N_1 f_2^{3\mathrm{d}},\ \text{two free pairs of faces},\\
\beta F_{\mathrm{f}}^{3\mathrm{d}} &= N f_0^{3\mathrm{d}} + \sum_{i,j=1}^{3} N_iN_j f_1^{3\mathrm{d}} + 4\sum_{i=1}^{3} N_i f_2^{3\mathrm{d}} + f_3^{3\mathrm{d}},\ \text{fully free BC}.
\end{aligned}
\tag{II.2.117}
$$

These results suggest to interpret the free energy with fully free boundary conditions geometrically: We consider the term proportional to $N_1N_2N_3$ as the volume contribution, the terms proportional to N_i, N_j for $i \neq j$ as surface contributions, the term proportional to $N_1+N_2+N_3$ as the contribution which corresponds to the integrated mean curvature and the size-independent term as the corner contribution. As a result, we can say that the free energy of the three-dimensional Gaussian model on **convex** domains is in full agreement with the decomposition Eq. (I.0.4) and the geometric interpretation which goes hand-in-hand with it. The case of **non-convex** domains has to be studied separately.

Critical coupling: Similar to one and two dimensions, see Sec. II.2.1.4, Sec. II.2.2.5, one can analyse the behaviour of the coefficients $f_i^{3\mathrm{d}}$ of the three-dimensional system in the limit of critical coupling $|K| \to 1/3$. One should note that the coefficient $f_i^{3\mathrm{d}}$ is a linear combination of previous coefficients $f_{i-1}^{3\mathrm{d}}, ..., f_0^{3\mathrm{d}}$ and one additional contribution. Thus, it seems appropriate to start with $f_0^{3\mathrm{d}}$. In order to do this we study the integrand of $f_0^{3\mathrm{d}}$, see Eq. (II.2.116). We only consider $K = 1/d$, as the case

$K = -1/d$ can be treated analogously. The integrand diverges for $K = 1/d$ if the angle variable $(\varphi_1, \varphi_2, \varphi_3)$ approaches $(0,0,0)$. Carrying out a series expansion of the integrand around $(\varphi_1, \varphi_2, \varphi_3) = (0,0,0)$, we obtain:

$$\begin{aligned}\log\left(1 + K\sum_{i=1}^{3}\cos\varphi_i\right) &= \log\left(1 - 3K + \frac{1}{2}\sum_{i=1}^{3}\varphi_i^2 + \mathcal{O}\left(\varphi_i^3\right)\right) \\ &= \log\left(\sum_{i}^{3}\varphi_i^2 + \mathcal{O}\left(\varphi_i^3\right)\right) - \log 2. \end{aligned} \tag{II.2.118}$$

The integration around the origin $(0,0,0)$, e.g. over the ball B_ϵ, in spherical coordinates (R, θ, ϕ) results in an integral of the type

$$\int_{B_\epsilon} \mathrm{d}^3\varphi \, \log\sum_{i=1}^{3}\varphi_i^3 = \frac{8}{3}\pi\int_0^\epsilon \mathrm{d}R \, R^2 \log R, \tag{II.2.119}$$

and we see that the integral remains finite. The coefficient $f_1^{3\mathrm{d}}$ additionally features the integrand

$$\log\left(1 - K - K\sum_{i=1}^{2}\cos\varphi_i\right), \tag{II.2.120}$$

which is divergent for $(\varphi_1, \varphi_2) \to (0,0)$ and $K = 1/d$. Carrying out a series expansion of the integrand around the singularity and integrating over a small sphere B_ϵ centered at the singularity results in

$$\int_{B_\epsilon} \mathrm{d}^2\varphi \, \log\left(\sum_{i=1}^{2}\varphi_i^2\right) = 4\pi\int_0^\epsilon \mathrm{d}R \, R \, \log R. \tag{II.2.121}$$

Again, this integral is finite. Similar to $f_0^{3\mathrm{d}}$ and $f_1^{3\mathrm{d}}$, the coefficient $f_2^{3\mathrm{d}}$ features a divergent integrand and the integration over the singularity can be reduced to the finite integral

$$\int_0^\epsilon \mathrm{d}R \, \log R. \tag{II.2.122}$$

Therefore, the only divergent coefficient is $f_3^{3\mathrm{d}}$ which can be written as

$$f_3^{3\mathrm{d}} = f_0^{3\mathrm{d}} - 3f_1^{3\mathrm{d}} + 3f_2^{3\mathrm{d}} - \frac{1}{8}\log(1 - K^2). \tag{II.2.123}$$

The only divergent contribution is $\log(1 - K^2)$.

II.2.3.3. Higher dimensions

After having seen the derivation of the partition sum for $d = 1, 2, 3$, the generalisation to higher dimensions is straight-forward. One can easily derive the partition sum of the fully periodical system (which corresponds to the bulk contribution) for arbitrary dimension d using the theory of circulants. To calculate other geometric contributions, one can consider the system with free boundaries and derive the eigenvalues $\lambda_{i_1,\ldots,i_d}$ of the interaction matrix as

$$\lambda_{i_1,\ldots,i_d} = -1 + K \sum_{j=1}^{d} \cos\left(\pi \frac{i_j}{N_j + 1}\right), \tag{II.2.124}$$

where $N_1, \ldots, N_d$ characterise the size of the system and the index i_j can be any integer between 1 and N_j. Using the eigenvalues and the Euler-Maclaurin summation formula, one can estimate all contributions to the free energy, up to contributions which decay exponentially with at least one of the side lengths N_i. Since these calculations are lengthy and do not contribute to the understanding of the system, we omit them and concentrate on studying the cases $d = 1$, 2 and 3. However, after having studied the behaviour of the thermodynamic coefficients f_i in the limit of critical coupling in one, two and three dimensions, we formulate the following **conjecture**: In d dimensions, the thermodynamic coefficients f_0, $f_1, \ldots$, f_{d-1} of the free energy of the Gaussian system remain finite at the critical coupling $|K| = 1/d$. The coefficient f_d of the contribution to the free energy which grows as $(\text{system size})^0$ in the thermodynamic limit diverges logarithmically for $K \to \pm 1/d$.

II.3. Magnetic field

In this section we study the influence of a magnetic field on the partition sum of the Gaussian model in one and two dimensions: Given a set of boundary conditions, which are encoded in the interaction matrix M, we introduce the magnetic field $\boldsymbol{h}$, which enters the Hamiltonian H in the following way:

$$-\beta H = \boldsymbol{s}^t M \boldsymbol{s} + \boldsymbol{h}^t \boldsymbol{s}, \tag{II.3.1}$$

$$Z = \pi^{-\frac{|\mathcal{D}|}{2}} \int \mathrm{d}^{|\mathcal{D}|}\boldsymbol{s} \, \exp\left(\boldsymbol{s}^t M \boldsymbol{s} + \boldsymbol{h}^t \boldsymbol{s}\right). \tag{II.3.2}$$

Again, the factor $\pi^{-\frac{|\mathcal{D}|}{2}}$ is merely a convenient normalisation constant. To evaluate the integral we perform the substitution $\boldsymbol{x} = T^t \boldsymbol{s}$, which diagonalises the interaction matrix M:

$$\pi^{-\frac{|\mathcal{D}|}{2}} \prod_{i=1}^{|\mathcal{D}|} \int \mathrm{d}x_i \, \exp\left(x_i^2 \lambda_i + m_i x_i\right), \tag{II.3.3}$$

where $\boldsymbol{m} := T^t \boldsymbol{h}$ is the transformed magnetic field. The Gaussian integral yields

$$Z = \frac{1}{\sqrt{|\det M|}} \exp\left(-\frac{1}{4} \boldsymbol{h}^t M^{-1} \boldsymbol{h}\right). \tag{II.3.4}$$

Thus, by introducing a magnetic field $\boldsymbol{h}$, the free energy of the system obtains an additive contribution which is quadratic in $\boldsymbol{h}$:

$$\beta F(\mathcal{D}; \beta, \boldsymbol{h}) = -\log Z(\mathcal{D}; \beta, \boldsymbol{h}) = \beta F(\mathcal{D}; \beta, \boldsymbol{0}) + \frac{1}{4} \boldsymbol{h}^t M^{-1} \boldsymbol{h}. \tag{II.3.5}$$

The magnetic contribution is the standard scalar product of $\boldsymbol{h}$ with the transformed field $M^{-1}\boldsymbol{h}$. In the rest of this section we study three different types of magnetic fields $\boldsymbol{h}$: Fields which are eigenvectors of M, constant fields and, in case of $d = 2$, boundary fields. One should note that for the case of a constant magnetic field we obtain:

$$\boldsymbol{h}^t = m\,(1,\, 1,\, ...,\, 1). \tag{II.3.6}$$

The partition sum then reads

$$Z = \frac{1}{\sqrt{|\det M|}} \exp\left[-\frac{m^2}{4} \sum_{i,j} \left(M^{-1}\right)_{i,j}\right]. \tag{II.3.7}$$

We have to calculate the sum over all entries of the inverse interaction matrix M^{-1}.

II.3.1. One dimension

We consider the one-dimensional Gaussian chain with periodic and free boundary conditions.

II.3.1.1. Periodic boundaries

We know the inverse matrix M_{p}^{-1} from Sec. A.2. To illustrate the calculations, we only consider the case of odd system sizes N.

$$\left(M_p^{-1}\right)_{i,j} = \frac{1}{N(-1+K)} + \frac{2}{N}\sum_{n=1}^{\frac{N-1}{2}} \frac{\sin 2\pi\frac{n}{N}i \sin 2\pi\frac{n}{N}j + \cos 2\pi\frac{n}{N}i \cos 2\pi\frac{n}{N}j}{-1+K\cos\left(2\pi\frac{n}{N}\right)}. \quad \text{(II.3.8)}$$

One can easily verify that

$$\sum_{i=1}^{n} \sin 2\pi\frac{n}{N}i = \sum_{i=1}^{n} \cos 2\pi\frac{n}{N}i = 0, \quad \text{for } n = 1, ..., \frac{N-1}{2}. \quad \text{(II.3.9)}$$

Thus, we immediately obtain

$$-\frac{1}{4}\boldsymbol{h}^t M_p^{-1}\boldsymbol{h} = -\frac{m^2}{4}\sum_{i,j}\left(M_{p,1d}^{-1}\right)_{i,j} = \frac{m^2}{4}\frac{N}{1-K}. \quad \text{(II.3.10)}$$

The free energy of the system reads

$$\beta F_{\mathrm{p}}(N,\beta,m) = \beta F_{\mathrm{p}}(N,\beta,0) - \frac{m^2}{4}\frac{N}{1-K}. \quad \text{(II.3.11)}$$

One should note that the constant field is an eigenvector of the interaction matrix $M_{\mathbf{p}}$ for periodic boundary conditions. In the next step we consider eigenvector fields.

Eigenvectors and general fields

We consider a magnetic field which is an arbitrary eigenvector of the interaction matrix $M_{\mathbf{p}}$. The possible eigenvalues $1/\lambda_n = -1/(1-K\cos 2\pi n/N)$ lie in the range

$$\frac{1}{\lambda_n} \in \left[-\frac{1}{1-|K|}, -\frac{1}{1+|K|}\right], \quad \text{(II.3.12)}$$

see Sec. A.2 for detailed calculations. The magnetic contribution to the free energy can assume the values

$$-\frac{1}{4}\boldsymbol{h}^t M_p^{-1}\boldsymbol{h} \in \left[\frac{m^2}{4}\frac{N}{1+|K|}, \frac{m^2}{4}\frac{N}{1-|K|}\right]. \quad \text{(II.3.13)}$$

If we assume the magnetic field to be an arbitrary linear combination of eigenvectors Φ of M_{p}^{-1}, i.e.

$$\boldsymbol{h} = \sum_{j=1}^{N} a_j \Phi_j, \quad a_i \in \mathbb{R}, \tag{II.3.14}$$

the magnetic contribution reads

$$-\frac{1}{4}\boldsymbol{h}^t M_p^{-1}\boldsymbol{h} = \frac{N m^2}{4}\sum_{j=1}^{N} a_j^2 \left|\lambda_j^{-1}\right|. \tag{II.3.15}$$

Thus, the magnetic contribution is always positive due to the fact that the interaction matrix and its inverse is negative definite.

II.3.1.2. Free boundaries

The interaction matrix $M_{f,1d}$ is Toeplitz, its inverse is known, see [14] for detailed derivation or Sec. A.2 for a brief summary of the important properties:

$$\left(M_f^{-1}\right)_{i,j} = \frac{2}{N+1}\sum_{k=1}^{N}\frac{\sin i\Theta_k \, \sin j\Theta_k}{-1+K\,\cos\Theta_k}, \tag{II.3.16}$$

$$\Theta_k = \pi\frac{k}{N+1}. \tag{II.3.17}$$

We rewrite the partition sum:

$$Z(N,\beta,\boldsymbol{h}) = Z_{f,1d}(N,\beta)\,\exp\left[-\frac{1}{4}\boldsymbol{h}^t M_{f,1d}^{-1}\boldsymbol{h}\right], \tag{II.3.18}$$

$$-\frac{1}{4}\boldsymbol{h}^t M_{f,1d}^{-1}\boldsymbol{h} = \frac{m^2}{2}\frac{1}{N+1}\sum_{i,j,k=1}^{N}\frac{\sin i\Theta_k \, \sin j\Theta_k}{1-K\,\cos\Theta_k}. \tag{II.3.19}$$

The difficulty lies in simplifying the sum

$$\Sigma_{1d} := \frac{1}{N+1}\sum_{i,j,k=1}^{N}\frac{\sin i\Theta_k \, \sin j\Theta_k}{1-K\,\cos\Theta_k}. \tag{II.3.20}$$

Using the additions theorem from Sec. A.1, we obtain

$$\sum_{i=1}^{N}\sin i\Theta_k = \begin{cases}\frac{\sin\Theta_k}{1-\cos\Theta_k}, & \text{if } k \text{ odd},\\ 0, & \text{else.}\end{cases} = \begin{cases}\frac{1+\cos\Theta_k}{\sin\Theta_k}, & \text{if } k \text{ odd},\\ 0, & \text{else.}\end{cases} \tag{II.3.21}$$

For the sake of simplicity, let N be odd and let n, the function f and the angles α_k be defined as:

$$2n+1 := N, \tag{II.3.22}$$

$$f(K,\varphi) := \frac{1}{1-K\,\cos\varphi}, \tag{II.3.23}$$

$$\alpha_k := \pi\,\frac{2k+1}{2(n+1)}. \tag{II.3.24}$$

Then we obtain

$$\Sigma_{1d} = \frac{1}{2(n+1)} \sum_{k=0}^{n} \frac{1+\cos\alpha_k}{1-\cos\alpha_k} f(K,\alpha_k). \tag{II.3.25}$$

One should note that the sum diverges for $N \to \infty$:

$$\frac{1+\cos\alpha_k}{1-\cos\alpha_k} f(K,\alpha_k) = \mathcal{O}\left(N^2\right). \tag{II.3.26}$$

We start by isolating the divergent part:

$$\begin{aligned}\Sigma_{1d} &= \frac{f(K,0)}{2(n+1)} \sum_{k=0}^{n} \frac{1+\cos\alpha_k}{1-\cos\alpha_k} + \frac{1}{2(n+1)} \sum_{k=0}^{n} \frac{1+\cos\alpha_k}{1-\cos\alpha_k} \left(f(K,\alpha_k) - f(K,0)\right) \\ &= \frac{f(K,0)}{2(n+1)} \sum_{k=0}^{n} \frac{1+\cos\alpha_k}{1-\cos\alpha_k} - \frac{K}{1-K} \frac{1}{2(n+1)} \sum_{k=0}^{n} \frac{1-\cos\alpha_k}{1-K\cos\alpha_k}. \end{aligned} \tag{II.3.27}$$

For large N, the second sum can be transformed into an integral using the Euler-Maclaurin formula, see Sec. A.4:

$$\begin{aligned}\frac{-K}{1-K} \frac{1}{(n+1)} \sum_{k=0}^{n} \frac{1-\cos\alpha_k}{1-K\cos\alpha_k} &= \frac{-K}{1-K} \frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1-\cos\varphi}{1-K\cos\varphi} + R_n \\ &= -\frac{1+K-\sqrt{1-K^2}}{(1-K^2)} + R_n. \end{aligned} \tag{II.3.28}$$

In the remaining part of this section, we omit all contributions R_n which result from transforming sums into integrals and vanish exponentially with the system size. Furthermore, we can simplify the terms in the first sum in Σ_{1d}:

$$\frac{1+\cos\alpha_k}{1-\cos\alpha_k} = \frac{2}{1-\cos\alpha_k} - 1. \tag{II.3.29}$$

Thus, for large N we obtain

$$\Sigma_{1d} = \frac{1}{1-K} \frac{1}{n+1} \sum_{k=0}^{n} \frac{1}{1-\cos\alpha_k} - \frac{1}{1-K} + \frac{1}{2\sqrt{1-K^2}}. \tag{II.3.30}$$

Here, all contribution which decay exponentially with N have been omitted. One should note that $\cos\alpha_k$ are the zeros of the Chebyshev polynomials of the first kind T_{n+1}, see Sec. A.3:

$$T_{n+1}(x) = \prod_{k=0}^{n} \left(x - \cos\alpha_k\right). \tag{II.3.31}$$

This helps us to further simplify the expressions. For any polynomial P with the zeros x_k, $k = 1, .., n$ the following relation holds:

$$\sum_{k=1}^{n} \frac{1}{x - x_k} = \frac{P'(x)}{P(x)}. \tag{II.3.32}$$

Using the properties of the Chebyshev polynomials we obtain

$$\sum_{k=0}^{n} \frac{1}{1-\cos\alpha_k} = \frac{T'_{n+1}(1)}{T_{n+1}(1)} = (n+1)^2. \tag{II.3.33}$$

Therefore, we have estimated Σ_{1d} up to exponentially vanishing contributions:

$$\begin{aligned}\Sigma_{1d} &= (n+1)\frac{1}{1-K} - \frac{1}{1-K} + \frac{1}{2\sqrt{1-K^2}} \\ &= \frac{N}{2}\frac{1}{1-K} - \frac{1}{2}\left[\frac{1}{1-K} - \frac{1}{\sqrt{1-K^2}}\right].\end{aligned} \tag{II.3.34}$$

The free energy βF of the one-dimensional Gaussian chain with free boundary conditions and a constant magnetic field reads

$$\begin{aligned}\beta F_{\mathrm{f}}(N,\beta,m) &= -\log Z(N,\beta,m) \\ &= \beta F_{\mathrm{f}}(N,\beta,0) - \frac{m^2}{4}\left[\frac{N}{1-K} - \frac{1}{1-K} + \frac{1}{\sqrt{1-K^2}}\right] \\ &= \beta F(N,\beta,0) + N\, m_0^{1\mathrm{d}} + m_1^{1\mathrm{d}}.\end{aligned} \tag{II.3.35}$$

Here we defined the magnetic volume and the surface contributions $m_0^{1\mathrm{d}}$, $m_1^{1\mathrm{d}}$ as

$$\begin{aligned}m_0^{1\mathrm{d}} &= -\frac{m^2}{4}\frac{1}{1-K}, \\ m_1^{1\mathrm{d}} &= \frac{m^2}{4}\left[\frac{1}{1-K} - \frac{1}{\sqrt{1-K^2}}\right].\end{aligned} \tag{II.3.36}$$

One can see these coefficients as a function of the coupling K in Fig. II.3.1.

II.3.2. Two dimensions

In this section we examine the influence of a magnetic field on the two-dimensional Gaussian model. For the sake of simplicity we consider the square consisting of $N \times N$ Gaussian spins. We discuss the case of a constant magnetic field in detail and briefly summarise the situation of the magnetic vector $\boldsymbol{h}$ as an eigenvector of the interaction matrix. We start with toroidal boundary conditions.

II.3.2.1. Toroidal boundaries

In accordance to Sec. II.2.2.1, the constant field

$$\boldsymbol{h} = m\,(1,...,1)^t \tag{II.3.37}$$

is an eigenvector of $M_{\mathfrak{t}}^{-1}$ with the eigenvalue $1/(-1+2K)$. Therefore,

$$-\frac{1}{4}\,\boldsymbol{h}^t\, M_{\mathfrak{t}}^{-1}\,\boldsymbol{h} = \frac{1}{4}\frac{1}{1-2K}\,\|\boldsymbol{h}\|^2 = \frac{m^2}{4}\frac{N^2}{1-2K}. \tag{II.3.38}$$

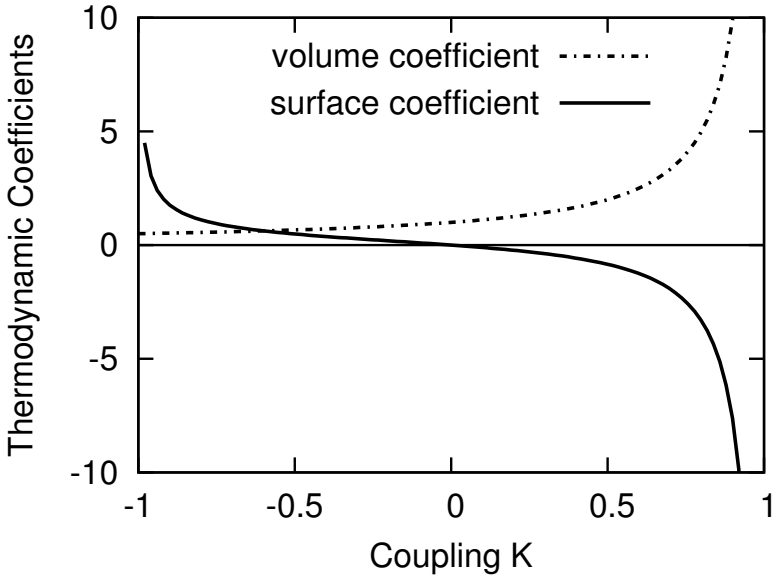

Figure II.3.1.: Thermodynamic coefficients which occur after applying a magnetic field $\boldsymbol{h}$ on a one-dimensional Gaussian chain, see Eq. (II.3.36). Dash-dotted: the volume coefficient $-4\,m_0^{1\mathrm{d}}/m^2$, which diverges linearly for $K \to 1$. Solid line: surface coefficient $-4\,m_1^{1\mathrm{d}}/m^2$. This coefficient diverges as $K^{1/2}$ for $K \to -1$ and linearly for $K \to 1$.

And the free energy reads

$$\beta F_{\mathrm{t}}^{2\mathrm{d}}(N,\beta,m) = \beta F_{\mathrm{t}}^{2\mathrm{d}}(N,\beta,0) - \frac{m^2}{4}\frac{N^2}{1-2K}. \tag{II.3.39}$$

In analogy to the toroidal system without a magnetic field, we consider this magnetic term contribution as the volume contribution.

II.3.2.2. Free boundaries

In the next step we discuss free boundary conditions. The inverse interaction matrix is known, see [14] and Sec. A.2:

$$\left(M_{f,2d}^{-1}\right)_{(i,j)(i',j')} = \frac{4}{(N+1)^2}\sum_{k,l=1}^{N}\frac{\sin i\Theta_k \,\sin j\Theta_k \,\sin i'\Theta_l \,j'\Theta_l}{-1+K\,\cos\Theta_k + K\,\cos\Theta_l}. \tag{II.3.40}$$

In analogy to the one-dimensional case, we define the sum Σ_{2d},

$$\Sigma_{2d} := \frac{1}{(N+1)^2}\sum_{i,i',j,j'=1}^{N}\sum_{k,l=1}^{N}\frac{\sin i\Theta_k \,\sin j\Theta_k \,\sin i'\Theta_l \,j'\Theta_l}{-1+K\,\cos\Theta_k + K\,\cos\Theta_l}. \tag{II.3.41}$$

We start with the summation over i, i', j, j' and assume $N = 2n+1$ odd:

$$\Sigma_{2d} = \frac{1}{2(n+1)} \sum_{l=0}^{n} \frac{1+\cos\alpha_l}{1-\cos\alpha_l} \frac{1}{2(n+1)} \sum_{k=0}^{n} \frac{1+\cos\alpha_k}{1-\cos\alpha_k} \frac{1}{-1+K\cos\alpha_k + K\cos\alpha_l}. \tag{II.3.42}$$

The second sum has been covered in the one-dimensional case:

$$\begin{aligned}\frac{1}{2(n+1)} \sum_{k=0}^{n} \frac{1+\cos\alpha_k}{1-\cos\alpha_k} \frac{1}{-1+K\cos\alpha_k + K\cos\alpha_l} = &-\frac{N-1}{2}\frac{1}{1-K-K\cos\alpha_l} \\ &- \frac{1}{2\sqrt{(1-K\cos\alpha_l)^2 - K^2}}.\end{aligned} \tag{II.3.43}$$

We evaluate both summands separately and the first summand $\Sigma_{2d}^{(1)}$, again, can be calculated in analogy to $d = 1$:

$$\begin{aligned}\Sigma_{2d}^{(1)} &:= -\frac{N-1}{2}\frac{1}{2(n+1)} \sum_{l=0}^{n} \frac{1+\cos\alpha_l}{1-\cos\alpha_l} \frac{1}{1-K-K\cos\alpha_l} \\ &= -\frac{(N-1)^2}{4}\frac{1}{1-2K} - \frac{N-1}{4\sqrt{1-2K}}.\end{aligned} \tag{II.3.44}$$

The second summand, $\Sigma_{2d}^{(2)}$, can be calculated with similar methods:

$$\Sigma_{2d}^{(2)} := -\frac{1}{4(n+1)} \sum_{l=0}^{n} \frac{1+\cos\alpha_l}{1-\cos\alpha_l} \frac{1}{\sqrt{(1-K\cos\alpha_l)^2 - K^2}}. \tag{II.3.45}$$

As in $d = 1$, both terms diverge with growing system size N^2. We define the function g:

$$g(K,\varphi) := \left[(1-K\cos\varphi)^2 - K^2\right]^{-\frac{1}{2}}, \tag{II.3.46}$$

and isolate the singularities:

$$\begin{aligned}\Sigma_{2d}^{(2)} = &-\frac{1}{4(n+1)} \sum_{l=0}^{n} \frac{1+\cos\alpha_l}{1-\cos\alpha_l}\, g(K,0) \\ &- \frac{1}{4(n+1)} \sum_{l=0}^{n} \frac{1+\cos\alpha_l}{1-\cos\alpha_l}\, \left(g(K,\alpha_k) - g(K,0)\right).\end{aligned} \tag{II.3.47}$$

In the next step we consider large system sizes and transform the second sum into an integral using the Euler-Maclaurin formula. Once again we omit all contributions which vanish exponentially with the system size:

$$\Sigma_{2d}^{(2)} = -\frac{N}{4}\,(1-2K)^{-1/2} - \frac{1}{4\pi}\int_0^{\pi} \mathrm{d}\varphi\, \frac{1+\cos\varphi}{1-\cos\varphi}\left[g(K,\varphi) - g(K,0)\right]. \tag{II.3.48}$$

We sort the different contributions from $\Sigma_{2d}^{(1)}$, $\Sigma_{2d}^{(2)}$ with respect to different powers of N and obtain

$$\begin{aligned}\Sigma_{2d} = &-\frac{N^2}{4}\frac{1}{1-2K}+\frac{N}{2}\left[\frac{1}{1-2K}-\frac{1}{\sqrt{1-2K}}\right]\\ &-\frac{1}{4}\left[\frac{1}{1-2K}-\frac{1}{\sqrt{1-2K}}+\frac{1}{\pi}\int_0^\pi \mathrm{d}\varphi\,\frac{1+\cos\varphi}{1-\cos\varphi}\left[g(K,\varphi)-g(K,0)\right]\right].\end{aligned} \tag{II.3.49}$$

Finally, the free energy reads

$$\beta F_f^{2\mathrm{d}}(N,\beta,m) = \beta F_f^{2\mathrm{d}}(N,\beta,0) + N^2\, m_0^{2\mathrm{d}} + 4N\, m_1^{2\mathrm{d}} + m_2^{2\mathrm{d}}. \tag{II.3.50}$$

Here we defined the magnetic coefficients $m_0^{2\mathrm{d}}$, $m_1^{2\mathrm{d}}$, $m_2^{2\mathrm{d}}$ which correspond to the volume, the surface and the corner contribution to the free energy respectively:

$$\begin{aligned} m_0^{2\mathrm{d}} &= -\frac{m^2}{4}\frac{1}{1-2K},\\ m_1^{2\mathrm{d}} &= \frac{m^2}{2}\left[\frac{1}{1-2K}-\frac{1}{\sqrt{1-2K}}\right],\\ m_2^{2\mathrm{d}} &= -\frac{m^2}{4}\left[\frac{1}{1-2K}-\frac{1}{\sqrt{1-2K}}+\frac{1}{\pi}\int_0^\pi \mathrm{d}\varphi\,\frac{1+\cos\varphi}{1-\cos\varphi}\left[g(K,\varphi)-g(K,0)\right]\right]. \end{aligned} \tag{II.3.51}$$

The coefficients are plotted on the left plot in Fig. II.3.2 as functions of the coupling K. Additionally, one can see the linear divergence of $m_2^{2\mathrm{d}}$ for $K \to -1/2$ in a double logarithmic plot on the right side of Fig. II.3.2.

II.3.2.3. Boundary field

One special choice of the magnetic field in two dimensions is the constant boundary field, i.e. a magnetic field which only interacts with the boundary spins. This type of magnetic field can also be interpreted as boundary conditions where the outer spins of the system linearly couple to an external potential. We decompose the field $\boldsymbol{h}$:

$$\begin{aligned} \boldsymbol{h} &= \boldsymbol{h}_1 + \boldsymbol{h}_2 \in \mathbb{R}^{N^2},\\ \boldsymbol{h}_1 &= m\ (\mathbf{1}, \mathbf{0}, ..., \mathbf{0}) \in \mathbb{R}^{N^2},\\ \boldsymbol{h}_2 &= m\ (\boldsymbol{e}_1, ..., \boldsymbol{e}_1) \in \mathbb{R}^{N^2},\\ \boldsymbol{e}_1 &= (1,0,...,0) \in \mathbb{R}^N,\\ \mathbf{1} &= (1,1,...,1) \in \mathbb{R}^N. \end{aligned} \tag{II.3.52}$$

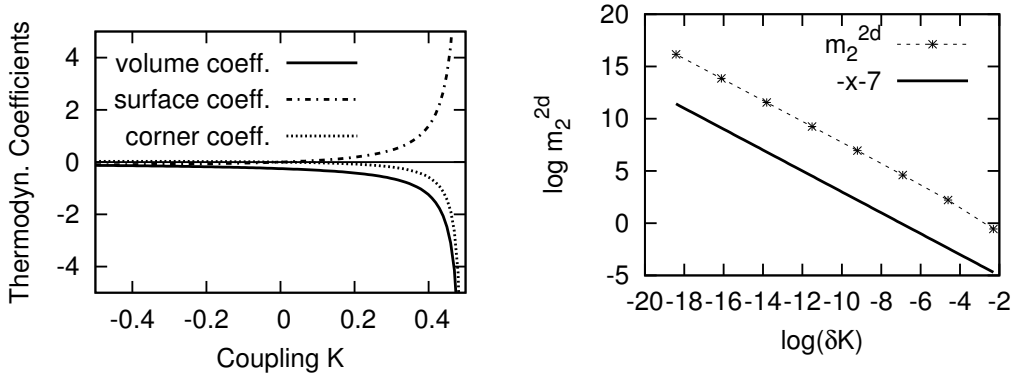

Figure II.3.2.: Left: thermodynamic coefficients which arise after applying a constant magnetic field to a $N \times N$ domain of Gaussian spins, see Eq. (II.3.51). Solid line: the volume coefficient $m_0^{2\mathrm{d}}/m^2$. Dash-dotted line: the surface coefficient $m_1^{2\mathrm{d}}/m^2$. Both coefficients diverge linearly as $K \to 0.5$, as can be seen from Eq. (II.3.51). Dashed line: topological coefficient $m_2^{2\mathrm{d}}/m^2$, which also diverges linearly for $K \to 0.5$, see the plot on the right-hand side. Right: topological coefficient $m_2^{2\mathrm{d}}$ as a function of $\delta K := 0.5 - K$ in a double-logarithmic plot for values $\delta K = 10^{-1}, ..., 10^{-8}$, see Eq. (II.3.51). Through comparison with the function $-\log \delta K - 7$ (solid line), one can recognise the linear divergence of $m_2^{2\mathrm{d}}$.

The scalar product $\boldsymbol{h}^t M_{f,2d}^{-1} \boldsymbol{h}$ reads:

$$-\frac{1}{4}\boldsymbol{h}^t \left(M_f^{2\mathrm{d}}\right)^{-1} \boldsymbol{h} = -\frac{m^2}{2} \sum_{i,j=1}^{N} \left[\left(M_f^{2\mathrm{d}}\right)^{-1}_{(1,1)(i,j)} + \left(M_f^{2\mathrm{d}}\right)^{-1}_{(1,i)(j,1)} \right] \tag{II.3.53}$$

$$= \frac{2\,m^2}{(N+1)^2} \sum_{i,j,k,l=1}^{N} \frac{\sin\Theta_k \, \sin j\Theta_l \, (\sin\Theta_k \, \sin i\Theta_l + \sin i\Theta_k \, \sin\Theta_l)}{1 - K\,\cos\Theta_k - K\cos\Theta_l}.$$

We decompose this expression into two components, A, B, and calculate them separately:

$$A := \frac{1}{(N+1)^2} \sum_{i,j,k,l=1}^{N} \frac{\sin^2\Theta_k \, \sin i\Theta_l \, \sin j\Theta_l}{1 - K\,\cos\Theta_k - K\cos\Theta_l}, \tag{II.3.54}$$

$$B := \frac{1}{(N+1)^2} \sum_{i,j,k,l=1}^{N} \frac{\sin i\Theta_k \, \sin\Theta_k \, \sin j\Theta_l \, \sin\Theta_l}{1 - K\,\cos\Theta_k - K\cos\Theta_l}. \tag{II.3.55}$$

One can recognise that A corresponds to the interaction of the magnetic field $\boldsymbol{h}_1$ or $\boldsymbol{h}_2$ with itself. On the other hand, B represents the interaction between both fields $\boldsymbol{h}_1$

and $\boldsymbol{h}_2$. Starting with A, we convert the k-sum into an integral:

$$A = \frac{1}{(N+1)\,K^2} \sum_{i,j,l=1}^{N} \sin i\Theta_l \, \sin j\Theta_l \left(1 - K\,\cos\Theta_l - \sqrt{(1-K\cos\Theta_l)^2 - K^2}\right). \tag{II.3.56}$$

To keep the calculations short we, once again, restrict them to the case $N = 2n+1$ odd and carry out the summation over i, j:

$$A = \frac{1}{2(n+1)\,K^2} \sum_{l=0}^{n} \frac{1+\cos\alpha_l}{1-\cos\alpha_l} \left(1 - K\,\cos\alpha_l - \sqrt{(1-K\cos\alpha_l)^2 - K^2}\right). \tag{II.3.57}$$

Isolating the divergent contribution results in

$$\begin{aligned} A = {} & \frac{N}{2}\,\frac{1-K-\sqrt{1-2K}}{K^2} + \frac{1}{2K} \\ & + \frac{1}{2\pi\,K^2} \int_0^\pi \mathrm{d}\varphi\, \frac{1+\cos\varphi}{1-\cos\varphi} \left[\sqrt{1-2K} - \sqrt{(1-K\cos\varphi)^2 - K^2}\right]. \end{aligned} \tag{II.3.58}$$

In the next step we approach the term B. In contrast to the one-dimensional calculations and the contribution A (which describes the self-interaction of a field with itself), no diverging sums occur in B. This leads to the fact that B features no extensive, i.e. growing linearly with the size N of the field, contributions. The summation over i, j yields

$$B = \frac{1}{4(n+1)^2} \sum_{k,l=0}^{n} \frac{(1+\cos\alpha_k)(1+\cos\alpha_l)}{1 - K\,\cos\alpha_k - K\cos\alpha_l}. \tag{II.3.59}$$

Performing the Euler-Maclaurin transformation once again gives us

$$\begin{aligned} B &= \frac{1}{4(n+1)} \sum_{l=0}^{n} (1+\cos\alpha_l)\,\frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi\, \frac{1+\cos\varphi}{1 - K\,\cos\varphi - K\,\cos\alpha_l} \\ &= -\frac{1}{4(n+1)\,K} \sum_{l=0}^{n} (1+\cos\alpha_l) \left[1 - \frac{\sqrt{(1-K\,\cos\alpha_l)^2 - K^2}}{1-K-K\,\cos\alpha_l}\right] \\ &= -\frac{1}{4\,K} \left[1 - \frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi\,(1+\cos\varphi)\,\frac{\sqrt{(1-K\,\cos\varphi)^2 - K^2}}{1-K-K\,\cos\varphi}\right]. \end{aligned} \tag{II.3.60}$$

We have finally calculated the total contribution of a boundary magnetic field to the free energy:

$$\begin{aligned}\frac{\beta F - \beta F\big|_{m=0}}{m^2} =& -N\,\frac{1-K-\sqrt{1-2K}}{K^2} \\ & -\frac{1}{K}-\frac{1}{\pi K^2}\int_0^\pi \mathrm{d}\varphi\,\frac{1+\cos\varphi}{1-\cos\varphi}\left[\sqrt{1-2K}-\sqrt{(1-K\cos\varphi)^2-K^2}\right] \\ & +\frac{1}{2K}\left[1-\frac{1}{\pi}\int_0^\pi \mathrm{d}\varphi\,(1+\cos\varphi)\,\frac{\sqrt{(1-K\,\cos\varphi)^2-K^2}}{1-K-K\,\cos\varphi}\right]. \quad \text{(II.3.61)}\end{aligned}$$

The first and the second line correspond to the extensive, i.e. growing with the system size, and the non-extensive contributions which arise from the interaction of $\boldsymbol{h}_1$ and $\boldsymbol{h}_2$ with itself. The third line corresponds to the interaction between both boundary fields $\boldsymbol{h}_1$ and $\boldsymbol{h}_2$. All three contributions are plotted in Fig. II.3.3.

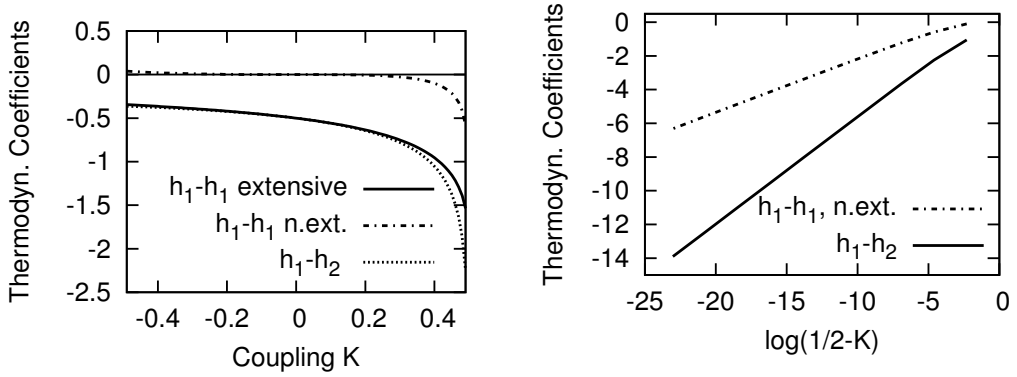

Figure II.3.3.: Left: contributions of a boundary field to the free energy of a $N \times N$ Gaussian stripe. The magnetic part of the free energy consists of the interaction of the boundary magnetic fields $\boldsymbol{h}_1$, $\boldsymbol{h}_2$ with itself – this contribution has an extensive and a non-extensive part, see Eq. (II.3.61). Furthermore, there is a non-extensive interaction between h_1 and h_2. While the extensive part of the interaction of a boundary field with itself (solid line) remains finite for all allowed coupling strengths, both the non-extensive part of the self-interaction (dash-dotted line) and the interaction coefficients between two boundary fields diverge for $K \to 1/2$. Right: divergent parts of the boundary field free energy plotted versus $\log 1/2 - K$ for values $1/2 - K \in \{10^{-1}, 10^{-2}, ..., 10^{-8}\}$, see Eq. (II.3.61). One can see that both functions are logarithmically divergent for $K \to 1/2$.

II.3.3. Summary

We applied a constant magnetic field to a Gaussian chain in one dimension and a constant volume magnetic field as well as a constant boundary field to a Gaussian $N \times N$ strip in two dimensions. The constant boundary field can also be interpreted as another type of boundary conditions, in addition to the free, the cylindric and the periodic boundary conditions from Sec. II.2.2.

The introduction of a magnetic field in one dimension expectedly leads to additive contributions to the free energy of the system and breaks the $K \mapsto -K$ symmetry between the ferromagnetic and the anti-ferromagnetic coupling, see Eq. (II.3.36). These additional contributions can be interpreted as volume and surface terms in accordance to Eq. (I.0.4). All additional contributions to the free energy beyond these geometric contributions decay exponentially with the system size.

The introduction of a bulk magnetic field in two dimensions leads to additional contributions to the free energy of the system, see Eq. (II.3.51). These contributions break the symmetry between the ferromagnetic and the anti-ferromagnetic coupling and can be interpreted as the volume, the surface and the corner contributions to the free energy, according to Eq. (I.0.4). A constant magnetic field along the boundary of the system leads to additional corner and surface contributions. All remaining terms vanish exponentially with the system size in the thermodynamic limit.

Part III.

Non-convex geometries

In the previous part of this thesis we discussed the Gaussian model in several dimensions for **convexly** shaped containers $\mathcal{D}$, i.e. for $N_1 \times N_2 \times ... \times N_d$ rectangular lattices. For this type of lattices, we estimated all contributions to the free energy which scale as $N^d, N^{d-1}, ..., N^0$ and interpreted these contributions as the volume energy, the surface energy, etc. However, in order to justify this interpretation and to verify the decomposition Eq. (I.0.4), we, in fact, have to calculate the partition sum for arbitrarily shaped containers $\mathcal{D}$, in particular for non-convex containers. The straight-forward way to calculate such partition sums is to write down the interaction matrix and evaluate its determinant. Unfortunately, even simple non-convex geometries feature a complicated interaction matrix. In this section we introduce the methods which allow us to evaluate the free energy for non-convex container geometries. We start by introducing two different analytical tools which help evaluate partition sums of Gaussian systems. After that we consider one special non-convex lattice container, the non-convex building block, and show that evaluating its partition sum allows us to evaluate the partition sum of a large variety of non-convex domains, see Eq. (III.1.42). Finally, we present examples of lattice domains which can not be treated with this method and lay out alternative methods to access the corresponding partition sums. The last section of this part of the thesis concerns itself with the evaluation of the partition sum of the non-convex building block.

III.1. Analytic approach

In this section we introduce two different methods to approach non-convex geometries: the spin freezing, which allows us to introduce defects in a convex container, and the zip method, which is used for building non-convex containers from convex building blocks. The mathematical background for this section is the treatment of the Gaussian model in presence of magnetic fields, see Chap. II.3. In the last part of this section, we apply the developed tools to calculate partition sums of non-convex lattice domains.

III.1.1. Freezing spins

We consider a rectangular d-dimensional Gaussian stripe consisting of N lattice sites with the attached spins $s_1, ..., s_N$ and a given choice of boundary conditions. For a n-tuple of pairwise different indices $i(1), ..., i(n) \in \{1, ..., N\}$, we define the index set

$$I := \{i(1), ..., i(n)\}\,. \tag{III.1.1}$$

We introduce the condition

$$s_i = 0 \;\; \forall\, i \in I. \tag{III.1.2}$$

The goal of this section is to calculate the partition sum of the system with the side condition Eq. (III.1.2). One should note that the "freezing" of the spins $s_i = 0 \;\; \forall\, i \in I$, i.e. setting their values to zero, impacts the general lattice geometry: In the one-dimensional case the system partitions in several one-dimensional subsystems. In higher dimensions, depending on the choice of I, this can lead to non-convex container geometries. The new system has the size $N - n$. We write down the partition sum using the Dirac delta function,

$$Z = \pi^{-\frac{N-n}{2}} \int_{\mathbb{R}^N} \mathrm{d}^N s \, \exp\left(\boldsymbol{s}^t M \boldsymbol{s}\right) \prod_{j=1}^{n} \delta(s_{i(j)}). \tag{III.1.3}$$

Representing the delta using the Fourier transformation,

$$\delta(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \, \exp\left(\mathrm{i}kx\right), \tag{III.1.4}$$

transforms the partition sum into

$$Z = \pi^{-\frac{N-n}{2}} \int_{\mathbb{R}^n} \frac{\mathrm{d}^n k}{(2\pi)^n} \int_{\mathbb{R}^N} \mathrm{d}^N s \, \exp\left(\boldsymbol{s}^t M \boldsymbol{s} + \mathrm{i}\boldsymbol{\kappa}^t \boldsymbol{s}\right). \tag{III.1.5}$$

Here, the vector $\boldsymbol{\kappa}$ reads

$$\kappa_i = \begin{cases} k_j, & \text{if } i = i(j) \text{ for any } j, \\ 0, & \text{else.} \end{cases} \tag{III.1.6}$$

Apparently, the side condition Eq. (III.1.2) results in a complex magnetic field i$\boldsymbol{\kappa}$, which has to be integrated. Applying the results from Chap. II.3, we obtain

$$Z = \frac{1}{\sqrt{\det(-M)}} \int_{\mathbb{R}^n} \frac{\mathrm{d}^n k}{(2\pi)^n} \exp\left(\frac{1}{4}\boldsymbol{\kappa}^t M^{-1} \boldsymbol{\kappa}\right). \tag{III.1.7}$$

We define the matrix $M_I^{-1} \in \mathrm{Mat}\,(n \times n, \mathbb{R})$ as the matrix obtained from M^{-1} by omitting all rows and columns except for the rows and columns $i(1), ..., i(n)$. Using this definition, we rewrite the partition sum as:

$$Z = \frac{1}{\sqrt{\det(-M)\det(-M_I^{-1})}}. \tag{III.1.8}$$

The challenge lies in calculating the determinant of the sub-matrix M_I^{-1}.

III.1.1.1. Examples

This section demonstrates the application of the spin freezing method. We discuss examples of already known systems in one and two dimensions and present new results in two dimensions.

One-dimensional systems

As our first example, we study the application of the spin freezing on the $1d$ Gaussian chain with periodic boundary conditions. The interaction matrix and its inverse is known from Sec. A.2. All results, in particular the entries of the inverse interaction matrix, are considered in the limit $N \to \infty$. We discuss both cases of $n = 1$ and $n = 2$ frozen spins.

For $n = 1$ the submatrix $M_{\mathrm{p},I}^{-1}$ is a 1×1 matrix, the only entry (which is also the determinant of the matrix) reads for $N \to \infty$

$$\det\left(-M_{\mathrm{p},I}^{-1}\right) = \frac{1}{\sqrt{1-K^2}}. \tag{III.1.9}$$

The free energy of the one-dimensional periodic Gaussian chain and one frozen spin reads

$$\beta F = (N-1) f_0^{1\mathrm{d}} + f_1^{1\mathrm{d}}, \tag{III.1.10}$$

with the thermodynamic coefficients f_0^{1d}, f_1^{1d} of the Gaussian model in one dimension, see Sec. II.2.1.4. As expected, the freezing of the spin breaks the periodicity and introduces free boundary conditions: The free energy equals the free energy of a Gaussian chain of the length $N-1$ with free boundary conditions.

For $n=2$ frozen spins we have to distinguish: either both spins lie next to each other or they are separated by one or more spins. In the second case, the separation grows linearly with N as we consider the thermodynamic limit. Since the original system has periodic boundary conditions and is translational invariant we can chose the first and the j-th spin to be set to zero. The case of neighbouring spins corresponds to $j=2$ (or $j=N$) while the case of separated spins results in $j \propto N \to \infty$. In the case of adjacent spins, the 2×2 matrix $M_{\mathrm{p},I}^{-1}$ has the form:

$$M_{\mathrm{p},I}^{-1} = \begin{bmatrix} -\frac{1}{\sqrt{1-K^2}} & \frac{-1+\sqrt{1-K^2}}{K\sqrt{1-K^2}} \\ \frac{-1+\sqrt{1^2-K^2}}{K\sqrt{1-K^2}} & -\frac{1}{\sqrt{1-K^2}} \end{bmatrix}, \quad \text{for } N \to \infty. \tag{III.1.11}$$

Thus, the free energy of the one-dimensional periodic Gaussian chain with two adjacent frozen spins reads

$$\beta F = (N-2) f_0^{1d} + f_1^{1d}. \tag{III.1.12}$$

As expected, the free energy equals the free energy of the one-dimensional free Gaussian chain of length $N-2$. In case of separated frozen spins, $j \propto N \to \infty$, the off-diagonal entries of $M_{\mathrm{p},I}^{-1}$ vanish:

$$M_{\mathrm{p},I}^{-1} = \begin{bmatrix} -\frac{1}{\sqrt{1-K^2}} & 0 \\ 0 & -\frac{1}{\sqrt{1-K^2}} \end{bmatrix}, \quad \text{for } N \to \infty, \tag{III.1.13}$$

and we obtain

$$\beta F = (N-2) f_0^{1d} + 2 f_1^{1d}. \tag{III.1.14}$$

This free energy corresponds to two separated Gaussian chains with free boundary conditions with the lengths N_1, N_2 which fulfill the side condition $N_1 + N_2 = N-2$.

Cylindric boundary conditions in two dimensions

As a more sophisticated example of the freezing method we consider the $N \times M$ Gaussian strip with toroidal boundary conditions, see Sec. II.2.2.1. We set the values of the first row, i.e. the first N spins to zero. In this example we demonstrate that using the freezing method we end up with the two-dimensional $N \times (M-1)$ Gaussian strip with **cylindric** boundary conditions. The index set I and the partition sum Z read

$$I = \{1, 2, ..., N\}, \tag{III.1.15}$$

$$Z = \left[\det(-M_{\mathrm{t}}) \det\left(-M_{\mathrm{t},I}^{-1}\right)\right]^{-\frac{1}{2}}. \tag{III.1.16}$$

The matrix M_{t} is the interaction matrix of the two-dimension $N \times M$ system with toroidal boundary conditions, see Sec. II.2.2.1. The matrix $M_{\mathrm{t},I}^{-1}$ is the upper left $N \times N$ submatrix of $M_{\mathrm{t}^{-1}}$ and reads for large N, up to exponentially decaying contributions:

$$\left(M_{\mathrm{t},I}^{-1}\right)_{k,l} = \left(M_{\mathrm{t,I}}^{-1}\right)_{(i,j)(k,l)}\Big|_{i=j=1} = \frac{1}{2\pi^2}\int_{[0,2\pi]^2} \mathrm{d}^2\varphi\, \frac{\cos\varphi_2(k-l)}{-1+K\sum_{m=1}^{2}\cos\varphi_m}. \quad \text{(III.1.17)}$$

The matrix $M_{\mathrm{t},I}^{-1}$ is Toeplitz and circulant. To calculate its determinant, we apply the Szegö theorem, see [4], [24]. The symbol f reads for large system sizes

$$f(x) = \frac{1}{\sqrt{(1-K\cos x)^2 - K^2}}. \quad \text{(III.1.18)}$$

Applying the Szegö theorem yields

$$\log\det\left(-M_{\mathrm{t},I}^{-1}\right) = \frac{N}{2\pi}\int_0^{2\pi}\mathrm{d}x\,\log\frac{1}{\sqrt{(1-K\cos x)^2-K^2}} + R\,(N,K)\,. \quad \text{(III.1.19)}$$

If we assume that the Fourier series of the symbol f converges exponentially fast towards f, then the remaining contribution R vanishes faster than any power of the system size as we consider the thermodynamic limit. We rewrite the result omitting the term R:

$$\beta F = -\log Z = NM f_0^{\mathrm{2d}} + \frac{1}{2}\log\det\left(-M_{t,I}^{-1}\right) \quad \text{(III.1.20)}$$

$$= NM f_0^{\mathrm{2d}} + \frac{N}{2\pi}\int_0^{\pi}\mathrm{d}\varphi\,\log\frac{1}{\sqrt{(1-K\cos\varphi)^2-K^2}} = N(M-1)f_0^{\mathrm{2d}} + 2Nf_1^{\mathrm{2d}}. \quad \text{(III.1.21)}$$

As expected, this is the free energy of the $N \times (M-1)$ Gaussian strip with cylindric boundary conditions, see Sec. II.2.2.2.

III.1.2. Zip method

In this section we introduce another method which allows us to approach non-convex Gaussian domains: the so-called zip method. The basic idea behind this method is to partition a non-convex lattice into rectangular blocks (which scale in both directions as the system grows) which are connected (or separated) by single spin lines. Treating the spin lines as arbitrary magnetic fields then allows us to calculate the partition sums of the convex blocks (with the values of the spin lines as variables) and afterwards integrate the magnetic "zips". It is shown in Sec. III.1.3 that this method allows us to calculate any arbitrary non-convex lattice configuration which scales "reasonably" in the thermodynamic limit. We start by introducing the zip method using the already known examples of two-dimensional rectangular stripes with free boundary conditions.

III.1.2.1. Introduction

We introduce the zip method by considering the two-dimensional Gaussian stripe with free boundary conditions, which is partitioned by a zip magnetic field in two different ways. For the sake of simplicity, we only consider a $N \times (N+1)$ and a $N \times (2N+1)$ stripe. The generalisation to arbitrary side lengths will be obvious from these calculations.

One convex block

We consider a $N \times N$ Gaussian block with an applied magnetic field $\boldsymbol{h}$ (the zip) at the boundary which is to be considered part of the system and integrated in order to obtain the partition sum. See Fig. III.1.1 for an illustration of the system. The

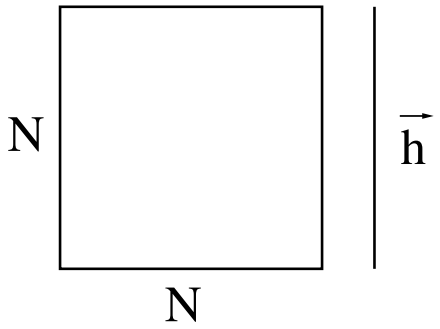

Figure III.1.1.: Two-dimensional Gaussian block with an applied magnetic field $\boldsymbol{h}$ at the boundary.

partition sum Z_1 of the $N \times N$ block without the magnetic field reads

$$Z_1 = \pi^{-\frac{N^2}{2}} \int \mathrm{d}^{N^2}\boldsymbol{s} \exp\left(\boldsymbol{s}^t M \boldsymbol{s}\right) = |\mathrm{det} M|^{-\frac{1}{2}}, \tag{III.1.22}$$

here we omit the indices of the matrix to keep the notation short: M is the interaction matrix of the $N \times N$ Gaussian stripe with free boundary conditions, see Sec. II.2.2.4. The full partition sum Z of the system can be obtained by integrating the magnetic field.

$$\begin{aligned} Z =& \pi^{-\frac{N(N+1)}{2}} \int \mathrm{d}^N \boldsymbol{h} \int \mathrm{d}^{N^2}\boldsymbol{s} \, \exp\left(\boldsymbol{s}^t M \boldsymbol{s} + K \boldsymbol{h}^t \boldsymbol{s} + \boldsymbol{h}^t M_\mathrm{f} \boldsymbol{h}\right) \\ =& \frac{\pi^{-\frac{N}{2}}}{|\det M|^{\frac{1}{2}}} \int \mathrm{d}^N \boldsymbol{h} \, \exp\left(-\frac{K^2}{4} \boldsymbol{h}^t M_I^{-1} \boldsymbol{h} + \boldsymbol{h}^t M_\mathrm{f} \boldsymbol{h}\right) = Z_1 \, \Delta Z. \end{aligned} \tag{III.1.23}$$

The matrix M_I^{-1} corresponds to the index set $I = \{1, ..., N\}$ according to Sec. III.1.1, i.e. it is the upper left $N \times N$ submatrix of M^{-1} (see Sec. A.2 for details on M^{-1}). The matrix M_f is the interaction matrix of the one-dimensional Gaussian chain of length N with free boundary conditions. By applying and integrating the magnetic

field $\boldsymbol{h}$, the partition sum Z_1 is multiplied by an additional partition sum ΔZ which describes the interaction of $\boldsymbol{h}$ with itself and the main system. In order to calculate ΔZ, we can diagonalise M_I^{-1} using the orthonormal transformation F which also diagonalises M_f

$$F_{i,j} = \sqrt{\frac{2}{N+1}} \sin ij \frac{\pi}{N+1}. \tag{III.1.24}$$

Applying the transformation, we obtain

$$-\frac{K^2}{4} F M_I^{-1} F = \frac{K^2}{2(N+1)} \sum_{l=1}^{N} \sin^2 \Theta_l \operatorname{diag} \left(1 - K\cos\Theta_l - K\cos\Theta_n\right)_n^{-1}, \tag{III.1.25}$$

$$\Theta_i := i\frac{\pi}{N+1}. \tag{III.1.26}$$

The notation $\operatorname{diag}(a_n)_n$ corresponds to a diagonal matrix with the entries $a_1, ..., a_N$ on its main diagonal. Once again, we apply the Euler-Maclaurin summation formula and omit all contributions which decay exponentially with N:

$$\begin{aligned}
-\frac{K^2}{4} F M_I^{-1} F &= \frac{K^2}{2(N+1)} \sum_{l=1}^{N} \operatorname{diag} \left(\frac{1-\cos^2\Theta_l}{1 - K\cos\Theta_l - K\cos\Theta_n} \right)_n \\
&= \frac{K^2}{2} \frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \operatorname{diag} \left(\frac{1-\cos^2\varphi}{1 - K\cos\Theta_n - K\cos\varphi} \right)_n \\
&= \frac{1}{2} \operatorname{diag} \left(1 - K\cos\Theta_n - \sqrt{\left(1 - K\cos\Theta_n\right)^2 - K^2} \right)_n .
\end{aligned}$$

From Sec. A.2 we already know the eigenvalues of M_f:

$$F M_\mathrm{f} F = \operatorname{diag} \left(-1 + K\cos\Theta_n\right)_n . \tag{III.1.27}$$

Thus, the interaction matrix in the exponent of Eq. (III.1.23) reads

$$F \left(-\frac{K^2}{4} M_I^{-1} + M_\mathrm{f} \right) F = -\operatorname{diag} \left(\frac{1 - K\cos\Theta_n + \sqrt{(1 - K\cos\Theta_n)^2 - K^2}}{2} \right)_n . \tag{III.1.28}$$

To evaluate the zip partition sum ΔZ, we calculate the determinant of this matrix:

$$\log \left| \det \left(-\frac{K^2}{4} M_I^{-1} + M_\mathrm{f} \right) \right| = \sum_{n=1}^{N} \log \left[\frac{1 - K\cos\Theta_n + \sqrt{(1 - K\cos\Theta_n)^2 - K^2}}{2} \right].$$

Applying the Euler-Maclaurin formula results in

$$\begin{aligned}\sum_{n=1}^{N} \log[...] &= \frac{N+1}{\pi}\int_0^\pi \mathrm{d}\varphi\, \log\frac{1-K\cos\varphi+\sqrt{(1-K\cos\varphi)^2-K^2}}{2} \\ &\quad -\frac{1}{2}\log\left[\frac{\left(1-K+\sqrt{1-2K}\right)\left(1+K+\sqrt{1+2K}\right)}{4}\right] \\ &= 2(N+1)f_0^{2\mathrm{d}} - \frac{1}{2}\log\left[\frac{\left(1-K+\sqrt{1-2K}\right)\left(1+K+\sqrt{1+2K}\right)}{4}\right].\end{aligned} \tag{III.1.29}$$

Therefore, the additional contribution $\log \Delta Z$ of the magnetic zip to the free energy $\log Z_1$ of the $N \times N$ Gaussian stripe reads

$$-\log \Delta Z = N f_0^{2\mathrm{d}} + 2 f_1^{2\mathrm{d}}. \tag{III.1.30}$$

As introduced in Sec. II.2.2.5, $f_0^{2\mathrm{d}}$, $f_1^{2\mathrm{d}}$ is the volume and the surface coefficient of the two-dimensional Gaussian model. As expected, the magnetic zip increases the volume of the system by N and the surface by 2.

Two blocks

As another example of the zip method and in order to prepare further calculations, we consider the following system: two $N \times N$ Gaussian blocks connected by a chain of Gaussian spins of length N (the magnetic zip), see Fig. III.1.2 for details. We start by calculating the partition sums of both block systems and integrate the magnetic field afterwards. We denote the partition sums of the blocks without the magnetic

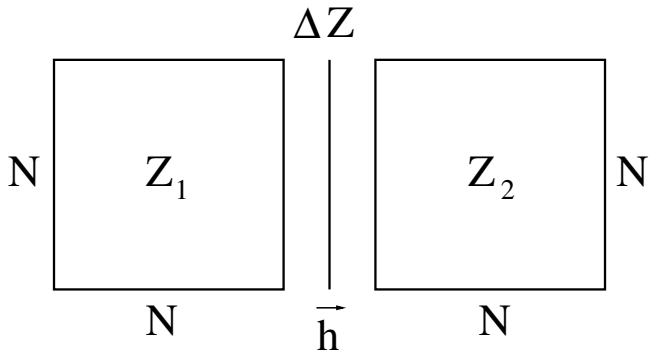

Figure III.1.2.: Two $N \times N$ Gaussian blocks zipped together by a magnetic chain of length N. We denote the partition sums of both block systems without the magnetic field with Z_1, Z_2. The partition sum which arises from integrating the magnetic field is denoted as ΔZ.

field with $Z_1,\ Z_2$ (see Sec. II.2.2.4 for results and details on calculations):

$$-\log Z_1 = -\log Z_2 = N^2 f_0^{2\mathrm{d}} + 4N f_1^{2\mathrm{d}} + f_2^{2\mathrm{d}}. \tag{III.1.31}$$

The total partition sum Z can be written as

$$Z = Z_1 Z_2 \Delta Z. \tag{III.1.32}$$

ΔZ is the partition sum of the magnetic field. There are two ways to estimate ΔZ: We can consider the whole system as one $N \times (2N+1)$ Gaussian stripe with free boundary conditions. The partition sum of this system is known from Sec. II.2.2.4. Since both subsystems $Z_1,\ Z_2$ are equal, we obtain

$$-\log Z = -2\log Z_1 - \log \Delta Z = N(2N+1) f_0^{2\mathrm{d}} + 2(3N+1) f_1^{2\mathrm{d}} + f_2^{2\mathrm{d}}. \tag{III.1.33}$$

Solving for ΔZ yields:

$$-\log \Delta Z = N f_0^{2\mathrm{d}} - 2(N-1) f_1^{2\mathrm{d}} - f_2^{2\mathrm{d}}. \tag{III.1.34}$$

Alternatively, we can estimate the interaction matrix of the magnetic field (after tracing out the subsystems $Z_1,\ Z_2$) and calculate the partition sum explicitly. In analogy to Eq. (III.1.23), we obtain

$$Z = \frac{\pi^{-\frac{N}{2}}}{|\mathrm{det} M|} \int \mathrm{d}^N \boldsymbol{h}\, \exp\left(-\frac{K^2}{2} \boldsymbol{h}^t M_I^{-1} \boldsymbol{h} + \boldsymbol{h}^t M_\mathrm{f} \boldsymbol{h} \right) = Z_1\, \Delta Z.$$

The matrix M_I^{-1} is, once again, the upper left $N \times N$ submatrix of the $N^2 \times N^2$ inverse interaction matrix of the subsystems $Z_1,\ Z_2$. In the previous example we have already diagonalised both M_I^{-1} and M_f using the discrete sine transformation F:

$$F^t \left(M_\mathrm{f} - \frac{K^2}{2} M_I^{-1} \right) F = -\mathrm{diag}\left(\sqrt{(1 - K\cos\Theta_n)^2 - K^2} \right)_n. \tag{III.1.35}$$

The determinant can be calculated via the Euler-Maclaurin summation formula

$$\begin{aligned} -\log \Delta Z &= -\log \left| \left(\sqrt{(1 - K\cos\Theta_n)^2 - K^2} \right)_n \right| \\ &= \frac{N}{4} \log \frac{\left(1 + K + \sqrt{1+2K}\right)\left(1 - K + \sqrt{1-2K}\right)}{4} \\ &\quad + \frac{1}{4} \log \frac{\left(1 + K + \sqrt{1+2K}\right)\left(1 - K + \sqrt{1-2K}\right)}{4\sqrt{1-4K^2}} \\ &= N f_0^{2\mathrm{d}} - 2(N-1) f_1^{2\mathrm{d}} - f_2^{2\mathrm{d}}. \end{aligned} \tag{III.1.36}$$

As expected the zip partition sum modifies the volume by N and reduces the surface of the whole system by $2(N-1)$. Additionally, it removes four corners from the system: Both subsystems $Z_1,\ Z_2$ have eight corners while the final system after the integration of the zip has only four corners, thus the contribution $-f_2^{2\mathrm{d}}$.

III.1.2.2. Non-convex building block

Consider the system depicted in Fig. III.1.3: three $N \times N$ blocks separated by spin lines $\boldsymbol{h}_1$, $\boldsymbol{h}_2$ of length N, arranged such that they build a corner. The choice of equal side lengths is arbitrary, the generalisation to different side lengths is straightforward. In the remaining part of this thesis this lattice domain is referred to as the non-convex building block. By partitioning the system in this way we obtain three

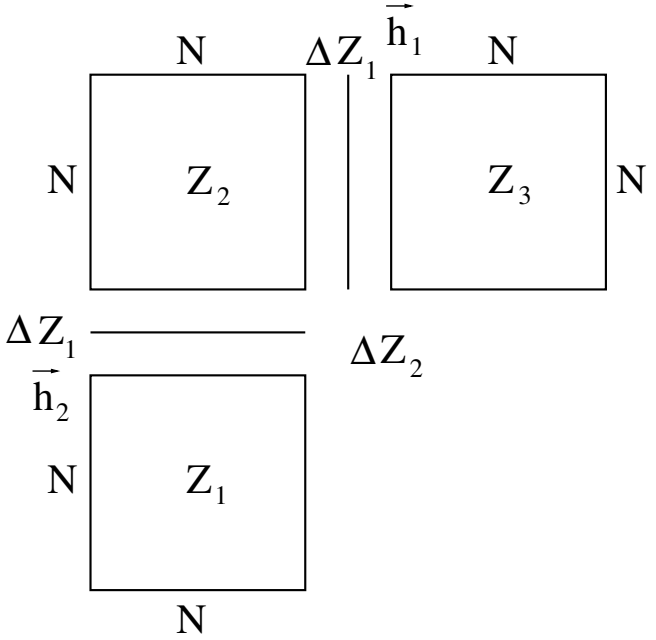

Figure III.1.3.: Basic non-convex domain configuration. The partition sums Z_1, Z_2, Z_3 are the partition sums of the $N \times N$ Gaussian blocks without magnetic field. The partition sum ΔZ_1 refers to the partition sum of a spin line between two blocks (the degrees of freedom of the blocks already traced out) and has been discussed in Sec. III.1.2.1. The partition sum ΔZ_2 corresponds to the interaction between both magnetic fields.

different types of partition sums: Partition sums Z_1, Z_2, Z_3, which correspond to $N \times N$ Gaussian blocks with free boundary condition without magnetic fields. Partition sum ΔZ_1, which describes the interaction of a spin line between two blocks and was discussed in the examples in Sec. III.1.2.1. And, finally, partition sum ΔZ_2, which is responsible for the interaction of both spin zips between each other. We can write down the total partition sum Z in a straight-forward manner:

$$Z = \pi^{-N} Z_1^3 \int \mathrm{d}^N \boldsymbol{h}_1 \int \mathrm{d}^N \boldsymbol{h}_2 \exp\left(\boldsymbol{h}^t A \boldsymbol{h}\right). \tag{III.1.37}$$

The contribution Z_1 is known. The magnetic field $\boldsymbol{h}$ and the matrix A read

$$\boldsymbol{h} = (\boldsymbol{h}_1, \boldsymbol{h}_2)^t \in \mathbb{R}^{2N}, \tag{III.1.38}$$

$$A = \begin{bmatrix} M_{\mathrm{f}} - \frac{K^2}{2} M_I^{-1} & \Delta M \\ \Delta M & M_{\mathrm{f}} - \frac{K^2}{2} M_I^{-1} \end{bmatrix} \tag{III.1.39}$$

The matrices M_I^{-1}, ΔM are $N \times N$ submatrices of the inverse M^{-1} of the interaction matrix of the two-dimensional Gaussian block with free boundary conditions. The index set $I = \{1, ..., N\}$ is the same as in the previous examples in Sec. III.1.2.1. The matrix ΔM is given by

$$(\Delta M)_{i,j} = -\frac{K^2}{4} M^{-1}_{(1,i)(j,1)}. \tag{III.1.40}$$

M^{-1} is a block matrix, the first pair of indices numerates the blocks, the second pair of indices numerates the entries in the block. It should be pointed out that the matrix $M_{\mathrm{f}} - \frac{K^2}{2} M_I^{-1}$ is the interaction matrix of a spin line consisting of N spins, which connects two $N \times N$ spin blocks, see Sec. III.1.2.1. Its determinant equals ΔZ_1 and is known from the second example in Sec. III.1.2.1. Obviously, the matrix ΔM is responsible for the interaction between both magnetic fields $\boldsymbol{h}_1$, $\boldsymbol{h}_2$. We discuss the properties of ΔM and A in detail and evaluate the relevant determinants in Chap. III.2. For now, we assume that the determinant of A is known. It is important to point out that the matrix A is tightly related to the partition sum of three blocks which are arranged in a line and connected by two magnetic zips, i.e. a $N \times (3N + 2)$ Gaussian rectangle, in the following way: The free energy difference

$$\Delta F = -\log \frac{|A|^{-\frac{1}{2}}}{\Delta Z_1^2} \tag{III.1.41}$$

is the energy needed to transform the convex $N \times (3N + 2)$ Gaussian rectangle, see Fig. III.1.4 into the non-convex configuration Fig. III.1.3. From the geometrical standpoint, the energy ΔF is the energy needed to create one additional convex corner and one additional concave corner. Since the energy of one convex corner is $f_2^{2\mathrm{d}}/4$ the energy of a concave corner is $\Delta F - f_2^{2\mathrm{d}}/4$. We denote this energy with $\tilde{f}_2^{2\mathrm{d}}$

$$\tilde{f}_2^{2\mathrm{d}} := 4\,\Delta F - f_2^{2\mathrm{d}} = -4 \log \frac{|A|^{-\frac{1}{2}}}{\Delta Z_1^2} - f_2^{2\mathrm{d}}. \tag{III.1.42}$$

In the remaining part of this section we show that the calculation of the partition sum of the Gaussian system on a large class of non-convex domains can be reduced to the calculation of the partition sum of the non-convex building block.

III.1.3. Generalisation to non-convex domains

In this section we apply the zip method to evaluate the partition sum of large class of non-convex domains. We start out by presenting representative examples of non-convex domains and reducing the calculation of the corresponding partition sums to

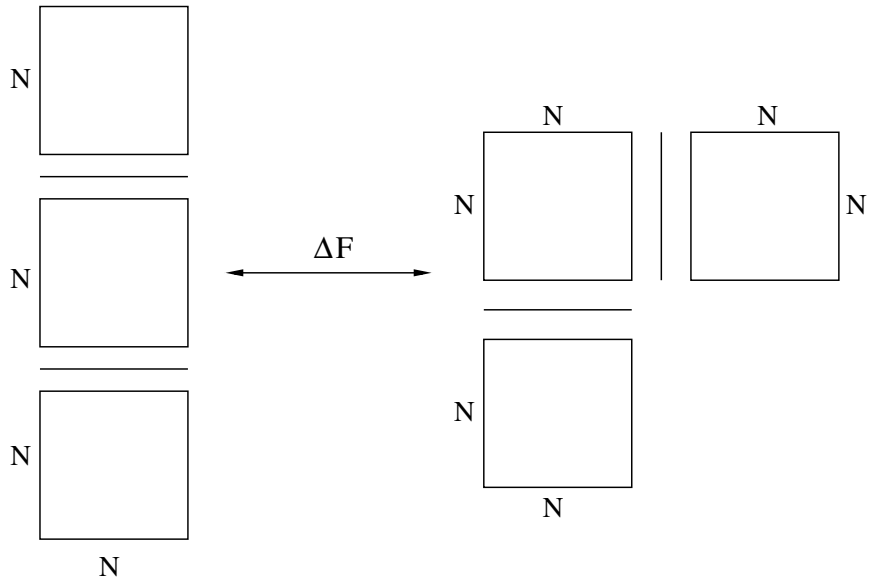

Figure III.1.4.: The energy ΔF, is the energy needed to transform the basic non-convex building block (right-hand side) into three linearly arranged Gaussian blocks (left-hand side).

the calculation of the partition sum of the non-convex building block. Afterwards, we define a large class of non-convex domains, the *proper* domains: Domains which scale reasonably in the thermodynamic limit, i.e. all side lengths of the domain are supposed to grow linearly with the size of the system as the number of spins goes to infinity in the thermodynamic limit. In this case, the system can be partitioned into rectangular blocks separated by spin zips. The interaction between the blocks and the magnetic zips can be boiled down to two different cases (which are discussed in this section) and the calculation of the partition sum of the system can be reduced to the calculation of the non-convex building block. Finally, we demonstrate examples of domains which can not be treated with these methods and point out alternative routes to access the partition sums of such domains.

III.1.3.1. Examples

Two separated magnetic zips: We consider two spin lines, $\boldsymbol{h}_1$, $\boldsymbol{h}_2$, of length n which couple to a $N \times M$ spin block (M rows, N columns) in an arbitrary way, with the side condition that the separation between both spin lines grows linearly with the system size, see Fig. III.1.5. After tracing out the degrees of freedom of the spin block, only the degrees of freedom of the magnetic lines remain. The partition sum of the magnetic lines is given by the determinant of a 2×2 interaction block matrix, each block being a $n \times n$ matrix. In addition to the interaction of a magnetic line with itself, which is described by the block diagonal, the interaction matrix contains the

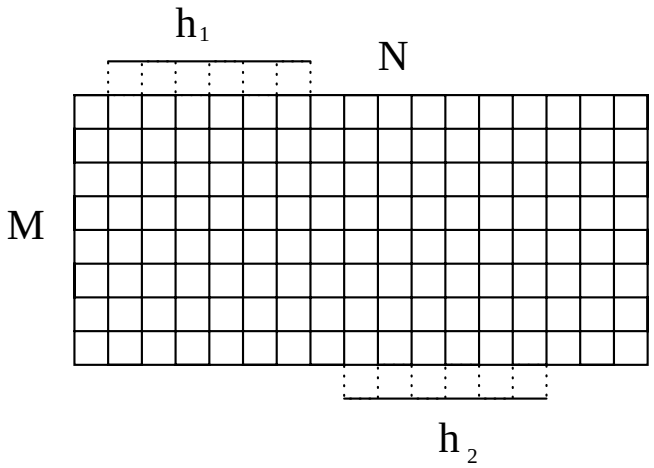

Figure III.1.5.: A $M \times N$ Gaussian spin block – a spin is attached at each lattice site. Additionally two spin lines, $\boldsymbol{h}_1$ and $\boldsymbol{h}_2$ couple to the spin block on two **opposite** sides (the coupling is illustrated by the dotted lines). As a result, the separation between the magnetic spin lines grows in the thermodynamic limit.

interaction coefficients between both zips – namely the off-diagonal blocks, which we denote as ϵ and ϵ^t. Assuming that the numeration of the spins of the spin block was chosen such that one zip couples to the first spin row and one to the last spin row, the off-diagonal blocks are of the form

$$\epsilon_{i,j} = -\frac{K^2}{4} M^{-1}_{(1,M)(\alpha_i,\beta_j)}. \tag{III.1.43}$$

where M is the interaction matrix of the $M \times N$ spin block and the index sets

$$\{\alpha_1, ..., \alpha_n\} \subset \{1, ..., N\} \text{ and} \tag{III.1.44}$$
$$\{\beta_1, ..., \beta_n\} \subset \{1, ..., N\} \tag{III.1.45}$$

and depend on the exact position of the magnetic zips. Writing out the zip interaction matrix ϵ, we obtain

$$\epsilon_{i,j} = -\frac{4}{(N+1)(M+1)} \sum_{l=1}^{N} \sum_{k=1}^{M} \frac{\sin^2\left(\pi \frac{k}{M+1}\right) (-1)^{k+1} \sin\left(\pi \frac{\alpha_i\, l}{N+1}\right) \sin\left(\pi \frac{\beta_j\, l}{N+1}\right)}{1 - K\cos\left(\pi \frac{k}{M+1}\right) - K\cos\left(\pi \frac{\alpha_i\, l}{N+1}\right)}. \tag{III.1.46}$$

We split the k-sum into even and odd contributions and apply the Euler-Maclaurin formula. As a result, it turns out that the entries of the interaction matrix ϵ vanish exponentially with the separation length M:

$$\epsilon_{i,j} = \mathcal{O}\left(M^{-k}\right), \forall k \in \mathbb{N}, \text{ as } M \to \infty. \tag{III.1.47}$$

This result allows us to neglect the interactions between two separated magnetic lines if the separation grows in the thermodynamic limit.

Two concave corners: In the next step, we consider a domain consisting of three different blocks, separated by two magnetic zips, such that it features two concave and six convex corners. See the left-hand side of Fig. III.1.6 for a schematic illustration. With the results of the previous example, we know that we can neglect the

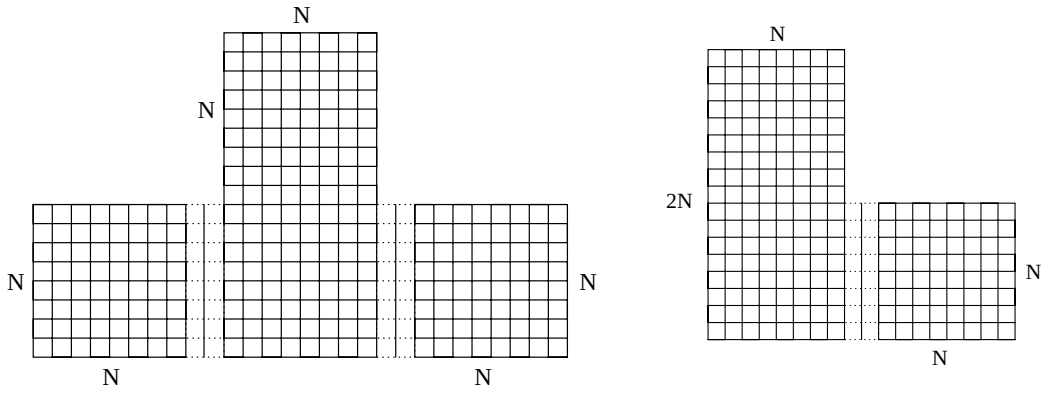

Figure III.1.6.: Left: three Gaussian spin blocks connected by two magnetic zip lines. The system features two concave and six convex corners. After tracing out the degrees of freedom of the spin blocks, the interaction between the magnetic zips can be neglected, since they are separated by a growing distance. It only remains to calculate the partition sum of one magnetic zip line between two spin blocks, as depicted on the right side.

interaction between both magnetic zips, since they a separated by a growing block. Therefore, after tracing out the three blocks, it only remains to estimate the partition sum ΔZ of a magnetic line, positioned between two blocks, as depicted on the right-hand side of Fig. III.1.6. However, this partition sum has already been treated as a part of the partition sum of the basic non-convex building block, see Sec. III.1.2.2: Assuming that the magnetic zips are of length N and the three blocks are $N \times N$ and $N \times 2N$, it reads

$$-\log \Delta Z = N f_0^{2\mathrm{d}} - 2(N-1) f_1^{2\mathrm{d}} - \frac{3}{4} f_2^{2\mathrm{d}} + \frac{1}{4} \tilde{f}_2^{2\mathrm{d}}. \tag{III.1.48}$$

Since there are two magnetic zips, ΔZ enters the total partition sum Z quadratically. We obtain the total partition sum Z of the configuration on the left-hand side of Fig. III.1.6:

$$-\log Z = 2N(2N+1) f_0^{2\mathrm{d}} + 2(5N+2) f_1^{2\mathrm{d}} + \frac{3}{2} f_2^{2\mathrm{d}} + \frac{1}{2} \tilde{f}_2^{2\mathrm{d}}. \tag{III.1.49}$$

Four concave corners: We consider a system consisting of two $N \times N$ blocks and one $N \times 3N$ block, separated by two magnetic zips of length N such that there are eight convex and four concave corners, see the left-hand side of Fig. III.1.7. The particular choice of the size of the blocks and magnetic lines is of no importance, the results can be generalised to arbitrary sizes. Since both magnetic zips are separated by a block

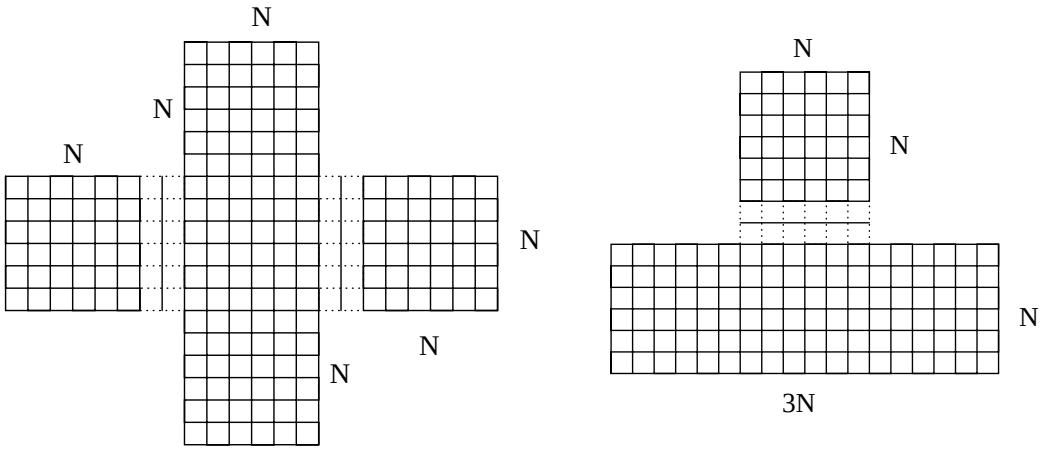

Figure III.1.7.: Left: three Gaussian spin blocks connected by two magnetic zip lines. The system features four concave and eight convex corners. After tracing out the degrees of freedom of the spin blocks, the interaction between both magnetic zips can be neglected, since they are separated by a growing distance. Therefore, the calculation of the partition sum goes back to the previous example of a system with two concave corners, as depicted on the right-hand side.

which grows linearly with the system size, we can trace out the degrees of freedom of the three blocks and neglect the interaction between both remaining spin lines. Therefore, it only remains to estimate the partition sum of a spin line between two blocks, as shown on the right-hand side of Fig. III.1.7. However, this partition sum is known from the previous example. The total free energy of the system F reads

$$F = -\log Z = N(5N+2) f_0^{2\mathrm{d}} + 3(3N+1) f_1^{2\mathrm{d}} + 2 f_2^{2\mathrm{d}} + \tilde{f}_2^{2\mathrm{d}}. \tag{III.1.50}$$

Rectangle with a hole: In the last example, we consider the simplest possible lattice domain with a zero Euler number. The system is depicted on the left-hand side of Fig. III.1.8 We decide to partition the system into eight blocks and eight magnetic zips as shown on the left-hand side of Fig. III.1.8. After tracing out the degrees of freedom of the blocks, the only remaining interactions between the magnetic lines are the interactions between two spin lines which form a corner (since the interactions between two magnetic lines separated by a block can be neglected), see the right-hand side of Fig. III.1.8. However, the interaction between two magnetic spin

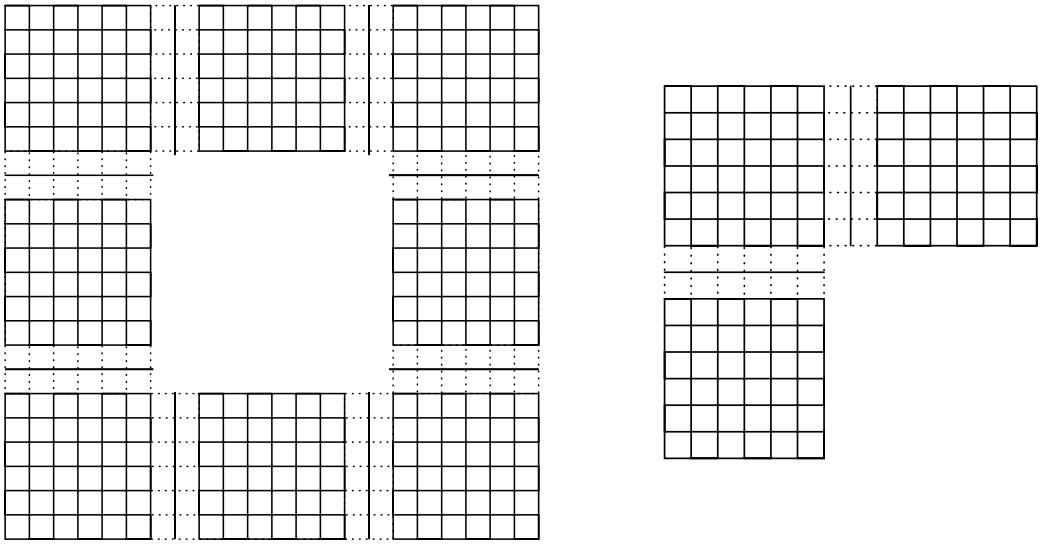

Figure III.1.8.: Left: the simplest lattice container featuring a hole. The size of the hole grows linearly with the system size. The Euler number of the lattice container is zero, see Sec. I.1. After tracing out the degrees of freedom of the eight quadratic lattices, the only remaining interactions are the interactions between two magnetic zips which form a corner, see the figure on the right-hand side. The partition sum of two zips which form a corner is part of the partition sum of the non-convex building block, see Sec. III.1.2.2.

lines forming a corner has been discussed as a part of the basic non-convex building block. Estimating the total partition sum of the system boils down to counting concave and convex corners:

$$-\log Z = 8N(N+1)f_0^{2\mathrm{d}} + 16(N+1)f_1^{2\mathrm{d}} + f_2^{2\mathrm{d}} + \tilde{f}_2^{2\mathrm{d}}. \tag{III.1.51}$$

III.1.3.2. Properly scaling domains

Motivated by these examples we consider the following class of domains $\mathcal{D} \subset \mathbb{Z}^2$: domains which can be decomposed into blocks $\mathcal{D}_1, .., \mathcal{D}_n$, which are connected by spin zips. All side lengths, holes and distances between magnetic zips are supposed to grow linearly with the system size in the thermodynamic limit. It should be pointed out that in order to apply the zip method, not the shape of the domain is important, but how the domain scales in the thermodynamic limit: E.g. consider a $N \times N$ lattice with spins attached to all lattice sites except one lattice site in the middle – i.e. a rectangular domain with a single hole. One can choose the hole to grow linearly with the system size as the system grows in the thermodynamic limit, or alternatively one can choose the hole to keep its size as the system grows and end

up with an infinite system featuring a single defect. The former case is a "properly scaling" domain and can be treated with the zip method, being essentially the last example in Sec. III.1.3.1, while the latter case requires different methods to calculate the partition sum. In order to put the concept of properly scaling domains in a precise mathematical formulation, we need some definitions. We start by defining the convex hull and the projections on the axes: Let $\mathcal{D} \subset \mathbb{Z}^2$ be finite, consisting of $|\mathcal{D}|$ points $x_1, ..., x_{|\mathcal{D}|}$. The *convex hull* $\mathrm{Conv}(\mathcal{D})$ is defined as

$$\mathrm{Conv}(\mathcal{D}) := \left\{ \sum_{i=1}^{|\mathcal{D}|} \alpha_i x_i;\ (\forall i : \alpha_i > 0) \wedge \sum_{i=1}^{|\mathcal{D}|} \alpha_i = 1 \right\}. \tag{III.1.52}$$

Obviously, the convex hull is no longer a subset of $\mathbb{Z}^2$. The *axis projections* of $\mathcal{D}$ are defined in a straight-forward way as

$$\mathrm{Pr}_x(\mathcal{D}) = \{x \in \mathbb{R};\ (x, y) \in \mathrm{Conv}(\mathcal{D})\}, \tag{III.1.53}$$
$$\mathrm{Pr}_y(\mathcal{D}) = \{y \in \mathbb{R};\ (x, y) \in \mathrm{Conv}(\mathcal{D})\}. \tag{III.1.54}$$

A *rectangular lattice domain* $\mathcal{Q} \subset \mathbb{Z}^2$ with side lengths $N_1,\ N_2$, otherwise called convex domain, is a set which fulfills

$$\begin{aligned} \mathrm{Conv}(\mathcal{Q}) \cap \mathbb{Z}^2 &= \mathcal{Q}, \\ \lambda\left(\mathrm{Pr}_x(\mathcal{Q})\right) &= N_1 - 1 > 0, \\ \lambda\left(\mathrm{Pr}_x(\mathcal{Q})\right) &= N_2 - 1 > 0, \end{aligned} \tag{III.1.55}$$

where λ is the Lebesgue measure on $\mathbb{R}$. In other words, a rectangular lattice domain is what we intuitively refer to as a convex domain. If a rectangular domain has horizontal edges consisting of N_1 spins, then the length of each of these edges is $N_1 - 1$. This definition excludes spin lines and single isolated spins from the set of rectangular lattice domains, as these sets would have at least one edge with the length zero. A *rectangular decomposition* $r(\mathcal{D})$ of a domain $\mathcal{D}$ is a set $\{\mathcal{Q}_1, ..., \mathcal{Q}_n\},\ n \in \mathbb{N}$, of rectangular domains, such that

$$\bigcup_{i=1}^{n} \mathcal{Q}_i = \mathcal{D}. \tag{III.1.56}$$

We call a domain $\mathcal{D}$ *proper*, if a rectangular decomposition $\mathcal{Q}_1, ..., \mathcal{Q}_n$ exists, such that

$$\mathcal{Q}_i \cap \mathcal{Q}_j > 0 \Rightarrow \mathcal{Q}_i \cap \mathcal{Q}_j > 1. \tag{III.1.57}$$

This side condition is needed to exclude domains which consist of two rectangular blocks overlapping only at the corner lattice site: While it is possible to calculate the free energy of the Gaussian system on such domains, they do not scale properly in the thermodynamic limit (the overlap will only be one lattice site, no matter how the system is scaled) and the underlying calculations can not be reduced to the partition sum of the non-convex building block. Given a proper domain $\mathcal{D}$, we can consider

the set R of rectangular decompositions of $\mathcal{D}$. R is finite, since $\mathcal{D}$ is a finite set. Now we can define the *scaled domain* $n\mathcal{D}$ for any $n \in \mathbb{N}$:

$$n\mathcal{D} := \left(\bigcup_{r \in R} \bigcup_{\mathcal{Q}_i \in r} n\mathrm{Conv}\left(\mathcal{Q}_i\right) \right) \bigcap \mathbb{Z}^2, \text{ where} \tag{III.1.58}$$

$$nM := \{nx;\ x \in M\}\,, \text{ for any } M \subset \mathbb{R}^2 \text{ is the scaled set.} \tag{III.1.59}$$

The basic idea is to decompose the underlying domain into rectangular blocks, rescale the rectangular blocks as subsets of $\mathbb{R}^2$ and then project the scaled set on the lattice $\mathbb{Z}^2$. Now, a *properly scaling* lattice domain is any domain which can be obtained by scaling a proper domain. On the other hand, starting with a proper domain $\mathcal{D}$, one can achieve the thermodynamic limit by considering the scaled domain $n\mathcal{D}$ and then letting n go to infinity. For large system sizes, a properly scaling domain can be decomposed into rectangular blocks connected by single spin zip lines similar to the examples in Sec. III.1.3.1. As the system grows to infinity, the zips are either separated by a growing distance, and thus the interaction between them can be neglected, or the zips are positioned similar to the zips of the non-convex building block, see Sec. III.1.2.2. After tracing out the degrees of freedom of the rectangular blocks, only the degrees of freedom of the magnetic zips remain. The partition sum of the magnetic zips can now be reduced to one of the examples in Sec. III.1.3.1.

Summary:

Summarising, one can say that the zip method allows to calculate the partition sum of an arbitrarily shaped properly scaling two-dimensional Gaussian system, once the partition sum of the non-convex building block is known. The total free energy can be calculated in an easy way by counting volume, surface and corner lattice sites and weighting them as following:

- Each lattice site multiplicatively contributes with the factor $\exp\left(-f_0^{2\mathrm{d}}\right)$ to the **partition sum**.
- Additionally, each lattice side which belongs to the surface of the system – i.e. has **exactly** three neighbouring spins – contributes with the factor $\exp\left(-f_1^{2\mathrm{d}}\right)$ to the partition sum.
- Additionally, each lattice site which forms a convex corner – i.e. has only two neighbouring spins – contributes with the factor $\exp\left(-f_2^{2\mathrm{d}}/4 - 2f_1^{2\mathrm{d}}\right)$ to the partition sum.
- Additionally, each lattice site which forms a concave corner contributes with the factor $\exp\left(-\tilde{f}_2^{2\mathrm{d}}/4\right)$ to the partition sum.

All additional contributions to the free energy decay exponentially with the system size in the thermodynamic limit. One should note that in order to be able to determine the partition sum in this simple geometric way, we have to restrict ourselves to

properly scaling container geometries, as defined in this section. In the next section, we give some examples of container geometries with partition sums, which can not be calculated as easily and present alternative methods to estimate these partition sums.

III.1.3.3. Non-properly scaling domains

In the previous section the partition sum of the Gaussian system on any properly scaling domain was calculated – i.e. domains whose edge lengths and holes grow with the system size in the thermodynamic limit. While this covers a large class of relevant domains there are other domains which can be interesting from the physical point of view, e.g. domains with single hole or line defects. In this section we present several examples of Gaussian spin systems on lattice containers which do not meet the requirement of being properly scaling in the thermodynamic limit: The partition sums of these systems can not be estimated in the simple way presented in this section, i.e. by counting volume, surface and corner spins. However, it turns out that it is possible to estimate some of these partition sums on a case-by-case basis using the methods developed here.

Single hole in a toroidal system

We start by considering a $N \times M$ Gaussian stripe with toroidal boundary conditions and a single hole defect which does not grow with the system size in the thermodynamic limit. Since the original system is translational invariant, the position of the hole does not affect the partition sum. We divide the system in M spin rows, each row consisting of N spins and choose the hole to be at the first lattice site of the first row. We can calculate the partition sum using the method of freezing spins, see Sec. III.1.1. The partition sum reads:

$$Z = \frac{1}{\sqrt{\det(-M)\det(-M_I^{-1})}} = Z_{\mathrm{t}}^{2\mathrm{d}} \frac{1}{\sqrt{\det(-M_I^{-1})}}. \tag{III.1.60}$$

Here, $M \equiv M_{\mathrm{t}}^{2\mathrm{d}}$ is the interaction matrix of the original system without defects, see Sec. II.2.2.1, $I = \{1\}$ the index set and M_I^{-1} the 1×1 upper left submatrix of M^{-1}, according to Sec. III.1.1. $Z_{\mathrm{t}}^{2\mathrm{d}}$ is the partition sum of the $N \times M$ toroidal system. Using the properties derived in Sec. A.2 and the Euler-Maclaurin summation formula, see Sec. A.4, we can calculate M_I^{-1} in the limit $M, N \to \infty$:

$$M_I^{-1} = -\frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1}{\sqrt{(1 - K\cos\varphi)^2 - K^2}}. \tag{III.1.61}$$

We define the bulk defect energy B as

$$B(K) := \frac{1}{2} \log \left| M_I^{-1} \right| = \frac{1}{2} \log \frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1}{\sqrt{(1 - K\cos\varphi)^2 - K^2}}. \tag{III.1.62}$$

The free energy reads

$$\beta F = \beta F_{\mathrm{t}}^{2\mathrm{d}} + B. \tag{III.1.63}$$

Here $\beta F_{\mathrm{t}}^{2\mathrm{d}}$ is the free energy of the original system without defects. The energy $B(K)$ of a single hole defect in the bulk of the system as a function of the coupling K is plotted in Fig. III.1.9.

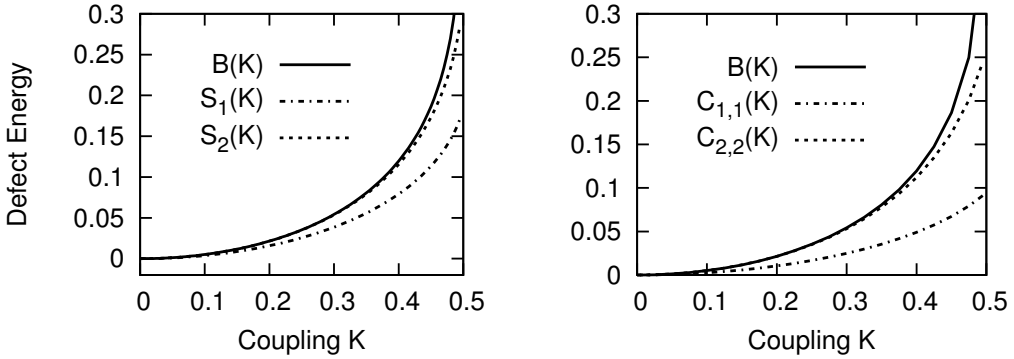

Figure III.1.9.: Left: the energy of a single hole defect as a function of the spin-spin coupling K. Solid line: $B(K)$, i.e. the hole defect is in the bulk, see Eq. (III.1.62). Dash-dotted line: $S_1(K)$, i.e. the hole defect is at the boundary of the system and far away from the corners of the system. Dashed line: $S_2(K)$, i.e. the hole defect is one lattice site away from the boundary of the system and far away from the corners, see Eq. (III.1.72). Right: the energy of a single hole defect as a function of K. Solid line: $B(K)$, i.e. the hole defect is in the bulk, see Eq. (III.1.62). Dash-dotted line: $C_{1,1}(K)$, i.e. the hole defect is at the corner site. Dashed line: $C_{2,2}(K)$, i.e. the hole defect is one lattice site away in each direction from the corner lattice site, see Eq. (III.1.65).

Single hole in a system with free boundaries

As our next example of non-properly scaling domains, we consider a $N \times M$ Gaussian stripe with free boundary conditions and a single hole which does not grow with the system size. In contrast to the toroidal boundary conditions this system is not translational invariant. Thus, the partition sum depends on the exact position of the defect. We choose the defect to be on the n-th lattice site of the m-th row and consider three cases: We start with m, n constant, not growing with the system size in the thermodynamic limit, i.e. $m, n \ll M, N$. This case corresponds to the defect being close to one of the corners of the system. The second case is $m = (M-1)/2$, $N = (N-1)/2$ with M, N odd. This choice corresponds to the defect in the bulk of the system, with the distance to the boundary growing with the system size. Finally, we consider $n = (N-1)/2$, m constant, with N odd. This case

corresponds to the defect being close to the boundary of the system, but far away from the corners. In analogy to the previous example, the partition sum reads

$$Z = Z_{\mathrm{f}}^{2\mathrm{d}} \frac{1}{\sqrt{\det\left(M_I^{-1}\right)}}. \tag{III.1.64}$$

$M \equiv M_{\mathrm{f}}^{2\mathrm{d}}$ is the interaction matrix of the Gaussian system with free boundary conditions, see Sec. II.2.2.4, and M_I^{-1} is a diagonal entry of M^{-1}. From Sec. A.2, we know the entries of M^{-1}:

$$M^{-1}_{(i,j)(m,n)} = \frac{4}{(N+1)(M+1)} \sum_{k=1}^{M} \sum_{l=1}^{N} \frac{\sin i\,k\frac{\pi}{M+1} \sin j\,k\frac{\pi}{M+1} \sin m\,l\frac{\pi}{N+1} \sin n\,l\frac{\pi}{N+1}}{-1 + K\cos k\frac{\pi}{M+1} + K\cos l\frac{\pi}{N+1}}.$$

We start with the hole close to one of the corners.

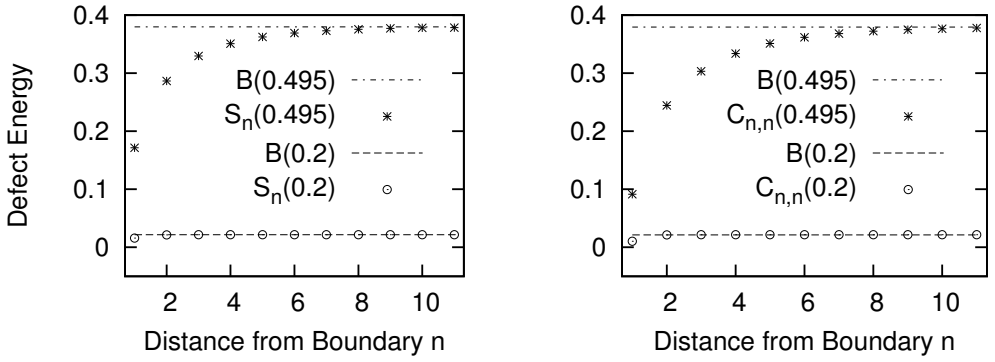

Figure III.1.10.: The energy of a single hole defect as a function of the distance n from the boundary. $n = 1$ means the hole defect is positioned at the boundary – either at the surface (left plot) or at the corner (right plot). The horizontal lines are the values $B(K)$ of the energy of a single hole defect in the bulk of the system at coupling strengths $K \in \{0.2, 0.495\}$. Left: the energy S_n of a hole defect close to the surface of the system but far away from the corners as a function of the distance n for values of the spin-spin coupling $K \in \{0.2, 0.495\}$, see Eq. (III.1.72). Right: the energy $C_{n,n}$ of a hole defect close to the corner of the system for values of the spin-spin coupling $K \in \{0.2, 0.495\}$, see Eq. (III.1.65). For any non-critical values of K, both $S_n(K)$ and $C_{n,n}(K)$ quickly converge to the energy $B(K)$ of a single hole defect in the bulk of the system as the distance n grows.

Defect close to a corner: We choose the defect to be on the n-the lattice site of the m-th row and keep m, n constant. Thus $I = (m-1)N + n$. Since M^{-1} is a block

matrix we have to calculate the n-th diagonal entry of the m-th diagonal block:

$$M_I^{-1} = M^{-1}_{(m,m)(n,n)} = \frac{4}{(N+1)(M+1)} \sum_{k=1}^{M} \sum_{l=1}^{N} \frac{\sin^2 m\, k \frac{\pi}{M+1} \, \sin^2 n\, l \frac{\pi}{N+1}}{-1 + K \cos k \frac{\pi}{M+1} + K \cos l \frac{\pi}{N+1}}.$$

We consider the thermodynamic limit M, $N \to \infty$ and apply the Euler-Maclaurin formula:

$$M_I^{-1} = \frac{4}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta \, \frac{\sin^2 m\varphi \, \sin^2 n\Theta}{-1 + K\cos\varphi + K\cos\Theta}.$$

We define the corner defect free energy $C_{n,m}$:

$$C_{n,m}(K) := \frac{1}{2} \log \left| M_I^{-1} \right| = \frac{1}{2} \log \frac{4}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta \, \frac{\sin^2 m\varphi \, \sin^2 n\Theta}{1 - K\cos\varphi - K\cos\Theta}. \quad \text{(III.1.65)}$$

Performing the Fourier decomposition of $\sin^2$ yields

$$\begin{aligned} M_I^{-1} = & \frac{1}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta \, \frac{1}{-1 + K\cos\varphi + K\cos\Theta} \\ & + \frac{1}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta \, \frac{\cos 2m\varphi \, \cos 2n\Theta}{-1 + K\cos\varphi + K\cos\Theta} \\ & - \frac{1}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta \, \frac{\cos 2m\varphi + \cos 2n\Theta}{-1 + K\cos\varphi + K\cos\Theta}. \end{aligned} \quad \text{(III.1.66)}$$

Finally, we can carry out one of the integrations:

$$\begin{aligned} M_I^{-1} = & -\frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1}{\sqrt{(1 - K\cos\varphi)^2 - K^2}} \\ & + \frac{1}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta \, \frac{\cos 2m\varphi \, \cos 2n\Theta}{-1 + K\cos\varphi + K\cos\Theta} \\ & + \sum_{k \in \{m,n\}} \frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{\cos 2k\varphi}{\sqrt{(1 - K\cos\varphi)^2 - K^2}}. \end{aligned} \quad \text{(III.1.67)}$$

As expected, the first term corresponds to the contribution of a single hole defect to the partition sum of the toroidal system. The second and the third terms are m, n-th Fourier modes of rational expressions of the cos function and describe the correlation of the hole defect with the boundary of the lattice domain. They vanish in the limit m, $n \to \infty$, i.e. when the hole defect is moved to the bulk of the system. The free energy βF reads

$$\beta F = \beta F_{\mathrm{f}}^{2\mathrm{d}} + C_{n,m}(K)$$

$\beta F_{\mathrm{f}}^{2\mathrm{d}}$ is the free energy of the $N \times M$ Gaussian stripe with free boundary conditions and no defect. The corner defect energy $C_{n,n}$ is plotted as a function of the coupling

strength K in Fig. III.1.9 and as a function of the distance n from the corner lattice site in Fig. III.1.10.

Defect in the bulk of the system: In the next example, we consider M, N odd and $m = (M-1)/2$, $N = (N-1)/2$. This choice corresponds to a single hole defect in the bulk of the system. The matrix entry M_I^{-1} reads

$$M_I^{-1} = \frac{4}{(N+1)(M+1)} \sum_{k=1}^{M} \sum_{l=1}^{N} \frac{\sin^2 k\frac{\pi}{2} \sin^2 l\frac{\pi}{2}}{-1 + K\cos k\frac{\pi}{M+1} + K\cos l\frac{\pi}{N+1}}. \tag{III.1.68}$$

In both the k- and the l-sum we consider only odd k, l, since the even contributions vanish due to $\sin^2$ terms. Applying the Euler-Maclaurin integration formula for large M, N results in

$$M_I^{-1} = -\frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1}{\sqrt{(1 - K\cos\varphi)^2 - K^2}}. \tag{III.1.69}$$

The free energy reads

$$\beta F = \beta F_{\mathrm{f}}^{2\mathrm{d}} + \frac{1}{2} \log \frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1}{\sqrt{(1 - K\cos\varphi)^2 - K^2}}. \tag{III.1.70}$$

Here, $\beta F_{\mathrm{f}}^{2\mathrm{d}}$ is the free energy of the original system without defects. As expected, the contribution of the hole defect to the free energy is the same for toroidal and free boundary conditions if the hole defect is positioned in the bulk of the system with a growing distance to the boundary of the container.

Defect close to the boundary, but far away from the corners: In the last example we consider the case $m = (M-1)/2$ and n constant. This describes a hole defect close to the boundary of the container but with a growing distance from the corners of the system. We can either explicitly calculate the partition sum or obtain it from the first case in this example by letting $m \to \infty$:

$$\begin{aligned} M_I^{-1} = \lim_{m\to\infty} \Bigg[& -\frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1}{\sqrt{(1 - K\cos\varphi)^2 - K^2}} \\ & + \frac{1}{\pi^2} \int_0^\pi \mathrm{d}\varphi \int_0^\pi \mathrm{d}\Theta \, \frac{\cos 2m\varphi \, \cos 2n\Theta}{-1 + K\cos\varphi + K\cos\Theta} \\ & + \sum_{k\in\{m,n\}} \frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{\cos 2k\varphi}{\sqrt{(1 - K\cos\varphi)^2 - K^2}} \Bigg] \\ = & -\frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1}{\sqrt{(1 - K\cos\varphi)^2 - K^2}} \\ & + \frac{1}{\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{\cos 2n\varphi}{\sqrt{(1 - K\cos\varphi)^2 - K^2}}. \end{aligned} \tag{III.1.71}$$

The surface defect free energy S_n is defined as

$$S_n(K) := \frac{1}{2}\log\frac{1}{\pi}\int_0^\pi \mathrm{d}\varphi\,\frac{1-\cos 2n\varphi}{\sqrt{(1-K\cos\varphi)^2-K^2}}, \tag{III.1.72}$$

And the free energy reads

$$\beta F = \beta F_{\mathrm{f}}^{2\mathrm{d}} + S_n.$$

In addition to the hole energy of a single hole in the middle of the container there is a energy contribution which describes the correlation of the hole with the boundary of the container. The surface defect free energy is plotted as a function of the coupling K in Fig. III.1.9 and as a function of the distance n from the boundary in Fig. III.1.10.

Further examples

In general, non-properly scaling lattice domains are domains with features which do not scale with the system size in the thermodynamic limit. It can be single holes (like the domains discussed in the previous examples), combinations of single holes with varying distance between the holes, line defects, where the defect grows linearly in one dimension, but has a constant length in the other dimension. Treating the corresponding partition sums turns out to be complicated, but can be done in some cases on a case-by-case basis with the methods presented in this section. For properly scaling containers, see Sec. III.1.3, we decomposed the lattice domain in growing rectangular blocks separated by growing magnetic zip lines where the interaction between the zip lines either vanished due to the growing distance between the zips or it could be reduced to the interaction of the zip lines in the non-convex building block, Sec. III.1.2.2. This can not be done in the case of non-properly scaling domains. Very often the calculation of the partition sum of the Gaussian model on such domains boils down to the calculation of the determinant of a submatrix of the inverse of the original interaction matrix of the system without defects. However, in some cases it can be more convenient to apply the zip method or an alternative numeration of the lattice sites. In this section, we give some examples of non-properly scaling domains.

Rectangles connected by zip lines: A simple example of non-properly scaling domains is the system consisting of two rectangular blocks connected by a single spin line. For the sake of simplicity we choose two $N \times N$ spin lattices connected by a spin line of the length N, see Fig. III.1.11. Alternatively, the spin line can connect to the corners of the rectangular blocks or to any of the boundary spins of the blocks. One can also add additional spin blocks and connect them by spin lines in a similar way. As $N \to \infty$ in the thermodynamic limit, the size of the spin blocks grows and the connecting spin lines become longer. However, the width of the spin lines stays constant equal 1, making such lattice domains non-properly scaling. The partition sum of such systems can be easily calculated by interpreting the boundary spins of

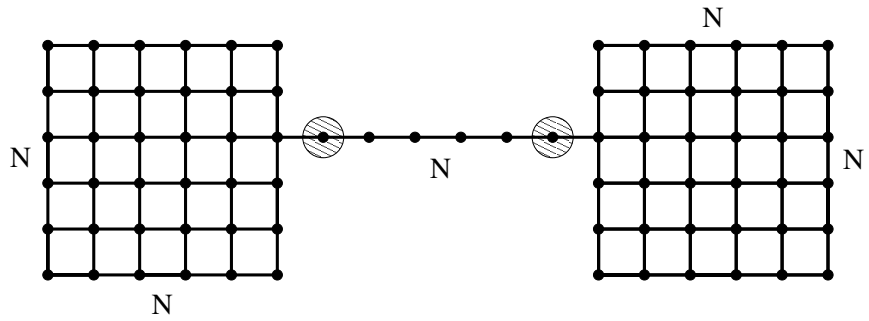

Figure III.1.11.: A lattice container consisting of two rectangular $N \times N$ blocks connected by a spin line of length N. The lattice sites in the shaded areas can be treated as magnetic zips, dividing the system in three simple subsystems.

the spin line (shaded spins in Fig. III.1.11) as magnetic zips, see Sec. III.1.2. The two magnetic zips divide the system in two $N \times N$ blocks and a spin line of length $N - 2$. After tracing out the degrees of freedom of these subsystems only a two-dimensional integral remains which describes the contribution of the zips to the partition sum. It should be pointed out that the interaction between the zips decays exponentially with the system size since they are separated by a growing distance. The interaction constant of a magnetic zip with itself is given by corresponding diagonal entries of the inverse interaction matrices of the $N \times N$ block or the spin line of length $N - 2$ with free boundary conditions.

Shifted rows: Another example of non-properly scaling lattice containers is a system consisting of N spin rows, M spins each, where each row is shifted by one lattice site relative to the previous row, see left side of Fig. III.1.12. We choose to connect the top and bottom row by periodic boundary conditions. Both zig-zag edges are subject to free boundary conditions. Alternatively, one can choose the shift length to be any integer. Each choice of the shift length would have to be treated separately. The system is similar to a rectangular domain. One should point out that the zig-zag edges prevent the application of the zip method and are the only feature of this lattice domain which makes it non-properly scaling. Instead of applying the zip method or interpret the zig-zag boundary as defects, it seems more appealing to calculate the

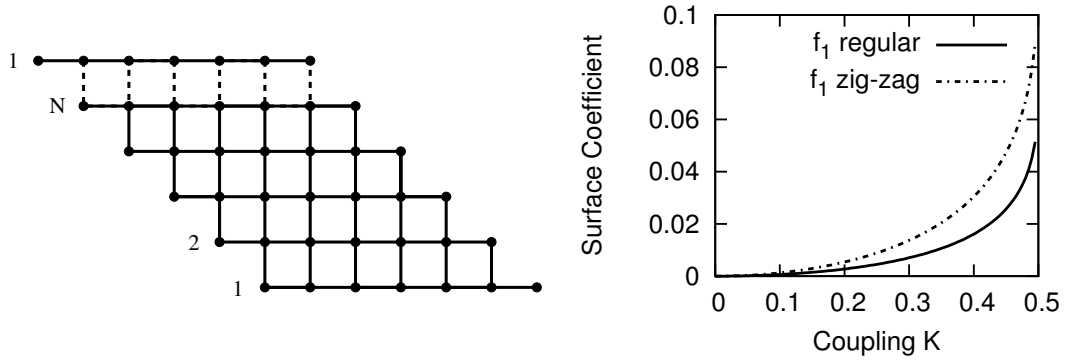

Figure III.1.12.: Left: N rows, each row consisting of M lattice sites. Each row is shifted by one lattice site relative to the previous row. Bottom and top rows interact with each other. Left and right edges of the system are subject to free boundary conditions. Right: regular surface coefficient $f_1^{2\mathrm{d}}$, see Sec. II.2.2.5 (solid line) and the surface coefficient of the zig-zag boundary (dash-dotted line), see the second term in Eq. (III.1.79).

eigenvalues and the determinant of the interaction matrix M:

$$M = \begin{bmatrix} M_{\mathrm{f}}^{1\mathrm{d}} & \Delta M & 0 & \cdots & 0 & 0 & \Delta M^t \\ \Delta M^t & M_{\mathrm{f}}^{1\mathrm{d}} & \Delta M & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \Delta M^t & M_{\mathrm{f}}^{1\mathrm{d}} & \Delta M \\ \Delta M & 0 & 0 & \cdots & 0 & \Delta M^t & M_{\mathrm{f}}^{1\mathrm{d}} \end{bmatrix}. \tag{III.1.73}$$

The matrix $M_{\mathrm{f}}^{1\mathrm{d}}$ on the main diagonal is the interaction matrix of the Gaussian chain with free boundary conditions and describes the interaction of the spins within each row, see Sec. II.2.1. The off diagonal blocks ΔM read

$$\Delta M = \begin{bmatrix} 0 & \frac{K}{2} & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \frac{K}{2} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & \frac{K}{2} \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 \end{bmatrix} \tag{III.1.74}$$

The matrix M is a block circulant. Thus, we can apply the same ansatz for the eigenvectors as in the two-dimensional case with toroidal boundary conditions, see

Sec. A.2. The equation system for NM eigenvalues $\lambda_{n,m}$ is reduced to an equation system for M eigenvalues:

$$\left(M_{\mathrm{f}}^{1d} + \Delta M z_n + \Delta M^t z_n^{-1}\right) \Psi = \lambda_{nm} \Psi. \tag{III.1.75}$$

Here, $z_n = \exp i\, 2\pi\, n/N$ is the n-th complex root of 1. However the determinant of this matrix obeys the same recurrence relation as the determinant of $M_{\mathrm{f}}^{1\mathrm{d}}$ with slightly modified matrix entries. As a result, we obtain the eigenvalues $\lambda_{n,m}$ of the interaction matrix M:

$$\lambda_{n,m} = -1 + K \cos\Theta_m \sqrt{2 + 2\cos\varphi_n}, \tag{III.1.76}$$

$$\Theta_m = \pi \frac{m}{M+1}, \quad m = 1, ..., M, \tag{III.1.77}$$

$$\varphi_n = 2\pi \frac{n}{N}, \quad n = 1, ..., N. \tag{III.1.78}$$

Applying Euler-Maclaurin summation formula for $N, M \to \infty$ and omitting all contributions which decay exponentially with the system size, we obtain the free energy βF:

$$\begin{aligned} \beta F = {} & \frac{NM}{2\pi} \int_0^\pi \mathrm{d}\varphi \, \log \frac{1 + \sqrt{1 - 2K^2(1+\cos\varphi)}}{2} \\ & + \frac{N}{2\pi} \int_0^\pi \mathrm{d}\varphi \, \log \frac{1 + \sqrt{1 - 2K^2(1+\cos\varphi)}}{2\sqrt{1 - 2K^2(1+\cos\varphi)}}. \end{aligned} \tag{III.1.79}$$

We compare this result to the free energy of the Gaussian system on a rectangular domain with cylindric boundary conditions, see Eq. (II.2.81). One can verify numerically that the volume contributions are equal, as one would expect. On the other hand, the contributions to the free energy proportional to N only, i.e. the surface contributions, are different: The zig-zag boundary has a higher energetic contribution than the straight boundary, see the right side of Fig. III.1.12.

Rectangles overlapping in one lattice site: Another example of non-properly scaling domains is a lattice domain consisting of two rectangular blocks which overlap only in one lattice site. In Fig. III.1.13, the system consists of two $N \times N$ blocks. As $N \to \infty$ in the thermodynamic limit, both blocks grow, but the overlap remains only one site, making this lattice domain non-properly scaling. The partition sum of this system is difficult to calculate with the methods developed and demonstrated throughout this thesis.

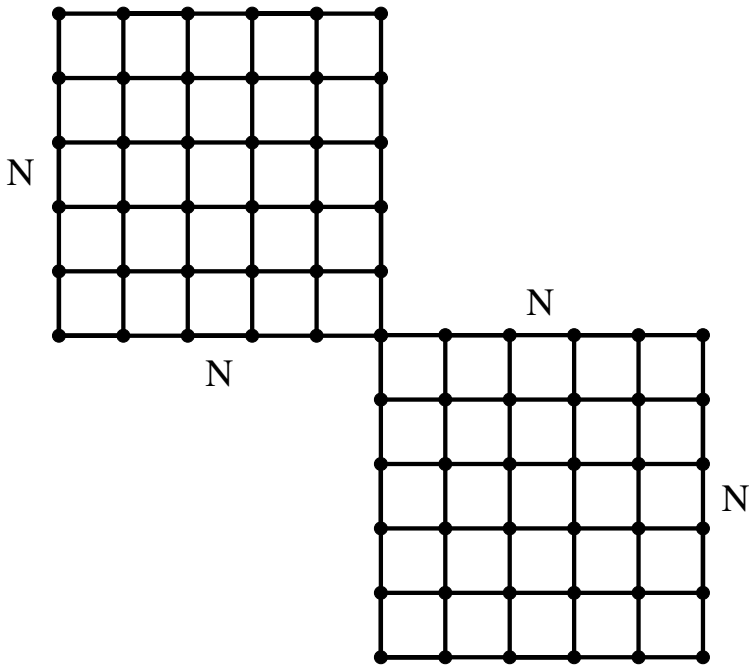

Figure III.1.13.: A lattice domain consisting of two rectangular $N \times N$ blocks overlapping in one lattice site. As the system grows in the thermodynamic limit the size of the overlap remains constant.

III.2. Evaluation of the non-convex building block

In this section we estimate the partition sum of the main non-convex building block, as introduced in Eq. (III.1.42) of Sec. III.1.2.2 and illustrated in Fig. III.2.1. As shown in Sec. III.1.3, this partition sum allows us to calculate the partition sum of the Gaussian model on an arbitrary properly scaling lattice container. We show analytically that the logarithm of the partition sum of the non-convex building block can not be written as a linear combination of $f_0^{2\mathrm{d}}$, $f_1^{2\mathrm{d}}$, $f_2^{2\mathrm{d}}$. Therefore, the contribution of the concave corner $\tilde{f}_2^{2\mathrm{d}}$ is genuinely different from the other geometric contributions and the free energy can not be written as a linear combination of Minkowski functionals, see Sec. I.1. Finally we evaluate the partition sum of the non-convex building block numerically. The system is partitioned such that it consists of three blocks and two spin zips which form a corner. We trace out the degrees of freedom of the three $N \times N$ blocks, which yields the partition sums $Z_1 = Z_2 = Z_3$, i.e. the partition sum of a $N \times N$ rectangle with free boundary conditions. The total partition sum Z can then be written as a partition sum of both magnetic zips $\boldsymbol{h}_1,\ \boldsymbol{h}_2$:

$$Z = Z_1^3 \pi^{-N} \int \mathrm{d}^N \boldsymbol{h}_1 \int \mathrm{d}^N \boldsymbol{h}_2 \, \exp\left(\boldsymbol{h}^t A \boldsymbol{h}\right), \tag{III.2.1}$$

where the total magnetic field $\boldsymbol{h}$ and the interaction matrix A read

$$\boldsymbol{h} = (\boldsymbol{h}_1, \boldsymbol{h}_2)^t \in \mathbb{R}^{2N}, \tag{III.2.2}$$

$$A = \begin{bmatrix} M_{\mathrm{f}} - \frac{K^2}{2} M_I^{-1} & \Delta M \\ \Delta M & M_{\mathrm{f}} - \frac{K^2}{2} M_I^{-1} \end{bmatrix}. \tag{III.2.3}$$

The matrices $M_I^{-1},\ \Delta M$ are $N \times N$ submatrices of the inverse M^{-1} of the interaction matrix of the two-dimensional Gaussian block. The index set $I = \{1, ..., N\}$ indicates that M_I^{-1} is the submatrix of M^{-1} obtained by erasing all rows and columns except $\{1, ..., N\}$. The matrix ΔM is given by

$$(\Delta M)_{i,j} = -\frac{K^2}{4} M^{-1}_{(1,i)(j,1)}. \tag{III.2.4}$$

M^{-1} is a block matrix, the first pair of indices numerates the blocks, the second pair of indices numerates the entries in the block. Obviously, the matrix ΔM is responsible for the interaction between both magnetic fields $\boldsymbol{h}_1,\ \boldsymbol{h}_2$. The goal is to estimate the determinant of A.

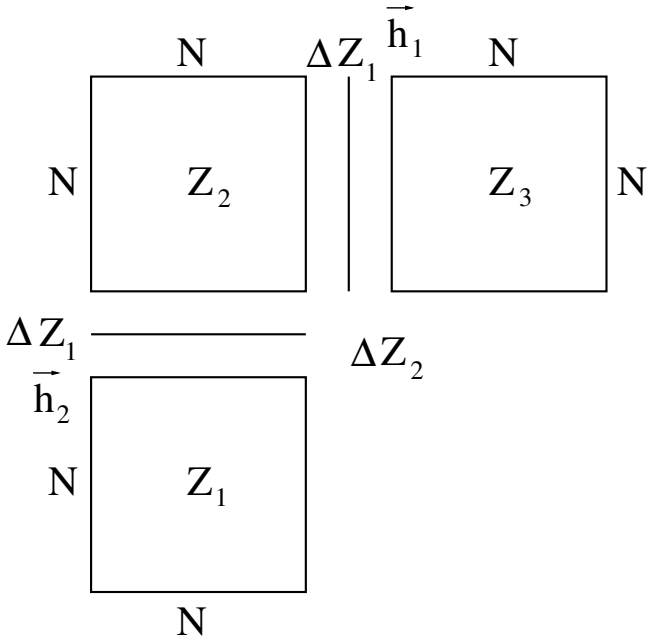

Figure III.2.1.: Basic non-convex domain configuration. The partition sums Z_1, Z_2, Z_3 are the partition sums of the $N \times N$ Gaussian blocks without magnetic field. The partition sum ΔZ_1 refers to the partition sum of a spin line between two blocks (the degrees of freedom of the blocks already traced out) and has been discussed in Sec. III.1.2.1. The partition sum ΔZ_2 corresponds to the interaction between both magnetic fields.

III.2.1. Orthonormal transformation

In order to evaluate the integral Eq. (III.2.1), we apply the orthonormal transformation T on the vector $\boldsymbol{h}$:

$$T = \frac{1}{\sqrt{2}} \begin{bmatrix} 1_N & 1_N \\ -1_N & 1_N \end{bmatrix}. \tag{III.2.5}$$

It is $\det T = 1$. The interaction matrix A transforms as follows:

$$T^t A T = \begin{bmatrix} M_\mathrm{f} - \frac{K^2}{2} M_I^{-1} - \Delta M & 0 \\ 0 & M_\mathrm{f} - \frac{K^2}{2} M_I^{-1} + \Delta M \end{bmatrix}. \tag{III.2.6}$$

Therefore, the remaining task is to evaluate the determinant of the matrices

$$A_\pm := M_\mathrm{f} - \frac{K^2}{2} M_I^{-1} \pm \Delta M, \tag{III.2.7}$$

$$\det A = \det A_+ \det A_-. \tag{III.2.8}$$

III.2.2. Discrete sine transform

Applying the matrix of the discrete sine transform F,

$$F_{i,j} := \sqrt{\frac{2}{N+1}} \sin\left(i\,j\,\frac{\pi}{N+1}\right), \tag{III.2.9}$$

on the interaction matrices $-\frac{K^2}{2}M_I^{-1} + M_\mathrm{f} \pm \Delta M$ yields

$$\begin{aligned}&\left(F^t A_\pm F\right)_{m,n} = \\ &-\delta_{m,n}\sqrt{(1-K\cos\Theta_m)^2 - K^2} \pm \frac{K^2}{2(N+1)}\,\frac{\sin\Theta_m \sin\Theta_n}{1+K\cos\Theta_m + K\cos\Theta_n}.\end{aligned} \tag{III.2.10}$$

In the next step we factorise the matrices $A_\pm$ as following:

$$\begin{aligned}F^t A_\pm F &= \left[F^t\left(M_\mathrm{f} - \frac{K^2}{2}M_I^{-1}\right)F\right] B_\pm, \quad \text{with the matrices } B_\pm : \\ B_\pm &= \left[F^t\left(M_\mathrm{f} - \frac{K^2}{2}M_I^{-1}\right)F\right]^{-1} F^t A_\pm F.\end{aligned} \tag{III.2.11}$$

The entries of $B_\pm$ read

$$\left(B_\pm\right)_{m,n} = \delta_{m,n} \mp \frac{K^2}{2(N+1)}\,\frac{\sin\Theta_m \sin\Theta_n}{(1+K\cos\Theta_m + K\cos\Theta_n)\sqrt{(1-K\cos\Theta_m)^2 - K^2}}. \tag{III.2.12}$$

We keep in mind that our goal is to calculate the determinant of A:

$$\det A = \det\left(M_\mathrm{f} - \frac{K^2}{2}M_I^{-1}\right)^2 \det B_+ B_-, \tag{III.2.13}$$

$$\Delta F = -\log\det B_+ B_-. \tag{III.2.14}$$

From the geometrical point of view, the determinant $\det B_+ B_-$ corresponds to the free energy difference ΔF needed to transform three $N \times N$ block connected by two magnetic zips and aligned linearly to the basic non-convex block configuration, see Sec. III.1.2.2 for details. In other words, ΔF is the energy need to create one convex and one concave corner, see Fig. III.2.2.

III.2.3. Vanishing spin-spin coupling

In the next step we consider the energy $\Delta F = -\log\det B_+ B_-$ at vanishing spin-spin coupling K. We perform a series expansion of ΔF in K around $K = 0$ and show that Δ is not a linear combination of $f_0^{2\mathrm{d}}$, $f_1^{2\mathrm{d}}$, $f_2^{2\mathrm{d}}$. In this section, we consider $\Delta F(K, N)$

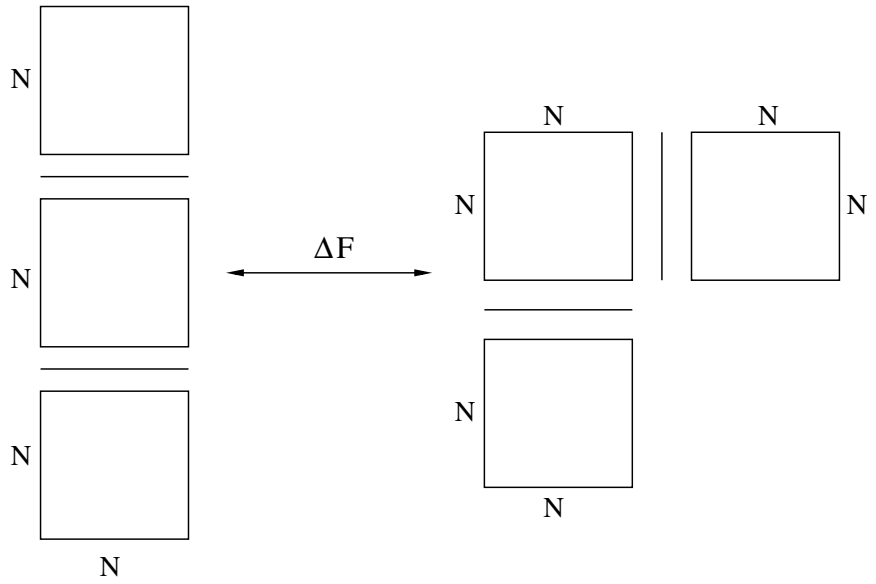

Figure III.2.2.: The energy ΔF is the energy needed to transform three linearly arranged Gaussian blocks (left-hand side) into the basic convex building block (right-hand side).

as a function of the coupling strength K and the length N of the magnetic zips. From the definition Eq. (III.2.12), we immediately obtain

$$\Delta F(0, N) = 0. \tag{III.2.15}$$

In the next step, we carry out the series expansion of the matrix $B_{\pm}$ in powers of K up to order K^8 and apply the discrete sine transformation Eq. (III.2.9) on the resulting matrix. The calculation can be performed by hand or using a Mathematica script. It turns out that the resulting matrix is a block diagonal matrix with an upper left 8×8 block matrix and a lower right $(N-8) \times (N-8)$ identity matrix, all other entries being zero. Evaluating the determinant yields

$$\Delta F(K, N) = -\frac{K^4}{16} - \frac{K^6}{4} - \frac{463}{512} K^8 + \mathcal{O}\left(K^{10}\right). \tag{III.2.16}$$

One should note that the result does not depend on N. The coefficients f_0, f_1, f_2 are known from Sec. II.2.2, the power series expansion is straight-forward:

$$\begin{aligned} f_0 &= -\frac{1}{4}K^2 - \frac{9}{32}K^4 - \frac{25}{48}K^6 - \frac{1225}{1024}K^8 + \mathcal{O}\left(K^{10}\right), \\ f_1 &= \frac{1}{16}K^2 + \frac{17}{128}K^4 + \frac{131}{384}K^6 + \frac{3985}{4096}K^8 + \mathcal{O}\left(K^{10}\right), \\ f_2 &= -\frac{3}{16}K^4 - \frac{25}{32}K^6 - \frac{1491}{512}K^8 + \mathcal{O}\left(K^{10}\right). \end{aligned} \tag{III.2.17}$$

If we assume that ΔF is a linear combination of $f_0,\ f_1,\ f_2$, the equation

$$\Delta F = x\, f_0 + y\, f_1 + z\, f_2. \tag{III.2.18}$$

has to hold for any power of K. It can be easily verified that this equation has no solution $(x,\ y,\ z)$. Therefore, the free energy ΔF is not a linear combination of f_0^{2d}, f_1^{2d}, f_2^{2d}.

III.2.4. Numerical evaluation

In this section we present and discuss the results of the numerical evaluation of ΔF. The determinants of the matrices $B_\pm$, see Eq. (III.2.12), have been evaluated numerically using the *np.linalg* package of Python. The main results have been obtained for $N = 2 \cdot 10^4$, where N is the length of the magnetic zip and the matrices $B_\pm$ are $N \times N$. Furthermore, we checked the dependence of the results on the system size. The energy ΔF as a function of coupling strength can be seen on the left-hand side of Fig. III.2.3 On the right-hand side of Fig. III.2.3, one can see the energy ΔF for values

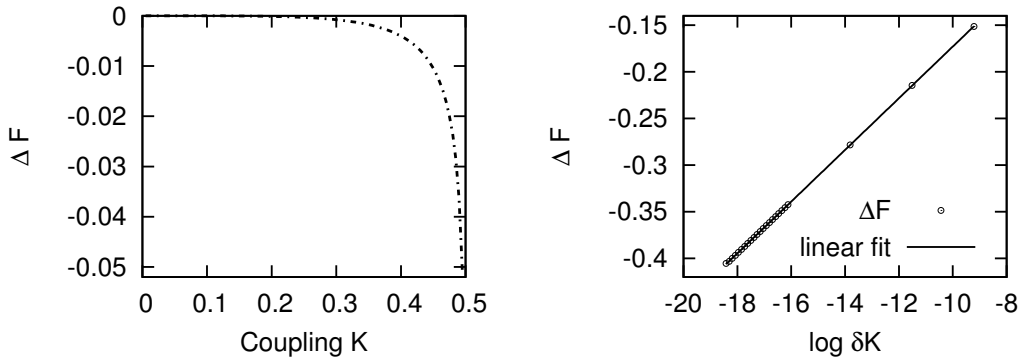

Figure III.2.3.: Left: the energy ΔF as a function of the coupling strength K. The size of the magnetic zips is $N = 2 \cdot 10^4$, see Eq. (III.2.14). ΔF is symmetric in K and diverges for $K \to \pm 1/2$. Right: the energy ΔF ($N = 2 \times 10^4$) as a function of $\log \delta K = \log(1/2 - K)$. The range of values of the coupling is $\delta K \in [10^{-8}...10^{-4}]$. Additionally, a linear function $a \log \delta K + b$ is fitted to the data.

of K close to the critical coupling $K = 0.5$ in a logarithmic plot. Additionally, a linear function $a \log \delta K + b$ is fitted to the plot, the fitting parameters read

$$\begin{aligned} f(x) &= a \log \delta K + b, \\ a &= 2{,}77 \times 10^{-2} \pm 2 \times 10^{-5}, \\ b &= 1{,}04 \times 10^{-1} \pm 4 \times 10^{-4}. \end{aligned} \tag{III.2.19}$$

The energy difference ΔF diverges logarithmically for $K \to \pm 0.5$ within the numerical precision of the data. In Fig. III.2.4 one can see the contribution $\tilde{f}_2 = 4\Delta F - f_2$ of four concave corners compared with the contribution f_2 of four convex corners. In the final step, we analyse the dependence of the results on the system size N.

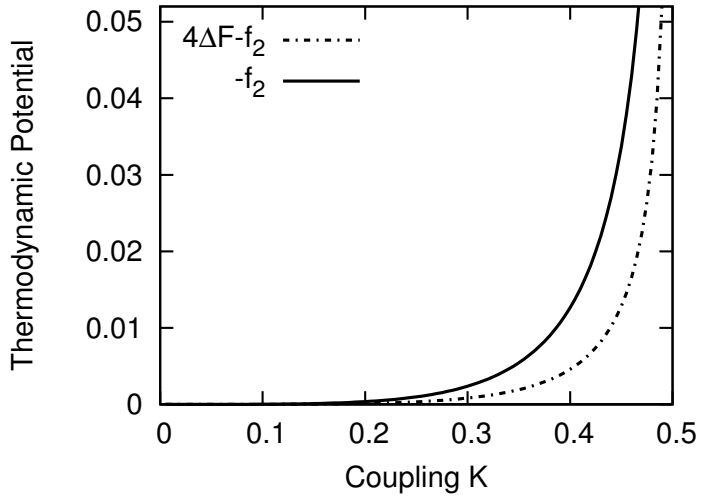

Figure III.2.4.: The contribution $\tilde{f}_2 = 4\Delta F - f_2$ of four concave corners and the contribution f_2 of four convex corners to the free energy as a function of the coupling K. Both functions are symmetric around $K = 0$ and have the opposite sign. Both functions diverge logarithmically as $K \to \pm 0.5$.

In Fig. III.2.5 one can see the relative error of $\Delta F(K, N)$ and $\Delta F(K, 10^4)$ for different values of K. One can safely assume that the precision of the numerical evaluation is high enough for $N = 10^4$.

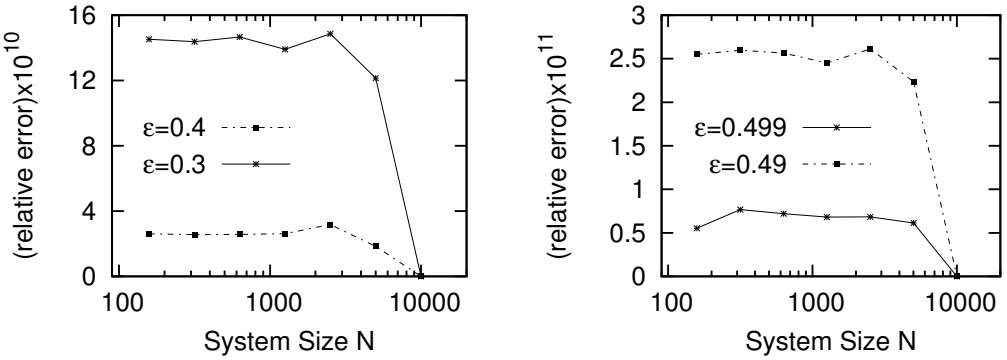

Figure III.2.5.: The relative error between $\Delta F(K, N)$ and $\Delta F(K, 10^4)$. Left: low coupling, $K \in \{0.3, 0.4\}$. Right: K close to the critical coupling, $K \in \{0.49, 0.499\}$. In all four cases, the precision at $N = 10^4$ is sufficiently high.

III.3. Summary

The methods developed in this section allow the calculation of the partition sum and the free energy of the Gaussian model on any *properly scaling* lattice domain with free boundary conditions. Roughly speaking a properly scaling lattice domain is a lattice domain whose edges and holes grow linearly with the system size in the thermodynamic limit, see Sec. III.1.3 for a precise definition. For properly scaling domains the partition sum can be evaluated by counting different types of lattice sites and assigning weights to them:

- Each lattice site multiplicatively contributes with the factor $\exp\left(-f_0^{2\mathrm{d}}\right)$ to the **partition sum**.

- Additionally, each lattice site which belongs to the surface of the system – i.e. has three neighbouring spins – contributes with the factor $\exp\left(-f_1^{2\mathrm{d}}\right)$ to the partition sum.

- Additionally, each lattice site which forms a convex corner – i.e. has only two neighbouring spins – contributes with the factor $\exp\left(-f_2^{2\mathrm{d}}/4 - 2f_1^{2\mathrm{d}}\right)$ to the partition sum.

- Additionally, each lattice site which forms a concave corner contributes with the factor $\exp\left(-\tilde{f}_2^{2\mathrm{d}}/4\right)$ to the partition sum.

Any additional contributions to the free energy beyond these contributions decay exponentially with the system size in the thermodynamic limit. One should point out that this result allows a simple geometric interpretation of the free energy: The free energy is a linear combination of the volume, the surface area, the number of convex corners and the number of concave corners of the lattice domain, with the coefficients of the linear combination being $f_0,\ f_1,\ f_2,\ \tilde{f}_2$. All coefficients are independent of the lattice geometry. All coefficients except the concave corner coefficient $\tilde{f}_2$ have been calculated analytically in Sec. II.2.2. The coefficient $\tilde{f}_2$ has been evaluated numerically in Sec. III.2.4. One important property of this coefficient is that $\tilde{f}_2$ can not be written as a linear combination of $f_0,\ f_1,\ f_2$, see Sec. III.2.3 for details. According to Sec. I.1, this means that the free energy, in general, can **not** be written as a linear combination of the volume, the surface area and the Euler number of the underlying lattice domain. Consequently the decomposition Eq. (I.0.4) has to be

modified to

$$\Omega(\lambda\mathcal{D}) = |\mathcal{D}|\,\lambda^2 f_0 + |\partial\mathcal{D}|\,\lambda\, f_1 + \frac{\#(\text{conv. corners})(\mathcal{D})}{4} f_2 + \frac{\#(\text{conc. corners})(\mathcal{D})}{4} \tilde{f}_2 + \mathcal{O}\left(\mathrm{e}^{-t\lambda}\right), \text{ as } \lambda \to \infty. \tag{III.3.1}$$

Once again $|\mathcal{D}|$, $|\partial\mathcal{D}|$ are the volume and the surface area of the underlying lattice domain. Expectedly, the calculation of the partition sum of the two-dimensional Gaussian model on *arbitrary*, i.e. not necessarily properly scaling domains, requires additional methods. Chap. III.1 presents some techniques which allow the calculation of such partition sums on a case-by-case method. Some examples are presented in Sec. III.1.3.3.

Motivated by these results, we formulate a conjecture for the free energy of the Gaussian model on arbitrary, properly scaling lattice domains in higher dimensions. In three dimensions we expect the free energy to be a linear combination of **seven** contributions (and otherwise only exponentially decaying terms): the volume contribution, the surface contribution, two different edge contributions which correspond to concave and convex edges and three different corner contributions. We expect different, linearly independent corner contributions from the three different possible types of corners: convex corners, i.e. the corners of a cuboid domain, concave corners, i.e. corners which are formed by a cavity inside a cuboid domain, and "saddle-type" corners, i.e. the inner corners of a L-shaped domain. We expect the respective coefficients f_i to be linearly independent. The thermodynamic coefficients f_i which correspond to the volume, the surface, the convex edge and the convex corner contributions have been calculated in Sec. II.2.3. Accordingly, in higher dimensions we expect linearly independent contributions from different geometric features of the domain: the volume, the surface area, the edges, the corners, etc.

Part IV.

Extensions of the basic model

In this part, we discuss two possible generalisations of the Gaussian model of ferro-magnetism: We start by considering the two-dimensional Gaussian model on the triangular and the hexagonal lattice instead of the $\mathbb{Z}^2$ and evaluate the corresponding partition sums. Furthermore, we extend the spin-spin interactions of the Gaussian model beyond the next-neighbour interactions: We discuss the impact of general spin-spin interactions on the partition sum of the one-dimensional Gaussian model and examine the corresponding convergence behaviour. We evaluate the partition sum of the one-dimensional Gaussian model with next-nearest-neighbour, quadratically and exponentially decaying interactions and the two-dimensional model with exponentially decaying interactions.

IV.1. Alternative lattices

In this section, we study the two-dimensional Gaussian model on the triangular and the hexagonal lattices. We evaluate the volume and the surface contributions of both lattice types. Additionally, we evaluate the corner contribution to the free energy of the Gaussian model on the hexagonal lattice.

IV.1.1. Triangular lattice

We start with the Gaussian model on a triangular lattice: Consider a $M \times N$ lattice domain with free boundary conditions. The lattice domain is subdivided in N rows, M spins each, subject to free boundary conditions, see Fig. IV.1.1. The interaction matrix M_N reads:

$$M_N = \begin{bmatrix} M_{\mathrm{f}}^{1\mathrm{d}} & M_{12} & 0 & \cdots & 0 & 0 & 0 \\ M_{12}^t & M_{\mathrm{f}}^{1\mathrm{d}} & M_{12} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & M_{12}^t & M_{\mathrm{f}}^{1\mathrm{d}} & M_{12} \\ 0 & 0 & 0 & \cdots & 0 & M_{12}^t & M_{\mathrm{f}}^{1\mathrm{d}} \end{bmatrix}. \tag{IV.1.1}$$

$M_{\mathrm{f}}^{1\mathrm{d}}$ is the interaction matrix of the one-dimensional spin chain with free boundary conditions. It describes the spin interactions within a row. M_{12} characterises the interaction between two neighbour rows and has the form:

$$M_{12} = \frac{K}{2} \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 1 \end{bmatrix}. \tag{IV.1.2}$$

The aim is to calculate the determinant of M_N.

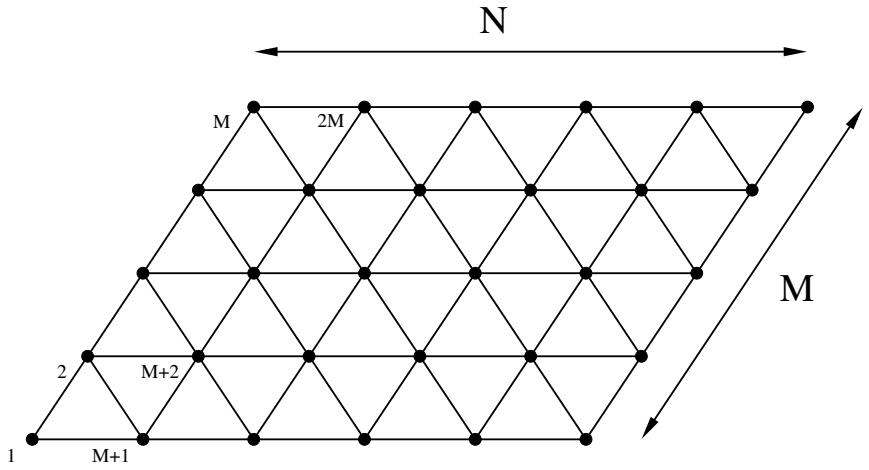

Figure IV.1.1.: A $M \times N$ triangular lattice. The black dots correspond to spins. Every two neighbour spins connected by a line interact with each other. For the enumeration, we group the spins in N rows, each consisting of M spins.

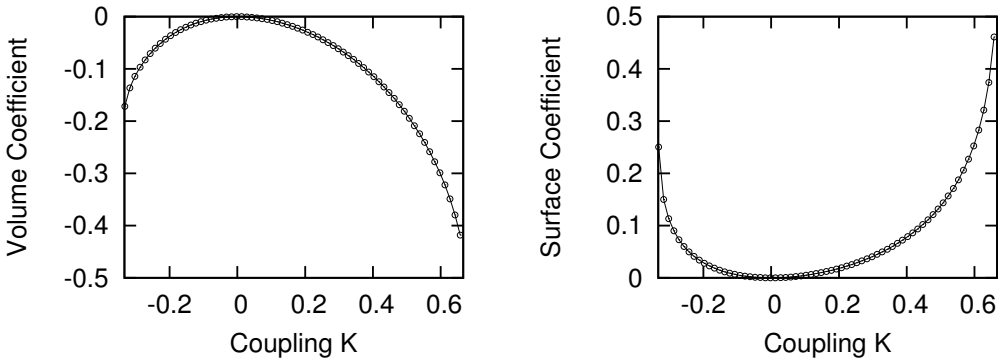

Figure IV.1.2.: Left figure: volume coefficient f_0 as a function of the coupling K. Right figure: surface coefficient f_1, see Eq. (IV.1.11) for both coefficients. Similar to the case of a rectangular lattice, both coefficients f_0, f_1 remain finite for $K \in [-1/3, 2/3]$.

Calculating the determinant $|M_N|$

In order to calculate the determinant we apply the Widom-Szegö theorem for block Toeplitz matrices, see [24]: The matrix valued symbol $\Phi_M(x)$ reads

$$\begin{aligned}\Phi_M(x) &= M_{\mathrm{f}}^{1\mathrm{d}} + M_{12}\,\mathrm{e}^{-\mathrm{i}\,x} + M_{12}^t\,\mathrm{e}^{\mathrm{i}\,x} \\ &= \begin{bmatrix} 1+K\cos x & \frac{K}{2}\left(1+\mathrm{e}^{-\mathrm{i}\,x}\right) & \cdots & 0 & 0 \\ \frac{K}{2}\left(1+\mathrm{e}^{\mathrm{i}\,x}\right) & 1+K\cos x & \cdots & 0 & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & \cdots & 1+K\cos x & \frac{K}{2}\left(1+\mathrm{e}^{-\mathrm{i}\,x}\right) \\ 0 & 0 & \cdots & \frac{K}{2}\left(1+\mathrm{e}^{\mathrm{i}\,x}\right) & 1+K\cos x \end{bmatrix}. \end{aligned} \tag{IV.1.3}$$

The Szegö theorem allows us to determine the leading contribution to det M_N:

$$\lim_{N\to\infty}\frac{1}{N}\log|-M_N| = G(\Phi) = \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}x\,\log\left|\det\Phi_M(x)\right|. \tag{IV.1.4}$$

Therefore, the remaining task is to calculate the determinant of $\Phi_M(x)$. We apply the Laplace expansion on the first row

$$\det\Phi_M(x) = (1+K\cos x)\det\Phi_{M-1}(x) - \frac{K^2}{2}(1+\cos x)\det\Phi_{M-2}(x), \tag{IV.1.5}$$

$$\det\Phi_1(x) = 1+K\cos x, \tag{IV.1.6}$$

$$\det\Phi_2(x) = (1+K\cos x)^2 - \frac{K^2}{2}(1+\cos x). \tag{IV.1.7}$$

This is the recursion which defines the determinant of the one-dimensional Gaussian chain with free boundaries, see Sec. II.2.1.2. We can calculate this determinant up to exponentially decaying terms:

$$\begin{aligned}\log\left|\det\Phi_M(x)\right| &= \frac{M+1}{2\pi}\int_0^{2\pi}\mathrm{d}y\,\log\left(1+K\cos x+K\sqrt{2}\sqrt{1+\cos x}\,\cos y\right) \\ &\quad -\frac{1}{2}\log\left[(1+K\cos x)^2 - 2\,K^2\,(1+\cos x)\right] \\ &= M\,\log\frac{1+K\cos x+\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}{2} \\ &\quad +\log\frac{1+K\cos x+\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}{2\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}. \end{aligned} \tag{IV.1.8}$$

We obtain the volume contribution to the partition sum of the Gaussian model on a triangular lattice:

$$\lim_{M,N\to\infty}\frac{\log|-M_N|}{MN} = \frac{1}{\pi}\int_0^{\pi}\mathrm{d}x\,\log\frac{1+K\cos x+\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}{2}. \tag{IV.1.9}$$

From Eq. (IV.1.8) we also know the contribution which grows linearly with N and is independent of M. For reasons of symmetry, a contribution proportional to M and independent of N with the same proportionality constant must exist. These two terms are the surface contribution to the free energy. Thus, the free energy reads:

$$\begin{aligned}\log|-M_N| = {} & \frac{MN}{2\pi}\int_0^{2\pi} \mathrm{d}x\, \log\frac{1+K\cos x+\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}{2} \\ & + \frac{M+N}{2\pi}\int_0^{2\pi} \mathrm{d}x\, \log\frac{1+K\cos x+\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}{2\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}} \\ & + \mathcal{O}(1), \quad \text{as} \quad M,N\to\infty. \end{aligned} \tag{IV.1.10}$$

Results

After having calculated the determinant of the interaction matrix we can write down the volume coefficient f_0 and the surface coefficients f_1:

$$\begin{aligned} f_0 &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}x\, \log\frac{1+K\cos x+\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}{2}, \\ f_1 &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}x\, \log\frac{1+K\cos x+\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}{2\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}}. \end{aligned} \tag{IV.1.11}$$

In the next step we study the range of the parameter K, for which the system is well defined. In order to do this we examine the integrand f of the volume contribution:

$$f(K,x) = \log\left[1+K\cos x+\sqrt{(1+K\cos x)^2-2K^2(1+\cos x)}\right]. \tag{IV.1.12}$$

The system is ill-defined if the argument of the logarithm or the square root is smaller than zero. We start by studying the zeros of the square root:

$$(1+K\cos x)^2-2K^2(1+\cos x) \stackrel{!}{=} 0, \tag{IV.1.13}$$

$$K_{1,2}(x) = -\frac{1}{\cos x \pm \sqrt{2+2\,\cos x}}. \tag{IV.1.14}$$

One can easily verify that

$$K_1\left([0,\pi]\right) = \left[-\infty,-\frac{1}{3}\right]\cup[1,\infty], \tag{IV.1.15}$$

$$K_2\left([0,\pi]\right) = \left[\frac{2}{3},1\right]. \tag{IV.1.16}$$

The only subset of $\mathbb{R}$ for which the argument of the square root does not possess any zeros is the interval $(-1/3,\, 2/3)$. It remains to prove that the argument of the

logarithm is always positive for $K \in (-1/3, 2/3)$ and $x \in \mathbb{R}$. The argument of the logarithm reads

$$1 + K\cos x + \sqrt{(1 + K\cos x)^2 - 2K^2(1 + \cos x)}. \tag{IV.1.17}$$

Since the square root is always positive and $|K\cos x| < 1$, the whole expression remains strictly positive. The volume coefficient and the surface coefficient are plotted in Fig. IV.1.2. One should note that in contrast to the square lattice, see Sec. II.2.2, f_0 and f_1 do not feature any symmetries in K. The reason for this behaviour is the fact that on a square lattice one can map the ferromagnetic system to the antiferromagnetic system by changing the sign of every second spin, while this is not possible on a triangular lattice.

IV.1.2. Hexagonal lattice

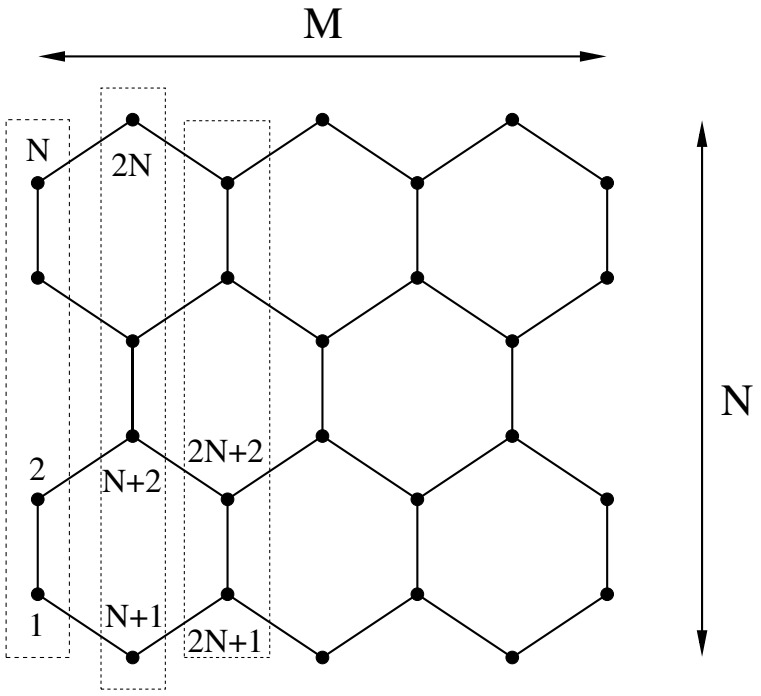

Figure IV.1.3.: A hexagonal lattice consisting of $M = 7$ columns, $N = 4$ spins each. The first three rows are marked by a dashed line. When using the illustrated enumeration of spins two neighbouring columns interact in the same way as in the case of a rectangular lattice. However, the interaction of spins within a column is different for odd and even rows.

In this section we study the Gaussian model on a hexagonal lattice. The exact form of the interaction matrix depends on the enumeration of the spins. We consider a

system of M columns, N spins each, the corresponding numeration is illustrated in Fig. IV.1.3. We assume M to be odd and N to be even, in order to fulfill the prerequisites for certain theorems, which are applied later in this section. The boundary spins are subject to free boundary conditions. For the chosen enumeration the interaction matrix $M \in \mathrm{Mat}(MN \times MN, \mathbb{R})$ reads

$$M = \begin{bmatrix} M^{(2)} & M_{12} & 0 & \cdots & 0 & 0 & 0 \\ M_{12} & M^{(1)} & M_{12} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & M_{12} & M^{(1)} & M_{12} \\ 0 & 0 & 0 & \cdots & 0 & M_{12} & M^{(2)} \end{bmatrix}. \tag{IV.1.18}$$

The off-diagonal blocks are $M_{12} = \frac{K}{2} 1_N$, same as for a rectangular lattice. They describe th interaction between the spins of two neighbouring spin columns. The entries on the main diagonal alternate between $M^{(1)}$ and $M^{(2)} \in \mathrm{Mat}(N \times N, \mathbb{R})$ and describe the interaction of the spins in one column. The interaction matrix of the spins in the odd columns $M^{(1)}$ reads

$$M^{(1)} = \begin{bmatrix} -1 & & & & & & & & \\ & -1 & \frac{K}{2} & & & & & & \\ & \frac{K}{2} & -1 & & & & & & \\ & & & -1 & \frac{K}{2} & & & & \\ & & & \frac{K}{2} & -1 & & & & \\ & & & & & \ddots & & & \\ & & & & & & -1 & \frac{K}{2} & \\ & & & & & & \frac{K}{2} & -1 & \\ & & & & & & & & -1 \end{bmatrix}. \tag{IV.1.19}$$

The interaction matrix of the spins in the even columns reads

$$M^{(2)} = \begin{bmatrix} -1 & \frac{K}{2} & & & & & & & \\ \frac{K}{2} & -1 & & & & & & & \\ & & -1 & \frac{K}{2} & & & & & \\ & & \frac{K}{2} & -1 & & & & & \\ & & & & \ddots & & & & \\ & & & & & -1 & \frac{K}{2} & & \\ & & & & & \frac{K}{2} & -1 & & \\ & & & & & & & -1 & \frac{K}{2} \\ & & & & & & & \frac{K}{2} & -1 \end{bmatrix}. \tag{IV.1.20}$$

Calculating the determinant

The interaction matrix M is a 2-periodic block tridiagonal block centrosymmetric matrix. The properties of such matrices, in particular their determinants, have been studied extensively, among others in [20]. In order to calculate the determinant we apply theorem 2 from [20] (The prerequisite is that M is a block matrix of odd size):

$$\det M = \left(\det M^{(2)}\right)^{\frac{M+1}{2}} \prod_{k=1}^{\frac{M-1}{2}} \det\left[M^{(1)} - \frac{K^2}{2}\left(1-\cos\left(2\pi\frac{k}{M+1}\right)\right)\left(M^{(2)}\right)^{-1}\right]. \tag{IV.1.21}$$

To evaluate this expression we need

$$\left(M^{(2)}\right)^{-1} = \frac{1}{1-\frac{K^2}{4}} \begin{bmatrix} -1 & -\frac{K}{2} & & & & & \\ -\frac{K}{2} & -1 & & & & & \\ & & -1 & -\frac{K}{2} & & & \\ & & -\frac{K}{2} & -1 & & & \\ & & & & \ddots & & \\ & & & & & -1 & -\frac{K}{2} \\ & & & & & -\frac{K}{2} & -1 \end{bmatrix}. \tag{IV.1.22}$$

To keep the notations short we introduce following abbreviations:

$$\begin{aligned} \alpha_k &:= 2\pi\frac{k}{M+1}, \\ a \equiv a(\alpha_k, K) &:= -1 + (1-\cos\alpha_k)\,\frac{K^2}{2}\frac{1}{1-\frac{K^2}{4}}, \\ b \equiv b(\alpha_k, K) &:= (1-\cos\alpha_k)\,\frac{K^3}{4}\frac{1}{1-\frac{K^2}{4}} = \frac{K}{2}\,(1+a)\,. \end{aligned} \tag{IV.1.23}$$

In the next step we calculate the determinant D_N:

$$\begin{aligned} D_N &:= \det\left[M^{(1)} - \frac{K^2}{2}\left(1-\cos\left(2\pi\frac{k}{M+1}\right)\right)\left(M^{(2)}\right)^{-1}\right] \\ &= \det \begin{bmatrix} a & b & & & & & \\ b & a & \frac{K}{2} & & & & \\ & \frac{K}{2} & a & b & & & \\ & & b & a & \frac{K}{2} & & \\ & & & & \ddots & & \\ & & & & & a & b \\ & & & & & b & a \end{bmatrix} \end{aligned} \tag{IV.1.24}$$

This matrix is a 2-periodic Toeplitz matrix. The determinants of such matrices are tightly connected to Chebyshev polynomials and have been studied, e.g. in [3]. In the remaining part of the calculations we apply results (in particular theorem 2.5) from [3]. We start by defining $\Delta_{N+1} \in \mathrm{Mat}(N+1 \times N+1)$, $\Delta_{N-1} \in \mathrm{Mat}(N-1 \times N-1)$, which are both of odd size:

$$\Delta_{N+1} := \begin{bmatrix} a & \frac{K}{2} & & & & & & \\ \frac{K}{2} & a & b & & & & & \\ & b & a & \frac{K}{2} & & & & \\ & & \frac{K}{2} & a & b & & & \\ & & & & & \ddots & & \\ & & & & & & a & b \\ & & & & & & b & a \end{bmatrix}$$

We obtain Δ_{N-1} from Δ_{N+1} by removing both last rows and columns. Applying the Laplace expansion on $|\Delta_{N+1}|$ yields:

$$D_N = \frac{|\Delta_{N+1}| + \frac{K^2}{4}|\Delta_{N-1}|}{a}. \tag{IV.1.25}$$

Applying theorem 2.5 from [3] allows to calculate both determinants on the right-hand side:

$$|\Delta_{N+1}| = a \prod_{l=1}^{N/2} \left[a^2 - b^2 - \frac{K^2}{4} - b\,K \cos\left(\pi \frac{l}{\frac{N}{2}+1} \right) \right]. \tag{IV.1.26}$$

Finally, we apply the Euler-Maclaurin summation formula to evaluate the logarithm for $N \to \infty$:

$$\begin{aligned} \log \left| \frac{1}{a} \Delta_{N+1} \right| = \frac{N}{2} \log & \frac{a^2 - b^2 - \frac{K^2}{4} + \sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2 K^2}}{2} \\ + \log & \frac{a^2 - b^2 - \frac{K^2}{4} + \sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2 K^2}}{2\sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2 K^2}}. \end{aligned} \tag{IV.1.27}$$

Here and in the remaining part of this section we omit and neglect all contributions which decay exponentially with the system size. We introduce following notations:

$$\chi_0(\alpha_k, K) := \log \frac{a^2 - b^2 - \frac{K^2}{4} + \sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}}{2},$$
$$\chi_1(\alpha_k, K) := \log \frac{a^2 - b^2 + \frac{K^2}{4} + \sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}}{2\sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}}. \tag{IV.1.28}$$

The determinant $|\Delta_{N-1}|$ reads for $N \to \infty$:

$$\log\left|\frac{1}{a}\,\Delta_{N-1}\right| = \frac{N}{2}\chi_0 - \log\sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}. \tag{IV.1.29}$$

Now we can write down the determinant D_N:

$$\begin{aligned}
\log D_N &= \log\left|\frac{1}{a}\,\Delta_{N-1}\right| + \log\left(1 + \frac{K^2}{4}\frac{|\Delta_{N-1}|}{|\Delta_{N+1}|}\right)\\
&= \log\left|\frac{1}{a}\,\Delta_{N-1}\right| + \log\left(1 + \frac{K^2}{4}\,\mathrm{e}^{-\chi_0}\right)\\
&= \log\left|\frac{1}{a}\,\Delta_{N-1}\right| + \log\left(1 + \frac{K^2}{4}\frac{2}{a^2 - b^2 - \frac{K^2}{4} + \sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}}\right)\\
&= \log\left|\frac{1}{a}\,\Delta_{N-1}\right| + \log\frac{a^2 - b^2 + \frac{K^2}{4} + \sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}}{a^2 - b^2 - \frac{K^2}{4} + \sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}}\\
&= \frac{N}{2}\,\chi_0 + \log\frac{a^2 - b^2 + \frac{K^2}{4} + \sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}}{\sqrt{\left(a^2 - b^2 - \frac{K^2}{4}\right)^2 - b^2K^2}},
\end{aligned} \tag{IV.1.30}$$

and rewrite this determinant in the following way:

$$\log D_N(\alpha_k, K) = \frac{N}{2}\,\chi_0(\alpha_k, K) + \chi_1(\alpha_k, K). \tag{IV.1.31}$$

One should keep in mind that the dependence on (α_k, K) is hidden in the variables $a,\ b$. Now we can concern ourselves with the partition sum of the system:

$$\begin{aligned}\log|\det M| &= \frac{M+1}{2}\log\det M^{(2)} + \sum_{k=1}^{\frac{N-1}{2}}\left[\frac{N}{2}\chi_0(\alpha_k,K)+\chi_1(\alpha_k,K)\right]\\ &= \frac{(M+1)}{2}\frac{N}{2}\log\left(1-\frac{K^2}{4}\right)+\frac{M+1}{2\pi}\int_0^\pi \mathrm{d}\alpha\,\left[\frac{N}{2}\chi_0(\alpha,K)+\chi_1(\alpha,K)\right]\\ &\quad -\frac{1}{2}\left[\frac{N}{2}\chi_0(0,K)+\chi_1(0,K)+\frac{N}{2}\chi_0(\pi,K)+\chi_1(\pi,K)\right]. \end{aligned} \tag{IV.1.32}$$

Results

In the last step we collect terms with respect to powers of M and N, keeping in mind that $\chi_0(0,K)=\log(1-K^2/4)$, and obtain:

$$\log|\det M| = MN\,f_0 + Nf_{1,N} + Mf_{1,M} + f_2, \tag{IV.1.33}$$

where the constants $f_0,\ f_{1,M},\ f_{1,N},\ f_2$ do not depend on $M,\ N$:

$$\begin{aligned} f_0(K) &= \frac{1}{4}\log\left(1-\frac{K^2}{4}\right)+\frac{1}{4\pi}\int_0^\pi \mathrm{d}\alpha\,\chi_0(\alpha,K),\\ f_{1,N}(K) &= \frac{1}{4\pi}\int_0^\pi \mathrm{d}\alpha\,\chi_0(\alpha,K)-\frac{1}{4}\chi_0(\pi,K),\\ f_{1,M}(K) &= \frac{1}{2\pi}\int_0^\pi \mathrm{d}\alpha\,\chi_1(\alpha,K),\\ f_2(K) &= \frac{1}{2\pi}\int_0^\pi \mathrm{d}\alpha\,\chi_1(\alpha,K)-\frac{\chi_1(0,K)+\chi_1(\pi,K)}{2}. \end{aligned} \tag{IV.1.34}$$

The functions $\chi_{0/1}$ are defined in Eq. (IV.1.28) and Eq. (IV.1.23). One should note that there are two different surface contributions. These contributions correspond to the boundaries of length M and N. The thermodynamic coefficients f_i as functions of the coupling K are plotted in Fig. IV.1.4. Of special note are the surface coefficients $f_{1,M},\ f_{1,N}$. In Fig. IV.1.5, the rate $f_{1,N}/f_{1,M}$ and the relative error $(2f_{1,M}-f_{1,N})/f_{1,N}$ are plotted as a function of the coupling K. From Fig. IV.1.5 one can recognise that $2\,f_{1,M}$ equals $f_{1,N}$ up to few percent error. In other words, the vertically oriented surfaces of the system, see Fig. IV.1.6, contribute (for $M=N$) twice as much to the free energy as the horizontally oriented surfaces. The reason for this is the chosen enumeration of spins: The number of surface spins in the left (right) surface column, grows proportionally to $2N$, since the spins of the second ($(M-1)$-st) spin column belong to this surface (these spins are marked with circles Fig. IV.1.6). However, the number of surface spins in the upper and lower surface rows grows linearly with M and not $2M$.

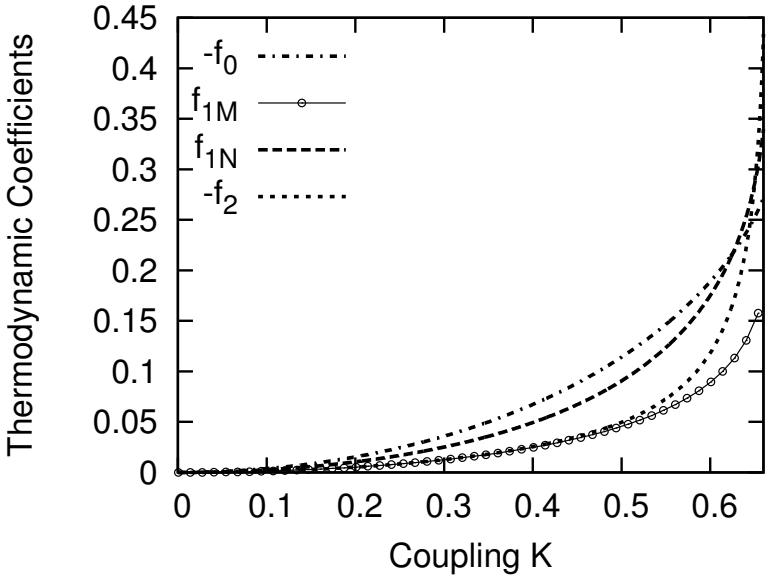

Figure IV.1.4.: Thermodynamic coefficients f_i of the Gaussian model on a hexagonal lattice plotted versus the spin-spin coupling K, see Eq. (IV.1.34) for details. All coefficients are symmetric under the transformation $K \mapsto -K$, all, except the corner contribution f_2 are defined on the whole interval $K \in [-2/3, 2/3]$. The coefficient f_2 diverges for $K \to \pm 2/3$.

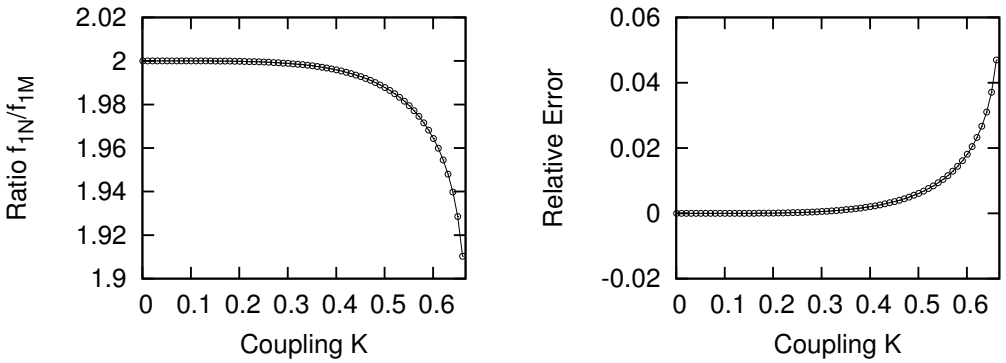

Figure IV.1.5.: Left: the ratio $f_{1,N}/f_{1,M}$ of the surface coefficients, see Eq. (IV.1.34). Right: relative error $(2f_{1,M} - f_{1,N})/f_{1,N}$. One can say that the coefficient $f_{1,N}$ equals twice the coefficient $f_{1,M}$ with very good approximation. The reason for this behaviour is the chosen enumeration of the spins.

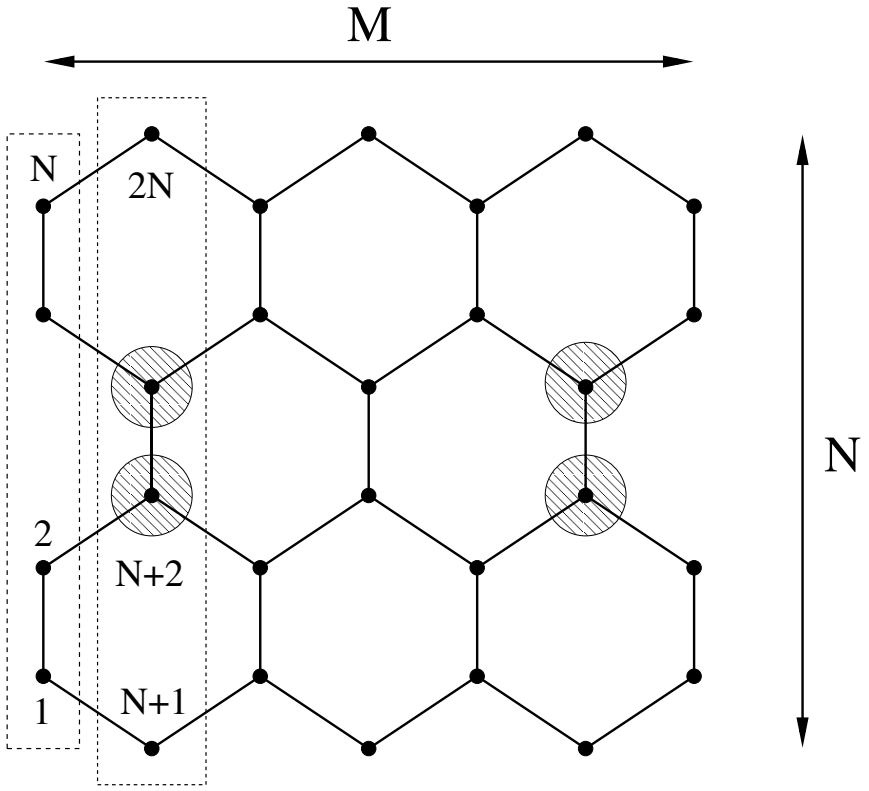

Figure IV.1.6.: Each vertically oriented surface consists of $\propto 2N$ spins, since the spins marked with the circles should be considered surface spins.

IV.1.3. Summary

We calculated the partition sum of the Gaussian model on the triangular and the hexagonal lattice with free boundary conditions. The free energy of the Gaussian model on the hexagonal lattice is a sum of four terms, see Eq. (IV.1.33), Eq. (IV.1.34): a volume term, proportional to the number of spins in the system, two different surface terms which correspond to the two different types of surfaces, see Fig. IV.1.3, and a constant contribution which can be interpreted as a corner contribution in accordance to Eq. (I.0.4). All additional contributions to the free energy beyond these four contributions decay exponentially with the system size.
The calculation of the full partition sum for the triangular lattice turns out to be more complicated. However, it was possible to determine the volume and the surface contribution, see Eq. (IV.1.10). The triangular system no longer features the symmetry $K \mapsto -K$ in contrast to the free energy of the Gaussian model on the rectangular and the hexagonal lattice.

Summarising, one can say that the calculation of partition sums on different lattice

types than the rectangular lattice involves more advanced mathematical techniques. The reason for this is that the underlying interaction matrices no longer possess simple mathematical properties which allow the application of the powerful Szegö and the Szegö-Widom theorems: The interaction matrices are no longer (Block)-Toeplitz, symmetric or tridiagonal.

IV.2. Alternative interactions

In this section we discuss the Gaussian model with other than next-neighbour interactions. We start by outlining the impact of general interactions on the interaction matrix and the partition sum in one dimension. As an example, we consider a one-dimensional system with quadratically decaying interactions and exponentially decaying interactions.

IV.2.1. General results

We consider a spin chain and assume that the first spin interacts with the n-th spin in the same way as the m-th spin with the $(m+n-1)$-th spin. Then the interaction can be fully characterised by a sequence of numbers $(a_k)_{k\in\mathbb{N}}$, where a_1 describes the interaction of two spins with the distance 1 to each other, a_2 the interaction of two spins with the distance 2 to each other, etc. For the sake of simplicity, we assume periodic boundary conditions and an odd number N of spins in the system. The first line of the interaction matrix M reads

$$(-1, a_1, a_2, ..., a_{(N-1)/2}, a_{(N-1)/2}, a_{(N-1)/2-1}, ..., a_1). \tag{IV.2.1}$$

The interaction matrix is a circulant, the n-th line is obtained by periodically shifting the first line $n-1$ times to the right. From the theory of circulants, see [4] for details, one can easily obtain the eigenvalues, eigenvectors and the determinant of M. We define the partial Fourier sum f_N and the symbol f as

$$f_N(\varphi) := 1 - 2\sum_{k=1}^{\frac{N-1}{2}} a_k \cos k\varphi, \tag{IV.2.2}$$

$$f(\varphi) := \lim_{N\to\infty} f_N(\varphi). \tag{IV.2.3}$$

We assume that the interaction between spins is chosen such that this limit exists. Since M is a circulant, its eigenvectors Ψ_n read

$$(\Psi_n)_m = \exp\left(2\pi \mathrm{i}\,\frac{nm}{N}\right), \quad n, m \in \{1, ..., N\}. \tag{IV.2.4}$$

The eigenvalues λ_n are given by

$$\lambda_n = -f_N(\varphi_n), \quad \text{where } \varphi_n = 2\pi\frac{n}{N}. \tag{IV.2.5}$$

Therefore, we obtain the bulk density of the free energy $(\beta F_N)/N$ of the finite system in a straight-forward way:

$$\frac{1}{N}\beta F_N = \frac{1}{2N}\sum_{n=1}^{N} \log f_N(\varphi_n). \tag{IV.2.6}$$

The bulk density of the free energy in the thermodynamic limit reads

$$\lim_{N\to\infty} \frac{1}{N}\beta F_N = \frac{1}{4\pi}\int_0^{2\pi} \mathrm{d}\varphi \, \log f(\varphi), \tag{IV.2.7}$$

assuming that the integral exists. The contributions beyond the volume contribution are contained in the remaining term R_N:

$$\begin{aligned} R_N &= \beta F_N - \frac{N}{4\pi}\int_0^{2\pi} \mathrm{d}\varphi \, \log f(\varphi) \\ &= \frac{1}{2}\sum_{n=1}^{N} \log f_N(\varphi_n) - \frac{N}{4\pi}\int_0^{2\pi} \mathrm{d}\varphi \, \log f(\varphi) \\ &= \frac{1}{2}\sum_{n=1}^{N} \log \frac{f_N(\varphi_n)}{f(\varphi_n)} + \frac{1}{2}\sum_{n=1}^{N} \log f(\varphi_n) - \frac{N}{4\pi}\int_0^{2\pi} \mathrm{d}\varphi \, \log f(\varphi). \end{aligned} \tag{IV.2.8}$$

Applying the triangle inequality results in

$$|R_N| \leq \left| \frac{1}{2}\sum_{n=1}^{N} \log \frac{f_N(\varphi_n)}{f(\varphi_n)} \right| + \left| \frac{1}{2}\sum_{n=1}^{N} \log f(\varphi_n) - \frac{N}{4\pi}\int_0^{2\pi} \mathrm{d}\varphi \, \log f(\varphi) \right|. \tag{IV.2.9}$$

As the system grows two limits are involved: the limit of the partial sum f_N, which converges to f, and the limit which allows to transform the sum over f into the integral. For the next-neighbour interactions and any other interactions with a finite interaction range, i.e. $a_k = 0$ for all k above a certain value, the partial sum f_N converges to f for a finite system size N. Thus, the first term on the right-hand side vanishes and all additional contributions to the free energy beyond the volume contribution stem from the Euler-Maclaurin summation formula, see Sec. A.4. However, if $(a_k)_{k\in\mathbb{N}}$ is an infinite sequence, additional contributions to the free energy can arise. The behaviour of these contributions in the limit $N \to \infty$ will be determined by the convergence behaviour of the partial sum f_N. As an example we consider quadratically decaying interactions.

IV.2.2. Quadratically decaying interactions

We start by defining the symbol f of the interaction matrix:

$$f(\varphi) := 1 + K - \frac{3K}{\pi^2}(\varphi - \pi)^2. \tag{IV.2.10}$$

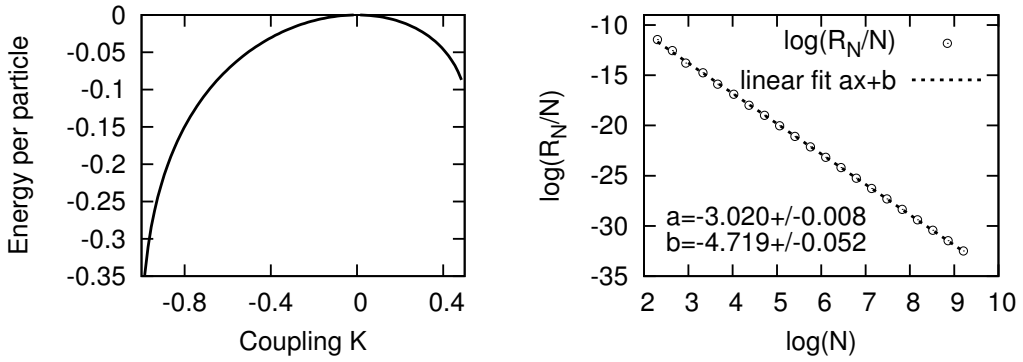

Figure IV.2.1.: Left: free energy per particle of the one-dimensional Gaussian system with quadratically decaying interactions as a function of the coupling strength K. In contrast to the next-neighbour model, the system is no longer symmetric around $K = 0$. Right: remaining term R_N/N (evaluated numerically) as a function of the system size N in a double logarithmic plot for $K = 0.1$ and $N = 10^1, ..., 10^4$. The linear fit indicates that R_N decays as N^{-2}. The decay is similar for other values of the coupling strength K.

The Fourier series of this function is given by

$$f(\varphi) = 1 - \frac{12K}{\pi^2} \sum_{k=1}^{\infty} \frac{\cos k\,\varphi}{k^2}. \tag{IV.2.11}$$

The coefficients a_k, which enter the interaction matrix read

$$a_k = \frac{6K}{\pi^2} \frac{1}{k^2}, \quad k \geq 1. \tag{IV.2.12}$$

thus the spin interaction decays quadratically with the distance between spins: The first spin couples with the strength -1 to itself (similar to the next-neighbour model), with the strength $6K/\pi^2$ to the second spins, with the strength $6K/(4\pi^2)$ to the third spin, etc. The eigenvalues λ_n of the interaction matrix read

$$\lambda_n = -1 + \frac{12K}{\pi^2} \sum_{k=1}^{\frac{N-1}{2}} \frac{\cos k\,\varphi}{k^2}. \tag{IV.2.13}$$

We can immediately write down the free energy per particle:

$$\begin{aligned}
\lim_{N\to\infty} \frac{1}{N} \beta F_N &= \frac{1}{4\pi} \int_0^{2\pi} \mathrm{d}\varphi\, \log f(\varphi) \\
&= \frac{1}{4\pi} \int_0^{2\pi} \mathrm{d}\varphi\, \log \left[1 + K - \frac{3K}{\pi^2} (\varphi - \pi)^2 \right] \\
&= -1 + \sqrt{\frac{1+K}{3K}} \mathrm{ArcTanh} \left(\sqrt{\frac{3K}{1+K}} \right) + \frac{1}{2} \log(1 - 2K).
\end{aligned} \tag{IV.2.14}$$

The system is defined for values of the coupling constant K between -1 and $1/2$. On the left-hand side of Fig. IV.2.1, the free energy per particle is depicted as a function of the coupling strength K. Additionally, on the right side of Fig. IV.2.1, the remaining term R_N/N is plotted in a double logarithmic plot as a function of the system size N. The linear fit indicates that the contributions to the free energy beyond the volume contribution no longer exponentially decay with the system size, as it was the case for the next-neighbour interactions, see Sec. II.2.1.2. Instead, R_N decays as N^{-2} in the limit of large N.

IV.2.3. Exponentially decaying interactions

In this section we extend the next-neighbours Gaussian model to the Gaussian model featuring spin-spin interactions which decay exponentially with the distance between spins. We consider the one-dimensional periodic system and discuss the bulk density of the free energy and the remaining terms. Consider the one-dimensional periodic chain of the size N. The Hamiltonian H reads

$$-\beta H = -\sum_{i=1}^{N} s_i^2 + K \sum_{i=1}^{N} \sum_{j>i}^{N} \rho^{\min(|i-j|, i-j+N)} s_i s_j, \tag{IV.2.15}$$

The parameter $\rho \in (-1, 1)$ governs the exponential decay of the spin-spin interactions. The first spin couples with the strength -1 to itself (same as in the next-neighbour model), with the strength $K\rho$ to the second spin, with the strength $K\rho^2$ to the third spin, etc. Therefore, negative ρ results in an alternating sign of the spin-spin interactions. Positive decay parameter ρ corresponds either to ferromagnetic interactions, if $K > 0$, or anti-ferromagnetic interactions, if $K < 0$. The system is subject to periodic boundary conditions. Thus, the interaction matrix M is a circulant, its first line reads

$$\left(-1, \frac{K}{2}\rho, \frac{K}{2}\rho^2, ..., \frac{K}{2}\rho^{\min(|1-j, 1-j+N)}, .., \frac{K}{2}\rho^2, \frac{K}{2}\rho\right). \tag{IV.2.16}$$

One obtains the n-th line by cyclically moving the entries of the first line to the right $n-1$ times. The eigenvalues λ_n of the interaction matrix can be obtained with the same ansatz as in the next-neighbour case, see Sec. II.2.1.1. We restrict our considerations to odd N. The eigenvalues read

$$\lambda_n = -f_N(\varphi_n) = -1 + K \sum_{k=1}^{\frac{N-1}{2}} \rho^k \cos(k\,\varphi_n), \quad \varphi_n = 2\pi \frac{n}{N}, \quad n = 1, .., N. \tag{IV.2.17}$$

The following limit is of interest for large systems:

$$\begin{aligned} \lim_{N\to\infty} f_N(\varphi) = f(\varphi) &= 1 - K\left(\frac{1-\rho\cos\varphi}{1-2\rho\cos\varphi+\rho^2} - 1\right) \\ &= \frac{1+\rho^2(1+K) - \rho\cos\varphi\,(2+K)}{1-2\rho\cos\varphi+\rho^2}. \end{aligned} \tag{IV.2.18}$$

The free energy of the system reads

$$\beta F = \frac{1}{2}\sum_{n=1}^{N} \log|\lambda_n| = \frac{N}{2}\int_0^{2\pi} \mathrm{d}\varphi\, \log f(\varphi) + R = N f_0^{\exp} + R. \tag{IV.2.19}$$

Here we applied the Euler-Maclaurin summation formula. R is the remaining term which depends on ρ, K and N. We will discuss its properties in the last part of this section. We can evaluate the integral in the bulk density $f_0^{\exp}$ of the free energy:

$$\begin{aligned} f_0^{\exp}(K,\rho) &= \frac{1}{2}\log\frac{1+\rho^2(1+K)+\sqrt{(1+\rho^2(1+K))^2-\rho^2(2+K)^2}}{2} \\ &= \frac{1}{2}\log\frac{1+\rho^2(1+K)+\sqrt{1-\rho^2}\sqrt{1-\rho^2(1+K)^2}}{2}. \end{aligned} \tag{IV.2.20}$$

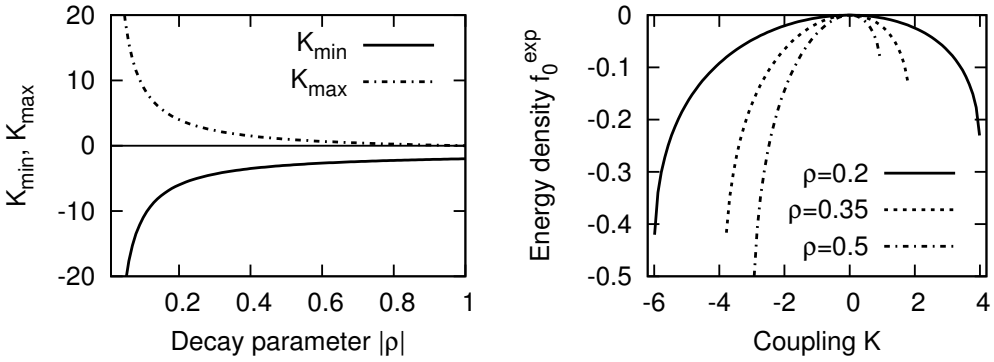

Figure IV.2.2.: Left: boundaries $K_{\min}$ and $K_{\max}$ as functions of the decay parameter ρ, see Eq. (IV.2.23) and Eq. (IV.2.24), of the interval for the coupling K in which the system is well-defined. Both functions diverge for quickly decaying interactions, i.e. $\rho \to 0$. For slowly decaying interactions, $\rho \to 1$, only anti-ferromagnetic coupling is allowed. Right: bulk density of the free energy $f_0^{\exp}$ as a function of the coupling K for values of the decay parameter $\rho \in \{0.2, 0.35, 0.5\}$, see Eq. (IV.2.20). In contrast to the next neighbour system, see Sec. II.2.1.1, the system is no longer symmetric under the transformation $K \mapsto -K$.

It is important to point out that the system is symmetric under the mapping $\rho \mapsto -\rho$, i.e. alternating spin-spin coupling yields the same energy as strictly ferromagnetic or strictly anti-ferromagnetic spin-spin coupling. The system is well-defined as long as the argument of the square root function in Eq. (IV.2.20) is not negative. The

argument of the square root is a quadratic function of K, its zeros K_1, K_2 are

$$K_1 = \frac{1-\rho}{\rho}, \tag{IV.2.21}$$

$$K_2 = -\frac{1+\rho}{\rho}. \tag{IV.2.22}$$

The coefficient of K^2 is $-\rho^2(1-\rho^2)$. Therefore, the system is well defined on the interval

$$K \in \left[-\frac{1+|\rho|}{|\rho|}, \frac{1-|\rho|}{|\rho|}\right]. \tag{IV.2.23}$$

The upper and the lower boundary of the definition interval are plotted as a function of the decay parameter ρ on the left-hand side of Fig. IV.2.2. Additionally, free energy density $f_0^{\exp}$ is plotted as a function of K for intermediate values of ρ on the right-hand side of Fig. IV.2.2. It should be pointed out that for general values of ρ the symmetry $K \mapsto -K$ between ferromagnetic and anti-ferromagnetic interactions of the next-neighbour model is broken for exponentially decaying interactions. In the next step, we consider strong exponential decay, $|\rho| \ll 1$, and weak exponential decay, $|\rho| \approx 1$.

Strong exponential decay: We consider the range of allowed temperatures K as a function of ρ, Eq. (IV.2.23). In the limit of strongly decaying spin-spin interactions, i.e. $\rho \ll 1$ we obtain

$$\begin{aligned} K_{\min} &\approx -\frac{1}{|\rho|}, \\ K_{\max} &\approx \frac{1}{|\rho|}. \end{aligned} \tag{IV.2.24}$$

Considering the free energy density $f_0^{\exp}$, Eq. (IV.2.20), we can rescale K with the factor $1/|\rho|$ and expand the argument of the logarithm around $\rho = 0$:

$$f_0\left(\frac{K}{|\rho|}, \rho\right) = \frac{1}{2}\log\frac{1+\sqrt{1-K^2}}{2} + \mathcal{O}(\rho). \tag{IV.2.25}$$

The system is essentially mapped on the next-neighbour system, see Sec. II.2.1.1. In particular, the symmetry between ferromagnetic and anti-ferromagnetic coupling is retained for very quickly decaying spin-spin interactions. One should note that the mapping $K \mapsto K/\rho$ in the interaction matrix Eq. (IV.2.16) causes the n-th spin to interact with the $(n+1)$-st spin via the coupling K. The exponential decay sets in starting with the $(n+2)$-nd spin, where the coupling is $K\rho$. The free energy density $f_0^{\exp}$ is plotted as a function of K for low values of ρ on the left-hand side of Fig. IV.2.3.

Weak exponential decay: Consider a Gaussian chain with a slow exponential decay of the spin-spin interactions, i.e. $|\rho| \approx 1$. For reasons of symmetry, it suffices to consider $\rho \approx 1$. We perform a series expansion of the argument of the logarithm in Eq. (IV.2.20):

$$f_0(K,\rho) = \frac{1}{2}\log\frac{2+K+\sqrt{1-\rho}\sqrt{-2K(2+K)}}{2} + \mathcal{O}(1-\rho). \tag{IV.2.26}$$

In the limit $\rho \to 1$ the system is defined only for $K \in [-2,0]$, meaning that only anti-ferromagnetic coupling is allowed. On the right-hand side of Fig. IV.2.3, the free energy density is plotted versus K for values of ρ close to 1.

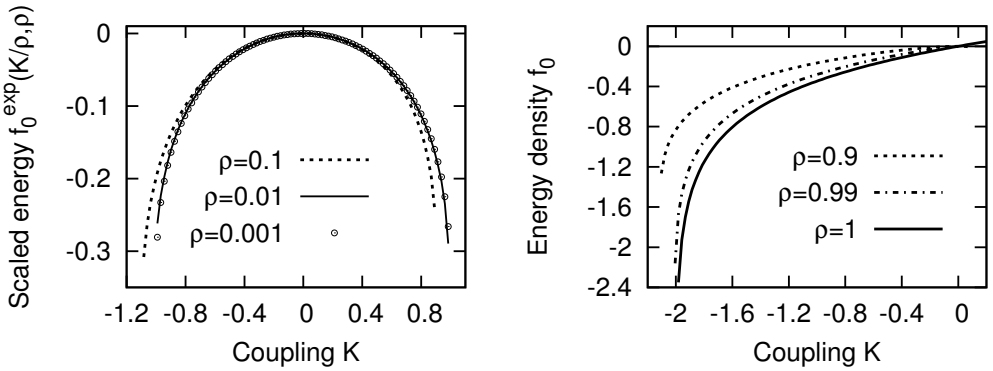

Figure IV.2.3.: Left: bulk density $f_0^{\exp}(K/\rho,\rho)$ of the free energy with a rescaled first argument as a function of the coupling K for quickly decaying spin-spin interactions, $\rho \in \{10^{-1}, 10^{-2}, 10^{-3}\}$, see Eq. (IV.2.20). For quickly decaying interactions, the system is similar to the next-neighbour system, see Eq. (IV.2.25). Right: bulk density $f_0^{\exp}$ as a function of K for slowly decaying spin-spin interactions, i.e. $\rho \approx 1$, see Eq. (IV.2.26). For slowly decaying interactions, the system is only defined for anti-ferromagnetic coupling, i.e. $K < 0$.

Remainder term R**:** The remaining term R in Eq. (IV.2.19) reads

$$R = \left|\sum_{n=1}^{N}\log f_N(\varphi_n) - \frac{N}{2\pi}\int_0^{2\pi}\mathrm{d}\varphi\,\log f(\varphi)\right|. \tag{IV.2.27}$$

We divide this expression in two contributions and apply the triangle inequality:

$$R \le \left|\sum_{n=1}^{N}\log\frac{f_N(\varphi_n)}{f(\varphi_n)}\right| + \left|\sum_{n}\log f(\varphi_n) - \frac{N}{2\pi}\int_0^{2\pi}\mathrm{d}\varphi\,\log f(\varphi)\right|. \tag{IV.2.28}$$

f is smooth for all allowed values of the parameters ρ, K. According to the Euler-Maclaurin formula the second term decays exponentially with the system size N:

$$\left|\sum_{n}\log f(\varphi_n) - \frac{N}{2\pi}\int_0^{2\pi}\mathrm{d}\varphi\,\log f(\varphi)\right| = \mathcal{O}\left(N^{-k}\right),\ \forall k \in \mathbb{N},\ \text{ as } N\to\infty. \tag{IV.2.29}$$

In the next step, we consider the first term in Eq. (IV.2.28):

$$\left| \sum_{n=1}^{N} \log \frac{f_N(\varphi_n)}{f(\varphi_n)} \right| . \tag{IV.2.30}$$

The partial sum f_N can be expressed using the geometric series:

$$\begin{aligned} f_N(\varphi) &= 1 + K - K \frac{1 - \rho\cos\varphi - \rho^{N+1}\cos(N+1)\varphi + \frac{1}{2}\rho^{2(N+1)}}{1 + \rho^2 - 2\rho\cos\varphi} \\ &= f(\varphi) - K\rho^{N+1}\frac{\cos(N+1)\varphi + \frac{1}{2}\rho^{N+1}}{1 + \rho^2 - 2\rho\cos\varphi} = f(\varphi) + \mathcal{O}\left(\rho^{N+1}\right). \end{aligned} \tag{IV.2.31}$$

The function f has no zeros for any allowed combinations of values of K, ρ. Thus, we can write

$$\frac{f_N(\varphi)}{f(\varphi)} = 1 + \mathcal{O}\left(N^{-k}\right),\ \forall k \in \mathbb{N},\ \text{ as } N \to \infty. \tag{IV.2.32}$$

And, finally,

$$\left| \sum_{n=1}^{N} \log \frac{f_N(\varphi_n)}{f(\varphi_n)} \right| = \mathcal{O}\left(N^{-k}\right),\ \forall k \in \mathbb{N},\ \text{ as } N \to \infty. \tag{IV.2.33}$$

We have shown that for all non-critical values of ρ, K the remaining term R decays exponentially with the system size in the thermodynamic limit:

$$\beta F = N f_0^{\text{exp.}} + \mathcal{O}\left(N^{-k}\right),\ \forall k \in \mathbb{N},\ \text{ as } N \to \infty. \tag{IV.2.34}$$

IV.2.4. Summary

In this section, we discussed the impact of different spin-spin interaction potentials on the partition sum of the Gaussian system. In one dimension, we calculated the partition sum of the Gaussian model with exponentially decaying interactions with periodic boundary conditions. We studied the limits of strongly and weakly decaying interactions. All contributions to the free energy beyond the volume contribution decay exponentially with the system size. In addition, we studied the partition sum of a Gaussian chain with quadratically decaying spin-spin interactions and periodic boundary conditions. In this system, the contributions to the free energy beyond the volume contribution – which is proportional to the number N of spins in the system – no longer exponentially decay in the thermodynamic limit. Instead, corrections to the free energy decay as N^{-2}. In general, one can assume that long-range spin-spin interactions in the Gaussian model lead to algebraically decaying corrections to the free energy.

Part V.

Back Matter

A. Appendices

A.1. Trigonometric relations

In this section we list some trigonometric relations which were used throughout this thesis.

Fourier decomposition of cos^j: In Chap. II.2, the Fourier decomposition of integer powers of trigonometric functions was used. We consider even and odd powers of $\cos^j$ for integer powers $j \in \mathbb{N}$:

$$\cos^{2n}(x) = \frac{1}{2^{2n}} \left[\binom{2n}{n} + 2 \sum_{k=1}^{n} \binom{2n}{n-k} \cos(2kx) \right], \tag{A.1}$$

$$\cos^{2n-1}(x) = \frac{1}{2^{2n-2}} \sum_{k=1}^{n} \binom{2n-1}{n-k} \cos((2k-1)x). \tag{A.2}$$

Addition theorem: The following addition theorem for the cosine function turned out to be useful:

$$\sum_{k=1}^{N} \cos(x+ky) = \cos\left(x + \frac{N+1}{2}y\right) \frac{\sin\left(\frac{Ny}{2}\right)}{\sin\frac{y}{2}}. \tag{A.3}$$

Discrete sine transformation: The transformation matrix $F \in \mathrm{Mat}(N \times N)$ of the discrete sine transformation,

$$F_{i,j} = \sqrt{\frac{2}{N}} \sin\left(ij\,\frac{\pi}{N+1}\right), \tag{A.4}$$

is symmetric and orthonormal due to the orthonormality of the discrete sine function:

$$\sum_{j=1}^{N} F_{i,j}F_{j,k} = \frac{2}{N} \sum_{j=1}^{N} \sin\left(ij\,\frac{\pi}{N+1}\right) \sin\left(jk\,\frac{\pi}{N+1}\right) = \delta_{i,k}. \tag{A.5}$$

A.2. Toeplitz matrices and circulants

In this section, we discuss the properties of circulants, Toeplitz and block Toeplitz matrices. We derive the eigenvalues, the eigenvectors, and, in some cases, the inverse matrices of the matrices which appear as interaction matrices of the Gaussian system. Some of the results are taken from [14] and [4], which is also a good summary on the topic of Toeplitz matrices and circulants. This section is structured in a similar fashion as the main section Part. II, which uses the results derived here: We start with interaction matrices of one-dimensional systems and discuss two and three-dimensional systems with different boundary conditions.

One dimension

We consider a string of N spins $s_i \in \mathbb{R},\ i = 1, .., N$.

Periodic boundary conditions

The interaction matrix $M_\mathrm{p} \in \mathrm{Mat}\,(N \times N, \mathbb{R})$ of the one-dimensional Gaussian chain with periodic boundary conditions reads.

$$M_\mathrm{p} = \begin{bmatrix} -1 & \frac{K}{2} & 0 & \cdots & 0 & 0 & \frac{K}{2} \\ \frac{K}{2} & -1 & \frac{K}{2} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2} & -1 & \frac{K}{2} \\ \frac{K}{2} & 0 & 0 & \cdots & 0 & \frac{K}{2} & -1 \end{bmatrix}. \tag{A.6}$$

The goal is to obtain the eigenvalues, eigenvectors and the inverse of this matrix. M_p is a circulant. All circulants share the same eigenvectors, see [4]. To obtain an eigenvector $\Psi = (\Psi_1, ..., \Psi_N)$ we try the ansatz $\Psi_n = z^n$. This vector has to fulfill

$$M_\mathrm{p}\Psi = \lambda\Psi \tag{A.7}$$

for an eigenvalue λ. Written out, this equation reads

$$-z + \tfrac{K}{2}\left(z^2 + z^N\right) = \lambda z, \tag{A.8}$$

$$-z^n + \tfrac{K}{2}\left(z^{n-1} + z^{n+1}\right) = \lambda z^n,\ \ \forall\, n = 2, ..., (N-1), \tag{A.9}$$

$$-z^N + \left(z + z^{N-1}\right) = \lambda z^{N-1}. \tag{A.10}$$

Choosing z such that $z^N = 1$ leads to N identical equations. We have N different choices for z: $z_n = \exp((2\pi\, i\, n)/N),\ n = 1, ..., N$. We denote the corresponding eigenvalues with λ_n:

$$\lambda_n = -1 + K\cos\left(2\pi\tfrac{n}{N}\right). \tag{A.11}$$

Constructing a real orthonormal basis

Our next step is to construct a real orthonormal basis of eigenvectors of M_p. With $\Psi_n^{(m)}$ we denote the m-th entry of the n-th complex eigenvector:

$$\Psi_n^{(m)} = z_n^m = \exp\left(2\pi \mathrm{i}\, \tfrac{mn}{N}\right). \tag{A.12}$$

These vectors are orthogonal with respect to the standard complex scalar product:

$$\Psi_n \cdot \Psi_m = \sum_{j=1}^{N} \left(\Psi_n^{(j)}\right)^* \Psi_m^{(j)} = \sum_{j=1}^{N} \mathrm{e}^{2\pi \mathrm{i} \frac{j}{N}(m-n)} = \begin{cases} N, \text{ if } m = n, \\ 0, \text{ else.} \end{cases} \tag{A.13}$$

This follows from applying trigonometric relations from Sec. A.1 to the real and imaginary part of the sum. One should note that the eigenvectors Ψ_n and Ψ_{N-n} share the same eigenvalue λ_n:

$$\lambda_n = -1 + K\cos\left(2\pi \tfrac{n}{N}\right), \tag{A.14}$$

meaning that for odd N all but the N-th eigenvalue are 2-fold degenerate. For even N, the $N/2$-th eigenvector is also non-degenerate. We start by considering

N **odd:** For each $n = 1, ..., (N-1)/2$ we define pairs of eigenvectors Φ_n:

$$\Phi_{2n}^{(j)} := \tfrac{1}{\sqrt{2N}}\left(\Psi_n^{(j)} + \Psi_{N-n}^{(j)}\right) = \sqrt{\tfrac{2}{N}}\cos 2\pi \tfrac{n}{N} j, \tag{A.15}$$

$$\Phi_{2n-1}^{j} := \tfrac{1}{\mathrm{i}\sqrt{2N}}\left(\Psi_n^{(j)} - \Psi_{N-n}^{(j)}\right) = \sqrt{\tfrac{2}{N}}\sin 2\pi \tfrac{n}{N} j. \tag{A.16}$$

and the vector

$$\Phi_0^{(j)} := \tfrac{1}{\sqrt{N}}. \tag{A.17}$$

These vectors are real, orthonormal and linearly independent. Since they are constructed as linear combinations of eigenvectors which share the same eigenvalue, they are also eigenvectors of M_p.

N **even:** For $n = 1, ..., N/2 - 1$ we define

$$\Phi_{2n}^{(j)} := \tfrac{1}{\sqrt{2N}}\left(\Psi_n^{(j)} + \Psi_{N-n}^{(j)}\right) = \sqrt{\tfrac{2}{N}}\cos 2\pi \tfrac{n}{N} j, \tag{A.18}$$

$$\Phi_{2n-1}^{j} := \tfrac{1}{\mathrm{i}\sqrt{2N}}\left(\Psi_n^{(j)} - \Psi_{N-n}^{(j)}\right) = \sqrt{\tfrac{2}{N}}\sin 2\pi \tfrac{n}{N} j, \tag{A.19}$$

and the vectors

$$\Phi_0^{(j)} := \tfrac{1}{\sqrt{N}}, \tag{A.20}$$

$$\Phi_{N-1}^{j} := \tfrac{(-1)^j}{\sqrt{N}}. \tag{A.21}$$

Which form an orthonormal basis of the $\mathbb{R}^N$ and are eigenvectors of M_p.

Calculating the inverse interaction matrix

In this section we calculate the inverse matrix of the interaction matrix M_p. M_p is real and symmetric, thus there exists an orthonormal matrix T such that

$$T^t M_\mathrm{p} T = \tilde{M}_\mathrm{p} = \mathrm{diag}(\lambda_1, ..., \lambda_N). \tag{A.22}$$

We can write the inverse matrix as

$$M_\mathrm{p}^{-1} = T\, \tilde{M}_\mathrm{p}^{-1}\, T^t. \tag{A.23}$$

The matrix T consists of columns which are orthonormal eigenvectors Φ of M_p. Using this, we rewrite the matrix entries $\left(M_\mathrm{p}^{-1}\right)_{ij}$

$$\left(M_\mathrm{p}^{-1}\right)_{ij} = \sum_m \frac{T_{im} T_{jm}}{\lambda_m} = \sum_m \frac{\Phi_m^{(i)} \Phi_m^{(j)}}{\lambda_m}. \tag{A.24}$$

We plug in the explicit form for Φ_n.

N **odd:**

$$\begin{aligned}\left(M_\mathrm{p}^{-1}\right)_{ij} &= \tfrac{1}{N(-1+K)} + \tfrac{2}{N} \sum_{n=1}^{\frac{N-1}{2}} \frac{\sin 2\pi\frac{n}{N} i \sin 2\pi\frac{n}{N} j + \cos 2\pi\frac{n}{N} i \cos 2\pi\frac{n}{N} j}{-1+K\cos\left(2\pi\frac{n}{N}\right)} \\ &= \tfrac{1}{N(-1+K)} + \tfrac{2}{N} \sum_{n=1}^{\frac{N-1}{2}} \frac{\cos\left[2\pi\frac{n}{N}(i-j)\right]}{-1+K\cos\left(2\pi\frac{n}{N}\right)}.\end{aligned} \tag{A.25}$$

N **even:**

$$\begin{aligned}\left(M_\mathrm{p}^{-1}\right)_{ij} &= \tfrac{1}{N(-1+K)} + \tfrac{(-1)^{i+j}}{N(-1-K)} \\ &\quad + \tfrac{2}{N} \sum_{n=1}^{\frac{N-2}{2}} \frac{\sin 2\pi\frac{n}{N} i \sin 2\pi\frac{n}{N} j + \cos 2\pi\frac{n}{N} i \cos 2\pi\frac{n}{N} j}{-1+K\cos\left(2\pi\frac{n}{N}\right)} \\ &= \tfrac{1}{N(-1+K)} + \tfrac{(-1)^{i+j}}{N(-1-K)} + \tfrac{2}{N} \sum_{n=1}^{\frac{N-2}{2}} \frac{\cos\left[2\pi\frac{n}{N}(i-j)\right]}{-1+K\cos\left(2\pi\frac{n}{N}\right)}.\end{aligned} \tag{A.26}$$

Properties of M_p^{-1}: We define the matrix $\hat{M}_p^{-1}$ as:

$$(\hat{M}_\mathrm{p}^{-1})_{ij} := \tfrac{1}{\pi} \int_0^\pi \mathrm{d}x\, \tfrac{\cos[(i-j)x]}{-1+K\cos(x)}. \tag{A.27}$$

Applying the trapezoidal rule for large N (see Sec. A.4) yields:

$$\left(M_\mathrm{p}^{-1}\right)_{ij} = \left(\hat{M}_\mathrm{p}^{-1}\right)_{ij} + \mathcal{O}\left(N^{-k}\right),\ \forall k \in \mathbb{N} \text{ as } N \to \infty. \tag{A.28}$$

Both matrices $M_\mathrm{p}^{-1}, \hat{M}_\mathrm{p}^{-1}$ are

- real
- symmetric
- Toeplitz.

Furthermore, M_{p}^{-1} is a circulant, see Sec. A.2. This can be illustrated as follows: We consider the first row of M_{p}^{-1} for odd N. For $j = 2, ..., (N+1)/2$ we have

$$\begin{aligned}\left(M_{\mathrm{p}}^{-1}\right)_{1,j} &= \tfrac{1}{M(-1+K)} + \tfrac{1}{N}\sum_{n=1}^{N-1} \tfrac{\cos\left[2\pi\frac{n}{N}(1-j)\right]}{-1+K\cos\frac{2}{\pi}nN} \\ &= \tfrac{1}{M(-1+K)} + \tfrac{1}{N}\sum_{n=1}^{N-1} \tfrac{\cos\left[2\pi\frac{n}{N}(j-1)+2\pi n\right]}{-1+K\cos\frac{2}{\pi}nN} \\ &= \tfrac{1}{M(-1+K)} + \tfrac{1}{N}\sum_{n=1}^{N-1} \tfrac{\cos\left[2\pi\frac{n}{N}(1-(N+2-j))\right]}{-1+K\cos\frac{2}{\pi}nN} \\ &= \left(M_{\mathrm{p}}^{-1}\right)_{1,(N+2-j)}. \end{aligned} \tag{A.29}$$

Using the symmetry and the Toeplitz property of M_{p}^{-1}, it follows that M_{p}^{-1} is a circulant. **One should note that $\hat{M}_{\mathbf{p}}^{-1}$ is not a circulant!**

Free boundaries

In the next step, we consider a Gaussian spin chain with free boundary conditions. The interaction matrix $M_{\mathrm{f}} \in \mathrm{Mat}\left(\mathbb{R}^N \times \mathbb{R}^N\right)$ reads

$$M_{\mathrm{f}} = \begin{bmatrix} -1 & \frac{K}{2} & 0 & \cdots & 0 & 0 & 0 \\ \frac{K}{2} & -1 & \frac{K}{2} & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2} & -1 & \frac{K}{2} \\ 0 & 0 & 0 & \cdots & 0 & \frac{K}{2} & -1 \end{bmatrix}. \tag{A.30}$$

Instead of guessing an eigenvector, we apply the Laplace expansion to directly calculate the determinant. We obtain the recursion

$$\det M_N = -\det M_{N-1} - \tfrac{K^2}{4}\det M_{N-2}, \tag{A.31}$$

$$\det M_1 = -1, \;\; \det M_2 = 1 - \tfrac{K^2}{4}. \tag{A.32}$$

The following ansatz fulfills this recursion relation

$$\det M_N = \tfrac{\tau_+^{N+1} - \tau_-^{N+1}}{\tau_+ - \tau_-} = \tau_+^N \sum_{n=0}^{N}\left(\tfrac{\tau_-}{\tau_+}\right)^n = \tau_-^N \sum_{n=0}^{N}\left(\tfrac{\tau_+}{\tau_-}\right)^n, \tag{A.33}$$

where

$$\tau_\pm(x,y) = \frac{x \pm \sqrt{1-y^2}}{2}, \tag{A.34}$$

$$\tau_\pm \equiv \tau_\pm(-1,K) = \tfrac{-1\pm\sqrt{1-K^2}}{2}. \tag{A.35}$$

This result already suffices to calculate the determinant and the partition sum. However, we also estimate the eigenvalues, since we need them for future calculations. We consider the equation for eigenvalues

$$0 \stackrel{!}{=} \det\left(M_N - \lambda\cdot 1\right) = \tfrac{\tau_+^{N+1}(-1-\lambda,K)-\tau_-^{N+1}(-1-\lambda,K)}{\tau_+(-1-\lambda,K)-\tau_-(-1-\lambda,K)}. \tag{A.36}$$

For this equation to hold, both following relations have to be true:

$$\tau_+^{N+1}(-1-\lambda,K) = \tau_-^{N+1}(-1-\lambda,K) \;\wedge\; \tau_+(-1-\lambda,K) \neq \tau_-(-1-\lambda,K) \tag{A.37}$$

$$\Leftrightarrow \quad \tfrac{\tau_-}{\tau_+} = \mathrm{e}^{2\pi i\,\frac{n}{N+1}} \;\wedge\; n \in \{1,...,N\}\,. \tag{A.38}$$

Thus, we have N possible choices for τ_-/τ_+. As we will see these choices correspond to the N eigenvalues λ_n.

$$\begin{aligned}\tfrac{\tau_-}{\tau_+} &= \tfrac{-1-\lambda-\sqrt{(-1-\lambda)^2-K^2}}{-1-\lambda+\sqrt{(-1-\lambda)^2-K^2}} = \tfrac{-1-\lambda-i\sqrt{K^2-(-1-\lambda)^2}}{-1-\lambda+i\sqrt{K^2-(-1-\lambda)^2}} \\ &= \tfrac{2(-1-\lambda)^2-K^2}{K^2} - 2\,i\,\tfrac{(-1-\lambda)\sqrt{K^2-(-1-\lambda)^2}}{K^2}.\end{aligned} \tag{A.39}$$

One can easily verify that $|\tau_-/\tau_+| = 1$. Thus, for every choice $n \in \{1,...,N\}$ both conditions *I*, *II* have to be true:

$$\text{I. } \mathrm{Re}\left(\tfrac{\tau_-}{\tau_+}\right) = \cos 2\Theta_n, \tag{A.40}$$

$$\text{II. } \mathrm{Im}\left(\tfrac{\tau_-}{\tau_+}\right) = \sin 2\Theta_n, \;\; \Theta_n = \pi\tfrac{n}{N-1}. \tag{A.41}$$

Condition I implies

$$\text{I. } \Rightarrow\; \lambda_n = -1 \pm K\cos\Theta_n. \tag{A.42}$$

To pin down the sign, we use II:

$$\text{II. } \Rightarrow\; \mathrm{sgn}(-1-\lambda_n) = \mathrm{sgn}(-\sin 2\Theta_n). \tag{A.43}$$

Thus, we finally obtain the eigenvalues of the interaction matrix for free boundary conditions:

$$\lambda_n = -1 + K\cos\Theta_n, \;\; \Theta_n = \pi\tfrac{n}{N+1}, \;\; n = 1,...,N. \tag{A.44}$$

One should note the similarity to the eigenvalues of the periodic system, Eq. (A.11).

Eigenvectors and the inverse

In this section, we briefly list and discuss the eigenvectors and the inverse M_{f}^{-1} of the interaction matrix of the one-dimensional free Gaussian chain. Most of the results are obtained from [14]. Similar to the eigenvectors of the periodic one-dimensional case the eigenvectors Φ_n of the $N \times N$ interaction matrix of the free Gaussian chain read

$$\Phi_n(k) = \sqrt{\frac{2}{N+1}} \sin\left(kn\frac{\pi}{N+1}\right). \tag{A.45}$$

These vectors are orthonormal due to the orthonormality of the sine function. The transformation matrix which diagonalises M_{f}^{-1} and M_{f} is the discrete sine transform F:

$$F_{i,j} = \sqrt{\frac{2}{N+1}} \sin\left(ij\frac{\pi}{N+1}\right). \tag{A.46}$$

Applying this transformation to the inverse interaction matrix in diagonal form we obtain M_{f}^{-1}:

$$\left(M_{\mathrm{f}}^{-1}\right)_{i,j} = \sum_{k=1}^{N} \frac{F_{i,k}F_{k,j}}{\lambda_k} = \frac{2}{N+1}\sum_{k=1}^{N} \frac{\sin i\,k\frac{\pi}{N+1}\,\sin j\,k\frac{\pi}{N+1}}{-1+K\cos k\frac{\pi}{N+1}}. \tag{A.47}$$

Two dimensions

In this section we derive the eigenvectors of the interaction matrix of the Gaussian model in two dimensions for toroidal, cylindric, Moebius strip and free boundary conditions. Additionally, we study the inverse for free and toroidal boundary conditions.

Toroidal boundaries

We start with toroidal boundary conditions

Interaction matrix, eigenvalues

We denote the interaction matrix as $M_{\mathrm{t}}^{2\mathrm{d}}$. The system size dictates that $M_{\mathrm{t}}^{2\mathrm{d}} \in \mathrm{Mat}\,(NM \times NM, \mathbb{R})$ and

$$M_{\mathrm{t}}^{2\mathrm{d}} = \begin{bmatrix} M_{\mathrm{p}} & \frac{K}{2}1_N & 0 & \cdots & 0 & 0 & \frac{K}{2}1_N \\ \frac{K}{2}1_N & M_{\mathrm{p}} & \frac{K}{2}1_N & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2}1_N & M_{\mathrm{p}} & \frac{K}{2}1_N \\ \frac{K}{2}1_N & 0 & 0 & \cdots & 0 & \frac{K}{2}1_N & M_{\mathrm{p}} \end{bmatrix}. \tag{A.48}$$

Here, $M_\mathrm{p} \in \mathrm{Mat}\,(N \times N, \mathbb{R})$ is the interaction matrix of the one-dimensional Gaussian model with periodic boundary conditions. To guess the eigenvectors $\Psi_{n,m} \in \mathbb{R}^{NM}$ we try the following ansatz:

$$\Psi_{n,m} = \left(z_m^1 u_n, z_m^2 u_n, ..., z_m^M u_n\right), \quad n \in \{1, ..., N\},\ m \in \{1, ..., M\}, \tag{A.49}$$

where $u_n \in \mathbb{R}^N$ is an eigenvector of M_p with the corresponding eigenvalue λ_n see Sec. II.2.1.1, and $z_m^M = 1$. We denote the nm-the eigenvalue with α_{nm}^t (the index t referring to toroidal boundaries) and write down the eigenvalue equation:

$$M_\mathrm{t}^\mathrm{2d} \Psi_{nm} = \alpha_{nm}^\mathrm{t} \Psi_{nm}. \tag{A.50}$$

Plugging in our ansatz for the eigenvectors reduces the number of linear equations from MN equations to N equations. We write these in matrix form:

$$\left[\tfrac{K}{2}\, 1_N \left(z_m + z_m^{-1}\right) + M_\mathrm{p}\right] u_n = \alpha_{nm} u_n. \tag{A.51}$$

Since u_n is an eigenvector of M_p,

$$M_\mathrm{p} u_n = \lambda_n u_n = \left(-1 + K \cos 2\pi \tfrac{n}{N}\right) u_n, \tag{A.52}$$

and $z_m = \exp((2\pi\, i\, m)/M)$, we obtain all eigenvalues α_{nm}^t of the interaction matrix M_t^2d:

$$\alpha_{nm}^\mathrm{t} = -1 + K \cos \varphi_n + K \cos \varphi_m = -1 + K \cos 2\pi \frac{n}{N} + K \cos 2\pi \frac{m}{M}. \tag{A.53}$$

The condition $2|K| < 1$ results from the requirement that all eigenvalues have to be negative. One should point out the similarity to the eigenvalues of the one-dimensional system, see Eq. (A.11).

Orthonormal eigenbasis

In the next step we determine a orthonormal set of real eigenvectors of M_t^2d. To simplify the notation we denote the interaction matrix of the system with toroidal boundary conditions with M_t (instead of M_t^2d) during this section. We consider only odd N, M, the generalisation to even system sizes will be obvious from the one-dimensional case. The eigenvalues of M_t read

$$\alpha_{n,m} = -1 + K \cos 2\pi \tfrac{n}{N} + K \cos 2\pi \tfrac{m}{M}, \tag{A.54}$$

and the corresponding complex eigenvectors are $\Psi_{n,m}$. We denote the $((i-1)M + j)$-th entry of $\Psi_{n,m}$ as $\Psi_{n,m}^{(i,j)}$:

$$\Psi_{n,m}^{(i,j)} = \mathrm{e}^{2\pi \mathrm{i} \frac{n}{N}} \mathrm{e}^{2\pi \mathrm{i} \frac{m}{M}}. \tag{A.55}$$

These eigenvectors are orthogonal with respect to the standard complex scalar product. For each $n = 1, ..., \frac{N-1}{2}$ and $m = 1, ..., \frac{M-1}{2}$ the eigenvalues $\alpha^{\mathrm{t}}_{n,m}$ are four-fold degenerate:

$$\alpha_{n,m} = \alpha_{n,M-m} = \alpha_{N-n,m} = \alpha_{N-n,M-m}. \tag{A.56}$$

Furthermore, for ($n = N$ and $m = 1, ..., \frac{M-1}{2}$) or ($m = M$ and $n = 1, ..., \frac{N-1}{2}$) the eigenvalues are two-fold degenerate. And, finally, the eigenvalue α_{NM} is not degenerate at all. Using these properties we construct the real eigenvectors Φ of M_{t}. For each choice of $n = 1, ..., \frac{N-1}{2}$ and $m = 1, ..., \frac{M-1}{2}$ the four eigenvectors

$$\Phi^{(i,j)} = \frac{2}{\sqrt{NM}} \begin{cases} \cos\left(2\pi \frac{m}{M} i\right) \cos\left(2\pi \frac{n}{N} j\right), \\ \cos\left(2\pi \frac{m}{M} i\right) \sin\left(2\pi \frac{n}{N} j\right), \\ \sin\left(2\pi \frac{m}{M} i\right) \cos\left(2\pi \frac{n}{N} j\right), \\ \sin\left(2\pi \frac{m}{M} i\right) \sin\left(2\pi \frac{n}{N} j\right). \end{cases} \tag{A.57}$$

For each choice of ($n = N$ and $m = 1, ..., \frac{M-1}{2}$) or ($m = M$ and $n = 1, ..., \frac{N-1}{2}$) the two eigenvectors

$$\Phi^{(i,j)} = \sqrt{\frac{2}{NM}} \begin{cases} \cos 2\pi i \frac{m}{M}, \\ \sin 2\pi i \frac{m}{M}, \quad \text{for } n = N. \end{cases} \tag{A.58}$$

or

$$\Phi^{(i,j)} = \sqrt{\frac{2}{NM}} \begin{cases} \cos 2\pi i \frac{n}{N}, \\ \sin 2\pi i \frac{n}{N}, \quad \text{for } m = M, \end{cases} \tag{A.59}$$

And, finally the eigenvector

$$\Phi^{(i,j)}_{N,M} = \frac{1}{\sqrt{NM}}. \tag{A.60}$$

The normalisation constant results from the relation

$$\sum_{j=1}^{N} \cos^2\left(2\pi \frac{n}{N} j\right) = \frac{N}{2}. \tag{A.61}$$

Estimating the inverse M_{t}^{-1}

In this section, we estimate the inverse matrix M_{t}^{-1} of the interaction matrix. The course of action is similar to the one-dimensional case: We calculate the inverse via the orthonormal transformation T:

$$T^t M_{\mathrm{t}} T = \tilde{M}_t = \mathrm{diag}\left(\alpha_{1,1}, ..., \alpha_{M,N}\right), \tag{A.62}$$

$$M_{\mathrm{t}}^{-1} = T \tilde{M}_t^{-1} T^t. \tag{A.63}$$

We obtain the entries of the matrix T using the eigenvectors Φ:

$$T_{(i,j)(n,m)} = \Phi^{(i,j)}_{n,m}. \tag{A.64}$$

The matrix T, as well as the interaction matrix and its inverse in two dimensions, is a block matrix. Therefore, the first index, (i,j), denotes the block and the second index, (n,m), denotes the position within the block. This notation for matrix entries of block matrices will be used throughout the thesis. The inverse M_t^{-1} can be written as:

$$\begin{aligned}\left(M_\mathrm{t}^{-1}\right)_{(i,j)(k,l)} &= \sum_{m=1}^{M}\sum_{n=1}^{N}\frac{\Phi^{(i,k)}_{n,m}\Phi^{(j,l)}_{n,m}}{\alpha_{n,m}} \\ &= \frac{1}{NM(-1+2K)} + \frac{2}{NM}\sum_{m=1}^{\frac{M-1}{2}}\frac{\cos 2\pi\frac{m}{M}(i-j)}{-1+K+K\cos 2\pi\frac{m}{M}} + \frac{2}{NM}\sum_{n=1}^{\frac{N-1}{2}}\frac{\cos 2\pi\frac{n}{N}(k-l)}{-1+K+K\cos 2\pi\frac{n}{N}} \\ &\quad + \frac{4}{MN}\sum_{m=1}^{\frac{M-1}{2}}\sum_{n=1}^{\frac{N-1}{2}}\frac{\cos 2\pi\frac{m}{M}(i-j)\cos 2\pi\frac{n}{N}(k-l)}{-1+K\cos 2\pi\frac{n}{N}+K\cos 2\pi\frac{m}{M}}.\end{aligned} \tag{A.65}$$

We define the matrix $\hat{M}_\mathrm{t}^{-1}$ through its matrix entries,

$$\left(\hat{M}_\mathrm{t}^{-1}\right)_{(i,k)(j,l)} := \frac{1}{(2\pi)^2}\int_0^{2\pi}\mathrm{d}x\int_0^{2\pi}\mathrm{d}y\,\frac{\cos x(i-j)\cos y(k-l)}{-1+K\cos x+K\cos y}, \tag{A.66}$$

one should note that the matrix entries of $\hat{M}_\mathrm{t}^{-1}$ are asymptotically equal to those of M_t^{-1} in the thermodynamic limit of large system size

$$\left(M_\mathrm{t}^{-1}\right)_{(i,k)(j,l)} = \left(\hat{M}_\mathrm{t}^{-1}\right)_{(i,k)(j,l)} + R(N,M,K), \text{ as } M,N\to\infty. \tag{A.67}$$

The remaining term R vanishes exponentially with the size of the matrix.

Properties of $\hat{M}_\mathrm{t}^{-1}$, M_t^{-1}: Using the definition of $\hat{M}_\mathrm{t}^{-1}$, M_t^{-1} we recognise the following properties:

- $\hat{M}_\mathrm{t}^{-1}$, M_t^{-1} are real and symmetric. Every block of $\hat{M}_\mathrm{t}^{-1}$, M_t^{-1} is real and symmetric. Thus, $\hat{M}_t$, M_t^{-1} are **symmetric as block matrices**.
- Every block is Toeplitz. Furthermore, $\hat{M}_t$, M_t^{-1} is Block-Toeplitz.
- **In contrast to** $\hat{M}_t^{-1}$, every block of M_t^{-1} is a circulant. M_t^{-1} is a block-circulant.

Cylindric boundaries

In this section we calculate the eigenvalues of the interaction matrix of the two-dimensional Gaussian system with cylindric boundary conditions. We omit the calculation of the eigenvectors, due to its similarity to the calculation of the eigenvectors of the toroidal and the free systems.

Interaction matrix

The interaction matrix $M_{\mathrm{c}}^{2\mathrm{d}}$ reads.

$$M_{\mathrm{c}}^{2\mathrm{d}} = \begin{bmatrix} M_{\mathrm{p}} & \frac{K}{2}1_N & 0 & \cdots & 0 & 0 & 0 \\ \frac{K}{2}1_N & M_{\mathrm{p}} & \frac{K}{2}1_N & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2}1_N & M_{\mathrm{p}} & \frac{K}{2}1_N \\ 0 & 0 & 0 & \cdots & 0 & \frac{K}{2}1_N & M_{\mathrm{p}} \end{bmatrix}. \tag{A.68}$$

Again, $M_{\mathrm{p}} \in \mathrm{Mat}\left(\mathbb{R}^N \times \mathbb{R}^N\right)$ is the interaction matrix of the one-dimensional periodic system. Since this matrix is no longer a block-circulant we have to come up with a new ansatz for the eigenvectors Ψ: Let u_n be the n-th eigenvector of the one-dimensional system M_{p}. To guess the eigenvectors Ψ of $M_{\mathrm{c}}^{2\mathrm{d}}$ we try the ansatz

$$\Psi = (z_1 u_n, ..., z_M u_n). \tag{A.69}$$

We are looking for M different M-tuples $(z_1, ..., z_M)$, such that the eigenvalue equation

$$M_{\mathrm{c}}^{2\mathrm{d}}\Psi = \alpha\Psi \tag{A.70}$$

is fulfilled for an eigenvalue α. We write down the equation explicitly:

$$\begin{aligned} &1.\ \left(z_1\lambda_n + z_2\tfrac{K}{2}\right) u_n = \alpha\, z_1 u_n, \\ &2.\ \left(z_M\lambda_n + z_{M-1}\tfrac{K}{2}\right) u_n = \alpha\, z_M u_n, \\ &3.\ \left(z_m\tfrac{K}{2} + z_{m+2}\tfrac{K}{2} + z_{m+1}\lambda_n\right) u_n = \alpha\, z_{m+1} u_n, \quad \forall\, m = 1, ..., M-2. \end{aligned} \tag{A.71}$$

Since all vectors u_n are different from the zero vector, we derive the following equation system:

$$\begin{aligned} &1.\ z_1\lambda_n + z_2\tfrac{K}{2} = \alpha\, z_1, \\ &2.\ z_M\lambda_n + z_{M-1}\tfrac{K}{2} = \alpha\, z_M, \\ &3.\ z_m\tfrac{K}{2} + z_{m+2}\tfrac{K}{2} + z_{m+1}\lambda_n = \alpha\, z_{m+1}, \quad \forall\, m = 1, ..., M-2. \end{aligned} \tag{A.72}$$

We interpret this equation as a homogeneous linear equation for $(z_1, ..., z_M)$. This equation possesses a solution if and only if the determinant of the corresponding matrix is different from zero. However, the corresponding matrix is the $M \times M$ interaction matrix of the one-dimensional free Gaussian chain, with the entry $\lambda_n - \alpha$ in the main diagonal, instead of -1. Using the same methods as in Sec. II.2.1.2, for each choice of u_n, we obtain M different M-tuples $(z_1, ..., z_M)$. We denote the corresponding eigenvalues with α_{nm}^{c}, $n = 1, ...N$, $m = 1, ..., M$:

$$\alpha_{nm}^{\mathrm{c}} = -1 + K\cos\varphi_n + K\cos\theta_m = -1 + K\cos 2\pi\tfrac{n}{N} + K\cos\pi\tfrac{m}{M+1}. \tag{A.73}$$

The index c refers to cylindric boundary conditions and will be omitted whenever it is obvious which type of boundary conditions is under consideration. One should point out the similarity to the eigenvalues of the toroidal system, see Eq. (A.53), as well as the one-dimensional systems, see Eq. (A.11) and Eq. (A.44).

Free boundary conditions

After having estimated the properties of the interaction matrix for toroidal and cylindric boundary conditions, we address the free boundary conditions in this section.

Interaction matrix

The interaction matrix $M_{\mathrm{f}}^{2\mathrm{d}}$ results from removing all entries which correspond to periodic interactions from the interaction matrix of cylindric boundaries $M_{\mathrm{c}}^{2\mathrm{d}}$:

$$M_{\mathrm{f}}^{2\mathrm{d}} = \begin{bmatrix} M_{\mathrm{f}} & \frac{K}{2}1_N & 0 & \cdots & 0 & 0 & 0 \\ \frac{K}{2}1_N & M_{\mathrm{f}} & \frac{K}{2}1_N & \cdots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{K}{2}1_N & M_{\mathrm{f}} & \frac{K}{2}1_N \\ 0 & 0 & 0 & \cdots & 0 & \frac{K}{2}1_N & M_{\mathrm{f}} \end{bmatrix}. \tag{A.74}$$

Instead of the circulant matrix M_{p} on the main block diagonal we use the matrix M_{f} of the one-dimensional system with free boundary conditions. To calculate the eigenvalues α_{nm}^{f}, we follow the same pattern as in the cylindric case: We make the same ansatz for the Ψ, but use eigenvectors u_n of the matrix M_{f} (instead of the eigenvectors of M_{p}):

$$\Psi = (z_1 u_n, ..., z_M u_n). \tag{A.75}$$

Performing exactly the same calculations as in Sec. II.2.2.2, we obtain the eigenvalues α_{nm}^{f}:

$$\alpha_{nm}^{\mathrm{f}} = -1 + K\cos\theta_n + K\cos\theta_m = -1 + K\cos\pi\tfrac{n}{N+1} + K\cos\pi\tfrac{m}{M+1}. \tag{A.76}$$

Again, one should note the similarity to the toroidal and the cylindric eigenvalues, see Eq. (A.53), Eq. (A.53).

Inverse interaction matrix

The interaction matrix of the two-dimensional Gaussian model with free boundary conditions is block Toeplitz. The results presented in this section are taken from [14], which also contains a detailed discussion of the properties of Toeplitz and block Toeplitz matrices. The inverse of the interaction matrix is again block Toeplitz: We

denote the position of the block with the first pair of indices and the position in the block with the second pair of indices. The inverse $M_{\mathrm{f}}^{2\mathrm{d}}$ reads

$$\left(M_{\mathrm{f}}^{2\mathrm{d}}\right)^{-1}_{(i,j)(m,n)} = \frac{4}{(N+1)(M+1)} \sum_{k=1}^{M} \sum_{l=1}^{N} \frac{\sin i\,k\frac{\pi}{M+1} \sin j\,k\frac{\pi}{M+1} \sin m\,l\frac{\pi}{N+1} \sin n\,l\frac{\pi}{N+1}}{-1 + K\cos k\frac{\pi}{M+1} + K\cos l\frac{\pi}{N+1}}. \tag{A.77}$$

Similar to the one-dimensional Gaussian chain with free boundaries, the eigenvectors $\Psi_{n,m}$ read

$$\Psi_{n,m}(i,j) = \sqrt{\frac{4}{(N+1)(M+1)}} \sin i\,n\frac{\pi}{N+1} \sin j\,m\frac{\pi}{M+1}. \tag{A.78}$$

A.3. Chebyshev polynomials

In this section we define the Chebyshev polynomials which are closely related to Toeplitz matrices. We list and briefly discuss the most important properties of the Chebyshev polynomials which were used throughout this work. One can define the **Chebyshev of the first kind** T_n through the following recursion relation:

$$T_{n+1}(x) = 2x\,T_n(x) - T_{n-1}, \tag{A.79}$$
$$T_0(x) = 1, \tag{A.80}$$
$$T_1(x) = x. \tag{A.81}$$

T_n is a polynomial of n-th degree. An alternative representation is

$$T_n(x) = \begin{cases} \cos(n \arccos(x)), & |x| \leq 1, \\ \cosh(n \operatorname{arccosh}(x)), & |x| > 1. \end{cases} \tag{A.82}$$

The zeros x_k of T_n are

$$x_k = \cos\left(\pi \frac{2k-1}{2n}\right), \quad k = 1, ..., n. \tag{A.83}$$

All zeros lie in the interval $[-1, 1]$. Furthermore the following equations hold:

$$T_n(1) = 1, \tag{A.84}$$
$$T_n(-1) = (-1)^n \tag{A.85}$$

The **Chebyshev polynomials of the second kind** U_n follow the recursion

$$U_{n+1}(x) = 2x\,U_n(x) - U_{n-1}(x), \tag{A.86}$$
$$U_0(x) = 1, \tag{A.87}$$
$$U_1(x) = 2x. \tag{A.88}$$

U_n is a polynomial of n-th degree. Alternatively it can be represented through trigonometric functions:

$$U_n(x) = \frac{\sin((n+1)\arccos x)}{\sin \arccos x}. \tag{A.89}$$

The zeros are

$$x_k = \cos\left(\pi \frac{k}{n+1}\right), \quad k = 1, ..., n. \tag{A.90}$$

Furthermore,

$$U_n(1) = n + 1, \tag{A.91}$$
$$U_n(-1) = (n+1)(-1)^n. \tag{A.92}$$

There is a relation between the Chebyshev polynomials of the first and the second kind:

$$T_n' = nU_{n-1}. \tag{A.93}$$

A.4. Euler-Maclaurin summation formula

In this section, we formulate the Euler-Maclaurin formula for numerical integration and discuss its most important properties (see [17] for details on the Euler-Maclaurin formula). Let $f : [a, b] \to \mathbb{R},\ f \in C^{2r+2},\ r \geq 0$. To approximate the integral $I(f)$,

$$I(f) := \int_a^b \mathrm{d}x\, f(x), \tag{A.94}$$

we define the N-th trapezoidal sum $T_N \equiv T_N(f)$:

$$T_N := h\frac{f(a) + f(b)}{2} + h\sum_{k=1}^{N-1} f(x_k) \tag{A.95}$$

where $h = (b-a)/N$ is the step width and $x_k = a + (b-a)k/N$ are the grid points. The Euler-Maclaurin summation formula reads:

$$T_N(f) - I(f) = \sum_{i=1}^{r} \tau_i(f)\, h^{2i} + R_{r+1}(h), \tag{A.96}$$

where the decay of the remaining term R is

$$R_{r+1}(h) = \mathcal{O}\left(h^{2r+2}\right) \tag{A.97}$$

and the coefficients τ_i read:

$$\tau_i(f) = \frac{B_{2i}(0)}{(2i)!}\left(f^{(2i-1)}(b) - f^{(2i-1)}(a)\right). \tag{A.98}$$

Here, $f^{(n)}$ is the n-th derivative of f and B_i is the i-th Bernoulli polynomial, see [1], [15]. Important properties of the Bernoulli polynomials, which are be used throughout this work are:

$$B_{2n-1}(x) = -B_{2n-1}(1-x), \tag{A.99}$$

$$B_{2n-1}\left(\frac{1}{2}\right) = 0, \tag{A.100}$$

$$B_1(0) = -\frac{1}{2}, \tag{A.101}$$

$$B_{2n-1}(0) = 0, \quad \text{for } n > 1. \tag{A.102}$$

A case of particular interest for this work is the case of periodic functions: Let $f \in C^n([a-\epsilon, b+\epsilon)),\ n \in \mathbb{N}$ be $(b-a)$-periodic, i.e. $f(x+b-a) = f(x)$. The error of the approximation of $I(f)$ by $T_N(f)$ can be expressed as:

$$|T_N(f) - I(f)| = \mathcal{O}(h^n). \tag{A.103}$$

Therefore, for smooth periodic function the difference decays faster than any natural power of N:

$$|T_N(f) - I(f)| = \mathcal{O}(N^{-n}), \quad \forall n \in \mathbb{N}. \tag{A.104}$$

Throughout this work the Euler-Maclaurin formula is being applied to smooth functions f, which are a function of the cosine for numerical integration over the interval $[0, \pi]$. Such functions are not necessarily π-periodic. Nevertheless the approximation error decays faster than any power of the number of discretisation steps N. The reason for this is that

1. The coefficients τ_k of the algebraically decaying contributions are proportional to $f^{(2k-1)}(\pi) - f^{(2k-1)}(0)$, $k \in \mathbb{N}$.
2. It is $f^{(2k-1)}(\pi) = f^{(2k-1)}(0)$, $\forall\, k \in \mathbb{N}$ for functions f which are functions of cos only.

We look closer at the second claim: Let f be a function of cos only:

$$f(\varphi) = g(\cos(\varphi)), \tag{A.105}$$

with a smooth g. We prove that all odd derivatives of f vanish at $\varphi = 0$ and $\varphi = \pi$. The first derivative reads

$$f'(\varphi) = -g'(\cos\varphi)\, \sin(\varphi), \tag{A.106}$$

in particular

$$f'(0) = f'(\pi) = 0. \tag{A.107}$$

The second derivative reads

$$\begin{aligned} f''(\varphi) &= g''(\cos(\varphi))\, \sin^2(\varphi) - g'(\cos\varphi)\, \cos(\varphi) \\ &= g''(\cos(\varphi))\, \left(1 - \cos^2(\varphi)\right) - g'(\cos\varphi)\, \cos(\varphi) = h(\cos\varphi). \end{aligned} \tag{A.108}$$

Obviously, the second derivative is a function of $\cos(\varphi)$ only. Therefore, the third derivative vanishes at 0 and π. The claim follows by induction.

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