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Faculty of Mathematics and Physics

DIPLOMA THESIS

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A link between lattice models and models of continuum mechanics

Mathematical institute

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I confess that I have written my diploma thesis on my own and using only the listed sources. I agree with lending of my diploma thesis.

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Contents

Název práce: ***Souvislost mezi mřížkovými modely a modely mechaniky kontinua***
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Abstrakt: Cílem této diplomové práce je studium mřížkových modelů v kontextu Lebowitz-Penrose limity a nalezení souvislosti mezi statistickou fyzikou a mezoskopickou van der Waalsovou teorií založenou na nelokálním funkcionálu volné energie. V prvé části práce je zaveden formalismus statické fyziky a zadefinován zobecněný Blume-Capel model (r-model). Poté je provedena aproximace teorií středního pole a jako ilustrace získaných výsledků je uveden fázový diagram klasického Blume-Capel modelu. V následující kapitole je dokázána Lebowitz-Penrose věta pro r-model včetně všech potřebných odhadů. Během důkazu je zaveden funkcionál volné energie a je diskutován přechod od diskrétních veličin k veličinám se spojitou proměnnou. Nakonec je ve stručnosti vyložena van der Waalsova teorie a pomocí funkcionálu volné energie ukázána souvislost se statistickou fyzikou r-modelu.
Klíčová slova: mřížkové modely, statistická mechanika, souvislost, mechanika kontinua, funkcionál volné energie.

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Abstract: The aim of this thesis is an investigation of lattice models in the context of Lebowitz-Penrose limit to provide a link between the underlying statistical mechanical models to the mesoscopic "continuous" description based on the nonlocal free energy functional. First, the basic formalism of statistical mechanics is introduced and an extended Blume-Capel model (r-model) defined. Then the mean-field approximation is discussed including a phase diagram of the classical Blume-Capel model. Fruther, the Lebowitz-Penrose theorem for the r-model is carried out from the scratch. All bounds are explicitly calculated. As a tool within the proof, the free energy functional is introduced and a transition from discrete to continuous variables is emerges. Finally, the basics of the van der Waals mesoscopic theory are discussed and a link with the original lattice model is established via the free energy functional.
Keywords: lattice models, statistical mechanics, link, continuum mechanics, free energy functional

Chapter 1

Introduction

The aim of this thesis is to broaden the understanding of the connection between the discrete theory (statistical mechanics) which studies the microscopical behaviour of systems to a "continuous" theory (van der Waals) describing averages of microscopical values at the mesoscopic level. The text is based on the Section 3.4 of [Pr] and extends its validity to the case of a general *r-model* which is defined in the second chapter of this thesis.

The outline of the proof of the main Theorem 4.1.4 is adopted from [Pr]. However, the whole prove including all lemmas is done from scratch and all bounds are explicitly calculated. The only thing we need from the statistical physics of lattice models is the Lemma 2.1.1 which gives us the existence of free energy, a fundamental thermodynamical quantity.

In the next chapter we give a short introduction to the statistical physics of lattice models, define the extended Blume-Capel model (r-model), discuss its mean-field approximation, and formulate an equivalent model. Further, we introduce the notion of phase transition and illustrate it on the mean-field approximation of the classical Blume-Capel model.

Next, in the third chapter, we make several observations concerning discrete and continuous entropies (especially inequalities among them) which will be used later and which are necessary to correctly perform the transition from discrete variables to their continuous counterparts. The basic tool here is the Stirling's formula.

Then, in the fourth chapter, we introduce Kac potentials and prove the Lebowitz-Penrose theorem for the r-model. Throughout the proof we introduce the free energy functional and discuss the transition from discrete to continuous description.

Finally, in the last chapter we introduce the van der Waals mesoscopic theory and provide the excess free energy functional for the r-model rounding off the link between the statistical mechanics and the van der Waals theory.

Chapter 2

Extended Blume-Capel model

2.1 Introduction to lattice models

In the first section of this chapter we present the basic abstract formalism of statistical mechanics for lattice models.

During the evolution of statistical mechanics, a discipline which investigates macroscopic behaviour of physical systems using the knowledge of their internal microscopic characteristics, it proved to be useful to study systems with configurations residing on discrete subsets of $\mathbb{R}^d$. The set is usually taken to be a periodic lattice and hence the name statistical mechanics of *lattice models*. We will take our underlying lattice to be $\mathbb{Z}^d$, the set of d-tuples $(x_1, x_2, \ldots, x_d)$ of integers.

Given a site $x \in \mathbb{Z}^d$ we choose a set of allowed "values" of the spin at x. We use Ω_x to denote the set and we assume it to be a compact metric space. For the sake of simplicity we also assume that Ω_x are the same at each site in the lattice and we use Ω_0 to denote it. Next we define $\mathscr{P}(\mathbb{Z}^d)$ and $\mathscr{P}_f(\mathbb{Z}^d)$, the sets of *all* and *all finite* subsets of $\mathbb{Z}^d$, respectively . Given a $\Lambda \in \mathscr{P}(\mathbb{Z}^d)$, configurations on Λ are mappings $\Lambda \to \Omega_0$. The set of configurations on Λ is then a Cartesian product Ω_0^Λ. We use $\mathbf{\Omega}$ instead of $\Omega_0^{\mathbb{Z}^d}$, the set of *all configurations of the* whole *system.* For $\Lambda' \subset \Lambda$ and $s \in \Omega_0^{\Lambda'}, t \in \Omega_0^{\Lambda \backslash \Lambda'}$, we use $s \times t$ for the obvious element of Ω_0^Λ

$$(s \times t)(x) = \begin{cases} s(x) & x \in \Lambda' \\ t(x) & x \in \Lambda \backslash \Lambda' \end{cases} . \tag{2.1}$$

Now we consider Ω_0^Λ with product topology and define the set $\mathcal{C}_\Lambda$ of all continuous functions $f : \Omega_0^\Lambda \to \mathbb{R}$. For $\Lambda' \subset \Lambda$ there exists a natural map $i_{\Lambda',\Lambda}$ from $\mathcal{C}_{\Lambda'}$ into $\mathcal{C}_\Lambda$ defined by

$$(i_{\Lambda',\Lambda} f)(s \times t) = f(s), \quad s \in \Omega_0^{\Lambda'}, t \in \Omega^{\Lambda \backslash \Lambda'}. \tag{2.2}$$

We drop the i's from the notation and regard $\mathcal{C}_{\Lambda'}$ as a subset of $\mathcal{C}_\Lambda$. Especially, we consider any $\mathcal{C}_\Lambda$ as a subset of $\mathcal{C}_{\mathbb{Z}^d}$. Accepting this agreement we can define the interaction potential and the Hamiltonian.

The *interaction potential* is a map Φ from $\mathscr{P}_f(\mathbb{Z}^d)$ into $\mathcal{C}_{\mathbb{Z}^d}$ such that $\Phi(X) \in \mathcal{C}_X$. $\Phi(X)$ describes the interaction among the spins inside X by assigning a value to each configuration $\sigma \in \Omega_0^X$. The assigned value is referred to as *energy* of the mutual interaction among spins in X. In physics it is the Hamilton function which has the meaning of energy and which determines the dynamics of physical models. The Hamiltonian of a lattice model is defined by

$$H_\Lambda(\Phi) = \sum_{\substack{X \in \mathscr{P}_f(\mathbb{Z}^d) \\ X \bigcap \Lambda \neq \emptyset}} \Phi(X). \tag{2.3}$$

The sum is in general case infinite and so as to converge we would have to state assumptions on Φ. Here we restrict ourselves to the case of a finite range Φ, i.e. $\exists k \in \mathbb{N} : |X| \geq k \Rightarrow \Phi(X) \equiv 0$. Then the sum is finite and Hamiltonian is a continuous function on $\mathbf{\Omega}$.

In the sequel we will be interested only in translational invariant potentials Φ, which is a natural assumption. We say that an interaction potential Φ is translational invariant if $\Phi\big(\tau_y(X)\big) = \Phi(X) \circ \tau_y^*$ for any $y \in \mathbb{Z}^d$, where $\tau_y(X) = \{x \in \mathbb{Z}^d : \exists \tilde{x} \in X, \textit{ such that } x = \tilde{x} + y\}$ and τ_y^* is a map $\mathbf{\Omega} \to \mathbf{\Omega}$ defined by $[\tau_y^*(\sigma)](x) = \sigma(x+y)$.

We are interested in the macroscopic behavior of our models, especially in thermodynamics and phase transitions. These can be obtained from thermodynamical potentials for large $|\Lambda|$. To introduce the thermodynamical potential we first define a partition function, then a free energy in a finite volume, and finally take a limit $|\Lambda| \to \infty$. In order to define the partition function we recall and equip Ω_0 with Borel σ-algebra $\mathcal{A}_0$ and a non-negative finite measure μ_0 on $(\Omega_0, \mathcal{A}_0)$ called "a priori measure". If Ω_0 is finite we usually use the counting measure.

Let $\beta = \frac{1}{k_B T}$ be the *inverse temperature* (k_B is the Boltzmann's constant and T the thermodynamical temperature). We define the *partition function on* Λ with a boundary condition $\tilde{\sigma} \in \mathbf{\Omega}$

$$Z(\Phi, \beta\,|\tilde{\sigma})_\Lambda = \int_{\Omega_0^\Lambda} e^{-\beta H(\Phi)_\Lambda(\tilde{\sigma})} \prod_{x \in \Lambda} d\mu_0(\tilde{\sigma}(x)). \tag{2.4}$$

Because μ_0 is non-negative and the Hamiltonian is real valued we can take a logarithm of the partition function and define the *free energy in a finite volume* Λ

$$f(\Phi, \beta\,|\tilde{\sigma})_\Lambda = -\frac{1}{\beta|\Lambda|} \log Z(\Phi, \beta\,|\tilde{\sigma})_\Lambda. \tag{2.5}$$

Finally, we take the limit $|\Lambda_n| \to \infty$. However, we must be careful about the choice of the sets Λ_n.

For $\Lambda \subset \mathbb{Z}^d$ we define $\partial\Lambda = \{x \in \Lambda^c : \exists y \in \Lambda\ |x-y| = 1\}$. We call a sequence $\{\Lambda_n\}_{n=1}^\infty \subset \mathscr{P}_f(\mathbb{Z}^d)$ a *van Hove sequence* if

$$\lim_{n \to \infty} \frac{|\partial\Lambda_n|}{|\Lambda_n|} = 0. \tag{2.6}$$

The *free energy* is then defined for a van Hove sequences by the limit

$$f(\Phi, \beta \,|\tilde{\sigma}) = \lim_{n\to\infty} -\frac{1}{\beta|\Lambda_n|} f(\Phi, \beta \,|\tilde{\sigma})_{\Lambda_n}, \tag{2.7}$$

if it exists.

The free energy is a thermodynamic potential used for investigating the lattice models. However, it depends on the interpretation of a particular model whether it corresponds to the Helmholtz free energy (for example in magnetic systems) or to the density of the grand canonical potential (lattice gas).

Now we state sufficient assumptions on Φ so that the free energy exists and does not depend on the choice of the boundary condition and the sequence $\{\Lambda_n\}_{n=1}^{\infty}$.

Lemma 2.1.1 *Let $\Phi : \mathscr{P}_f(\mathbb{Z}^d) \to \mathcal{C}_{\mathbb{Z}^d}$ be a uniformly bounded, translational invariant, finite range interaction potential:*

1. $\exists K \in \mathbb{R} : \forall X \in \mathscr{P}_f(\mathbb{Z}^d)\ |\Phi(X)| \leq K$,
2. $\exists k \in \mathbb{N} : |X| \geq k \Rightarrow \Phi(X) \equiv 0$,
3. $\Phi(\tau_y(X)) = \Phi(X) \circ \tau_y^*$ *for any* $y \in \mathbb{Z}^d$.

Further let $\tilde{\sigma} \in \mathbf{\Omega}$ be a fixed configuration and $\{\Lambda_n\}_{n=1}^{\infty} \subset \mathscr{P}_f(\mathbb{Z}^d)$ a van Hove sequence. Then the free energy exists,

$$f(\Phi, \beta, \tilde{\sigma}) = \lim_{n\to\infty} -\frac{1}{\beta|\Lambda_n|} \log Z(\Phi, \beta \,|\tilde{\sigma})_{\Lambda_n}, \tag{2.8}$$

and is independent of the choice of the sequence $\{\Lambda_n\}_{n=1}^{\infty}$. Moreover, for any other $\sigma \in \mathbf{\Omega}$ holds true

$$f(\Phi, \beta, \sigma) = f(\Phi, \beta, \tilde{\sigma}). \tag{2.9}$$

Proof. The lemma is a consequence of the subadditivity of the partition function. It can be proved in many ways. One of them is demonstrated in [BK] in Section *2.A* for the Ising model. However, the method is general enough to be used for this lemma without modification. □

2.2 r-model

Now we give an example of lattice model. We define the extended Blume-Capel model and formulate its mean-field approximation. Then we show an explicit formula for the mean-field free energy and further we formulate an equivalent model. Finally, as an illustration of the obtained results, we plot the phase diagram of the mean-field approximation of the standard Blume-Capel model.

When we investigate a particular model, we usually skip the interaction potential Φ from the notation and write down directly the Hamiltonian $H(\sigma) = H(\Phi)(\sigma)$.

Definition 2.2.1 (Extended Blume-Capel model) *Let* $r \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, $\Omega_0 = \{\omega_1, \omega_2, \ldots, \omega_r\} \subset \mathbb{R}$. [1] *We consider* Ω_0 *equipped with discrete topology and counting measure and we will use* Ω_0 *both for the set, the topological space, and the measurable space. We define the configuration space* $\mathbf{\Omega} = \Omega_0^{\mathbb{Z}^d}$ *with product topology (and the Borel* σ*-algebra). Let* $\sigma \in \mathbf{\Omega}$ *and* $\Lambda \in \mathscr{P}_f(\mathbb{Z}^d)$. *Then the Hamiltonian of the extended Blume-Capel model is given by*

$$H_h^o(\sigma)_\Lambda = \frac{1}{4}\sum_{x\in\Lambda}\sum_{\substack{y\in\Lambda\\|x-y|=1}}\big(\sigma(x)-\sigma(y)\big)^2-\sum_{i=1}^{r-1}h_i\sum_{x\in\Lambda}\sigma^i(x)+\frac{1}{2}\sum_{x\in\Lambda}\sum_{\substack{y\in\Lambda^c\\|x-y|=1}}\big(\sigma(x)-\sigma(y)\big)^2, \tag{2.10}$$

where σ^i *is the i'th power of* σ.

In the sequel we will refer to this model simply as to an *r-model.* For $r = 1$ this is a trivial model, for $r = 2$ and $\Omega_0 = \{-1, 1\}$ it is the Ising spin model, and for $r = 3$ with $\Omega_0 = \{-1, 0, 1\}$ it is the standard Blume-Capel model. The definition is thus a straightforward generalization of Ising and Blume-Capel models.

Now we define the configuration space with boundary condition:

Definition 2.2.2 (Configuration space with boundary condition) *For* $\Lambda \subset \mathbb{Z}^d$ *and* $\tilde{\sigma} \in \mathbf{\Omega}$ *we define*

$$\mathbf{\Omega}_\Lambda(\tilde{\sigma}) \stackrel{\text{df}}{=} \big\{\sigma \in \mathbf{\Omega},\ \sigma(y) = \tilde{\sigma}(y) \text{ for all } y \in \Lambda^c\big\}. \tag{2.11}$$

Here $\tilde{\sigma}$ stands for boundary condition as only the values outside Λ are considered. We will say that $\mathbf{\Omega}(\tilde{\sigma})_\Lambda$ is the configuration space on Λ with boundary condition $\tilde{\sigma}$. Notice that we use the elements of $\mathbf{\Omega}$ both for configurations σ and for the boundary conditions $\tilde{\sigma}$.

The partition function for the r-model is then

$$Z(\beta, h|\tilde{\sigma})_\Lambda = \sum_{\sigma\in\mathbf{\Omega}(\tilde{\sigma})_\Lambda} e^{-\beta H_h(\sigma)_\Lambda}. \tag{2.12}$$

Unfortunately, except the case $d = 1$, we are not able to compute the free energy explicitly.

2.3 Mean-field approximation

The first thing we can try to get some information about the phase transitions in such a model is the mean-field approximation. First of all we replace the Hamiltonian (2.10) with a more suitable one.

$$H_h(\sigma)_\Lambda = -\frac{1}{2}\sum_{x\in\Lambda}\sum_{\substack{y\in\Lambda\\|x-y|=1}}\sigma(x)\sigma(y)-\sum_{i=1}^{r-1}h_i\sum_{x\in\Lambda}\sigma^i(x)-\sum_{x\in\Lambda}\sum_{\substack{y\in\Lambda^c\\|x-y|=1}}\sigma(x)\sigma(y), \tag{2.13}$$

[1] We assume $i \neq j \Rightarrow \omega_i \neq \omega_j$.

This Hamiltonian slightly differs from the r-model Hamiltonian:

$$|H^0_{h_1,h_2,h_3,\dots,h_r}(\sigma)_\Lambda - H_{h_1,h_2-d,h_3,\dots,h_r}| \le d\,\omega^2_{max}|\partial\Lambda|, \tag{2.14}$$

where $\omega_{max} = \max_{\omega\in\Omega_0}|\omega|$. We can see from the inequality that for van Hove sequences of sets the difference is small in comparison to the volume $|\Lambda|$ and for the free energies of both models we have

$$f^0(\beta, h_1, h_2, h_3, \dots, h_r|\tilde{\sigma}) = f(\beta, h_1, h_2 - d, h_3, \dots, h_r|\tilde{\sigma}). \tag{2.15}$$

Now we look at the Hamiltonian (2.13) and identify the interaction potential Φ. There are only two types of interaction: one-site

$$\Phi_{\{x\}}(\sigma) = -\sum_{i=1}^{r-1} h_i\sigma^i(x) \tag{2.16}$$

and two site

$$\Phi_{\{x,y\}}(\sigma) = \begin{cases} -\sigma(x)\sigma(y) & \text{if } |x-y| = 1 \\ 0 & \text{otherwise} \end{cases}. \tag{2.17}$$

The two site interaction is the problematic one in the computation of the partition function. It relates the sites in Λ with its nearest neighbours only and does not allow to simplify the first sum in (2.13).

The idea of the *mean-field approximation* is to replace the two site nearest neighbour interaction with a one-site interaction of spins with an external *"mean" field* generated by the surrounding spins

$$\Phi_{\{x\}} = -\sigma(x)\ \left(\frac{1}{|\Lambda|}\sum_{y\in\Lambda}\sigma(y)\right). \tag{2.18}$$

It is an intuitive guess to make the situation easier. Even though the mean-field approximation has some unphysical properties (e.g. it predicts phase transitions for models even in $d = 1$) its main advantage is a possibility to calculate the free energy more explicitly. We use it and get the *mean-field Hamiltonian*

$$\mathcal{H}_h(\sigma)_\Lambda = -\frac{1}{2|\Lambda|}\sum_{x\in\Lambda}\sum_{y\in\Lambda}\sigma(x)\sigma(y) - \sum_{i=1}^{r-1} h_i \sum_{x\in\Lambda}\sigma^i(x). \tag{2.19}$$

In the following theorem we present an explicit formula for the free energy in terms of the entropy S_r, defined in previous chapter. First, let us introduce some notation.

Definition 2.3.1 *We define a mapping $L : \mathbb{R}^r \to \mathbb{R}^{r-1}$ given by the matrix L_{ij} with respect to the canonical bases*

$$L_{ij} = \begin{pmatrix} \omega_1 & \omega_2 & \dots & \omega_r \\ \omega_1^2 & \omega_2^2 & \dots & \omega_r^2 \\ \vdots & \vdots & \ddots & \vdots \\ \omega_1^{r-1} & \omega_2^{r-1} & \dots & \omega_r^{r-1} \end{pmatrix}. \tag{2.20}$$

Next, we define a set $\mathbb{M}_r = L(\mathbb{P}_r)$, *where* $\mathbb{P}_r$ *was defined in the previous chapter. Finally, we notice that we use* $\|L\|$ *to denote the norm of* L *in the space of linear maps* $\mathbb{R}^r \to \mathbb{R}^r$ *induced by the* ℓ^∞ *norm in* $\mathbb{R}^r$, $\|L\| = \max_{i\in\{1,\ldots,r-1\}} \sum_{j\in\{1,\ldots,r\}} |L_{ij}|$. *Then, for any* $x \in \mathbb{R}^d$, *we have* $|Lx| \le \|L\| |x|$.

Theorem 2.3.2 *Let* $r \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, $\boldsymbol{\Omega} = \Omega_0^{\mathbb{Z}^d}$ *be the configuration space,* $\tilde{\sigma} \in \boldsymbol{\Omega}$, $\Lambda \in \mathscr{P}_f(\mathbb{Z}^d)$, *and* $\mathcal{H}_h(\cdot)_\Lambda$ *be the mean-field Hamiltonian. The partition function of the* mean-field model *is*

$$\mathcal{Z}(\beta, h|\tilde{\sigma})_\Lambda = \sum_{\sigma\in\boldsymbol{\Omega}(\tilde{\sigma})_\Lambda} e^{-\beta\mathcal{H}_h(\sigma)_\Lambda}, \tag{2.21}$$

the free energy *exists, and for any sequence* $\{\Lambda_n\}_{n=1}^\infty \subset \mathscr{P}_f(\mathbb{Z}^d)$ *such that* $|\Lambda_n| \to \infty$ *for* $n \to \infty$ *one has*

$$\lim_{n\to\infty} -\frac{1}{\beta|\Lambda_n|} \log \mathcal{Z}(\beta, h|\tilde{\sigma})_{\Lambda_n} = \min_{m\in\mathbb{M}_r} \Psi_{\beta,h}(m), \tag{2.22}$$

where

$$\Psi_{\beta,h}(m) = -\frac{m_1^2}{2} - \sum_{i=1}^{r-1} h_i\, m_i \; - \frac{1}{\beta} S_r(L^{-1}(m)). \tag{2.23}$$

Proof. Introducing

$$m_1 = \frac{1}{|\Lambda|}\sum_{x\in\Lambda}\sigma(x), m_2 = \frac{1}{|\Lambda|}\sum_{x\in\Lambda}\sigma^2(x), \ldots, m_{r-1} = \frac{1}{|\Lambda|}\sum_{x\in\Lambda}\sigma^{r-1}(x), \tag{2.24}$$

and using $\mathbb{M}_{r,|\Lambda|}$ for the set of all such possible vectors $m = (m_1, m_2, \ldots, m_r)$, [2] we can rewrite the Hamiltonian

$$\mathcal{H}_h(\sigma)_\Lambda = -|\Lambda|\left(\frac{m_1^2}{2} + \sum_{i=1}^{r} h_i\, m_i\right) \tag{2.25}$$

and consequently, the partition function

$$\mathcal{Z} = \sum_{m\in\mathbb{M}_{r,|\Lambda|}} |\boldsymbol{\Omega}_m(\tilde{\sigma})_\Lambda|\, e^{-\beta|\Lambda|(-\frac{m_1^2}{2}+\sum_{i=1}^{r-1} h_i\, m_i)}. \tag{2.26}$$

Here,

$$\boldsymbol{\Omega}_m(\tilde{\sigma})_\Lambda = \left\{\sigma \in \boldsymbol{\Omega}(\tilde{\sigma})_\Lambda : \tfrac{1}{|\Lambda|}\textstyle\sum_{x\in\Lambda}\sigma^i(x) = m_i,\, i = 1, \ldots, r\right\}. \tag{2.27}$$

Before we compute $|\boldsymbol{\Omega}_m(\tilde{\sigma})_\Lambda|$, we notice that

$$|\Lambda| m_i = \sum_{x\in\Lambda}\sigma^i(x) = \sum_{j=1}^{r}(\omega_j)^i |\{x \in \Lambda : \sigma(x) = \omega_j\}| = \sum_{j=1}^{r} L_{ij} P_j, \tag{2.28}$$

[2] The coordinates m_i depend on Λ only through its volume $|\Lambda|$

where P_j is the number of ω_j's in Λ for the configuration σ. Hence, $P_j \in \{0, 1, \ldots, |\Lambda|\}$ and $\sum_{j=1}^{r} P_j = |\Lambda|$. If we define $p_j = \frac{1}{|\Lambda|} P_j$, then $(p_1, p_2, \ldots, p_r) \in \mathbb{P}_{r,|\Lambda|}$ and

$$\mathbb{M}_{r,|\Lambda|} = L(\mathbb{P}_{r,|\Lambda|}). \tag{2.29}$$

Now, let us assume that the restriction of L to $\mathbb{P}_r$ is a one to one map from $\mathbb{P}_r$ into $\mathbb{M}_r \overset{\text{df}}{=} L(\mathbb{P}_r)$. Then, for each $m \in \mathbb{M}_{r,|\Lambda|} \subset \mathbb{M}_r$ there is one and only one $p \in \mathbb{P}_{r,|\Lambda|}$ such that $m = L(p)$. Moreover, if we define

$$\mathbf{\Omega}^p(\tilde{\sigma})_\Lambda = \big\{\sigma \in \mathbf{\Omega}(\tilde{\sigma})_\Lambda : \, |\{x \in \Lambda : \ \sigma(x) = \omega_i\}| = |\Lambda| p_i, \, i = 1, \ldots, r\big\} \tag{2.30}$$

and consider (2.28), we find out that $\mathbf{\Omega}_m(\tilde{\sigma})_\Lambda = \mathbf{\Omega}^p(\tilde{\sigma})_\Lambda$. It is easy to observe that

$$|\mathbf{\Omega}^p(\tilde{\sigma})_\Lambda| = \frac{|\Lambda|!}{(|\Lambda| p_1)! \, (|\Lambda| p_2)! \, \ldots (|\Lambda| p_r)!} = e^{|\Lambda| S_{r,|\Lambda|}(p_1, p_2, \ldots, p_r)}. \tag{2.31}$$

With the help of equation above we can write down the partition function

$$\mathcal{Z}(\beta, h \,|\tilde{\sigma}) = \sum_{m \in \mathbb{M}_{r,|\Lambda|}} e^{-\beta |\Lambda| \Psi_{\beta,h}(m)_{|\Lambda|}}, \tag{2.32}$$

where

$$\Psi_{\beta,h}(m)_n \overset{\text{df}}{=} -\frac{m_1^2}{2} - \sum_{i=1}^{r-1} h_i m_i - \frac{1}{\beta} S_{r,n}(L^{-1}(m)). \tag{2.33}$$

Even though we cannot simplify $Z(\beta, h \,|\tilde{\sigma})_\Lambda$ any further, we are able to compute the limit free energy.

The summands in (2.32) are positive and we can use the maximal summand as lower bound and the maximal summand multiplied by the cardinality of he set $\mathbb{M}_{r,|\Lambda|}$ as the upper bound:

$$-\beta |\Lambda| \min_{m \in \mathbb{M}_{r,|\Lambda|}} \Psi_{\beta,h}(m)_{|\Lambda|} \leq \log \mathcal{Z}(\beta, h \,|\tilde{\sigma})_\Lambda \leq -\beta |\Lambda| \min_{m \in \mathbb{M}_{r,|\Lambda|}} \Psi_{\beta,h}(m)_{|\Lambda|} + \log |\mathbb{M}_{r,|\Lambda|}|. \tag{2.34}$$

Now, we recall lemma 3.3.2 and get

$$\min_{m \in \mathbb{M}_{r,n}} \Psi_{\beta,h}(m)_n \to \min_{m \in \mathbb{M}_r} \Psi_{\beta,h}(m) \quad \text{for} \quad n \to \infty. \tag{2.35}$$

Earlier in the proof, we assumed that L restricted to $\mathbb{P}_r$ is a one to one map into $L(\mathbb{P}_r)$. We use this fact once again:

$$|\mathbb{M}_{r,n}| = |L(\mathbb{P}_{r,n})| = |\mathbb{P}_{r,n}| \leq (n+1)^{r-1}. \tag{2.36}$$

In the last but one step we collect the previous (in)equalities for the sets Λ_n to produce the final claim

$$f(\beta, h \,|\tilde{\sigma}) = \lim_{n \to \infty} -\frac{1}{\beta |\Lambda_n|} \log Z(\beta, h, \,|\tilde{\sigma})_{\Lambda_n} = \min_{m \in \mathbb{M}_r} \Psi_{\beta,h}(m). \tag{2.37}$$

Finally, we show that L restricted to $\mathbb{P}_r$ is one to one. Let us define $\tilde{L}$: $\mathbb{R}^r \to \mathbb{R}^r$ given by the matrix

$$\tilde{L}_{ij} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ \omega_1 & \omega_2 & \dots & \omega_r \\ \omega_1^2 & \omega_2^2 & \dots & \omega_r^2 \\ \vdots & \vdots & \ddots & \vdots \\ \omega_1^{r-1} & \omega_2^{r-1} & \dots & \omega_r^{r-1} \end{pmatrix}. \tag{2.38}$$

This is the Vandermond matrix with a non-vanishing $\det(\tilde{L}) = \prod_{i<j}(\omega_j - \omega_i)$. This implies that $\tilde{L}$ is a one to one map $\mathbb{R}^d \to \mathbb{R}^d$ and the restriction $\tilde{L} \restriction_{\mathbb{P}_r}$ is then a one to one map $\mathbb{P}_r \to \tilde{L}(\mathbb{P}_r)$. Consequently, $x, y \in \mathbb{P}_r, x \neq y \Rightarrow \tilde{L}x \neq \tilde{L}y$. But from the definition of $\mathbb{P}_r$, it follows that $(\tilde{L}x)_1 = (\tilde{L}y)_1$. Hence, there must exist $j \in \{2, \dots, r\}$ such that $(\tilde{L}x)_j \neq (\tilde{L}y)_j$. Because $(Lx)_i = (\tilde{L}x)_{i+1}, i = 1, \dots, r-1$, it follows that $Lx \neq Ly$ and L $\mathbb{P}_r \to L(\mathbb{P}_r)$ is a one to one map. □

2.4 An equivalent model

In this section we introduce a slight modification or another point of view to the r-model. We start by discussing the sets $\mathbb{P}_{r,n}$ and $\mathbb{M}_{r,n}$.

To each configuration $\sigma \in \mathbf{\Omega}_\Lambda(\tilde{\sigma})$ we can assign a characteristic property $P = (P_1, P_2, \dots, P_r)$ bearing the information how many spins in Λ are equal to $(\omega_1, \omega_2, \dots, \omega_3)$. Another characteristic property of σ can be the "magnetization" $M = (M_1, M_1, \dots, M^{r-1})$ counting the "moments" of σ in Λ, $M_i = \sum_{x\in\Lambda} \tilde{\sigma}^i(x)$, $i = 1, \dots, r-1$. These two properties are equivalent and from (2.29) we know that $P = L(M)$.

We use this fact to transform the r-model which concerns M into another model, called a Spin r-model which concern P instead of M.

Definition 2.4.1 (Spin r-model) *Let $r \in \mathbb{N}$, $\tilde{h} \in \mathbb{R}^{r-1}$, $\Lambda \in \mathscr{P}_f(\mathbb{Z}^d)$, $\Omega_0 = \{\omega_1, \omega_2, \dots, \omega_r\} \subset \mathbb{R}^r$, $\mathbf{\Omega} = \Omega_0^{\mathbb{Z}^d}$, and $\sigma \in \mathbf{\Omega}$. We define*

$$\overline{H}_{\tilde{h}}(\sigma)_\Lambda = \frac{1}{4}\sum_{x\in\Lambda} \sum_{\substack{y\in\Lambda \\ |x-y|=1}} \big(\sigma(x) - \sigma(y)\big)^2 - \sum_{i=1}^{r-1} \tilde{h}_i |\{x \in \Lambda : \sigma(x) = \omega_i\}| + \frac{1}{2}\sum_{x\in\Lambda} \sum_{\substack{y\in\Lambda^c \\ |x-y|=1}} \big(\sigma(x) - \sigma(y)\big)^2. \tag{2.39}$$

Let us observe that

$$\overline{H}_{L^T(h)}(\sigma)_\Lambda = H_h^0(\sigma)_\Lambda, \tag{2.40}$$

where $L^T_{ij} = L_{ji}$. This tells us that these two models are completely equivalent, concerning the transformation between h and $\tilde{h}$ given by the map L^T.

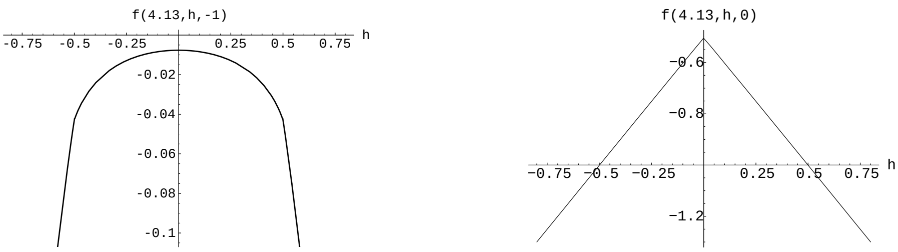

Figure 2.1: Profiles of the free energy of the Blume-Capel model for $\beta = 4.13$, $h \in [-0.8, 0.8]$, and $l \in \{-1, 0\}$

2.5 Mean-field phase diagram of Blume-Capel model

In the section before the last section we proved that the free energy of mean-field r-model equals to minimum of $\Psi_{\beta,h}$ over $\mathbb{M}_r$. Here, as a concrete illustration of this result for the (classical) Blume-Capel we show the function $\Psi_{\beta,h,l}$ $(h, l \in \mathbb{R})$, free energy $f(\beta, h, l)$, their relation to phase transitions and finally the phase diagram of the Blume-Capel model.

First of all, we introduce the notion of *phase transition.* We say that a model described by the free energy $f(\beta, h, l, \ldots)$ has a phase transition in the point of the parameters plain $h, l, \ldots$ if f is not an analytical function of these parameters at the concerned point. In particular, we say that there is a first-order phase transition if the first derivatives of f with respect to the parameters are not continuous.

This happens in the case of our mean-field Blume-Capel model. In Figure 2.1 we can see the profile of the free energy for the inverse temperature $\beta = 4.13$ and the values of the external field $l = -1, 0$ and $h \in [-0.8, 0.8]$. In the first one we can see that there is a phase transition near $h = \pm 0.5$ and in the other one for $h = 0$. In Figure 2.6 we plotted and numerically computed free energy $f(4.13, h, l)$.

Now, we take a look how phase transitions can be revealed directly from the function $\Psi_{\beta,h,l}$. For the sake of simplicity we illustrate this in the case of zero temperature (i.e. the limit $\beta \to \infty$). Figures 2.2 and 2.3 show the function $\Psi_{\beta,h,l}$ for several values of h and l. We can see that the external field h tilts the function up and lowers or raises the two local minima in $(m, w) = (1, 1)$ and $(m, w) = (-1, 1)$, while the external field w raises or lowers both of them and hence "preferring" or "punishing" the local minimum at $(m, w) = (0, 1)$. The three minima correspond to the three phases $\{-1, 0, 1\}$ which we have in the Blume-Capel. The global minimum chooses the "superior" phase presented in the model, while the coexistence of two or more minima determines the phase transition between the corresponding phases. Thus we can see, that for $h = 0$ and $l = -0.25$, there is a triple point. For nonzero temperature the graph of the function $\Psi_{\beta,h,l}$ deforms and becomes more complicated. However, there are still three local minima (for sufficiently small temperature, off course) which swap by the change of the external fields. In Figure 2.4 we plot the function $\Psi_{2.5,0,-0.25}$ for illustration.

Finally we present a schematic picture of the phase diagram for zero and one nonzero temperature in Figure 2.5. The areas separated by bold lines correspond to the regions with dominant phases -1, 0, or 1 and the lines themselves to the phase transitions among the phases. For zero temperature, there is a triple point at $h = 0$, $l = -0.5$. For nonzero temperature the phase transition curves move towards bigger values of l.

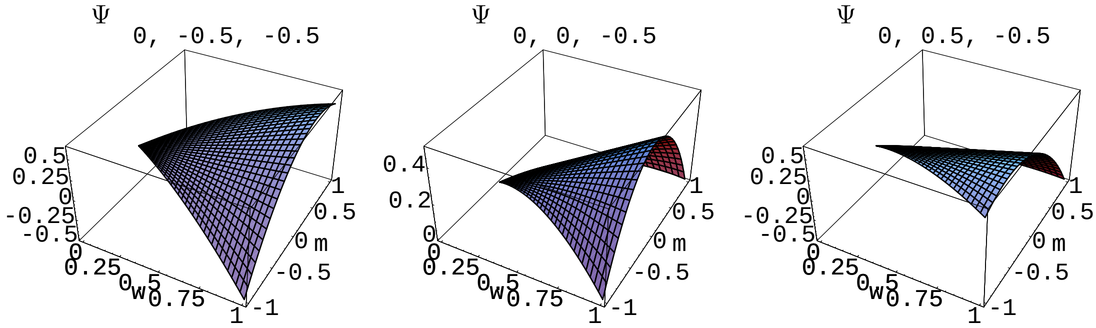

Figure 2.2: The function $\Psi_{\beta,h,l}$ for $l = -0.5$ and $h \in \{-0.5, 0, 0.5\}$.

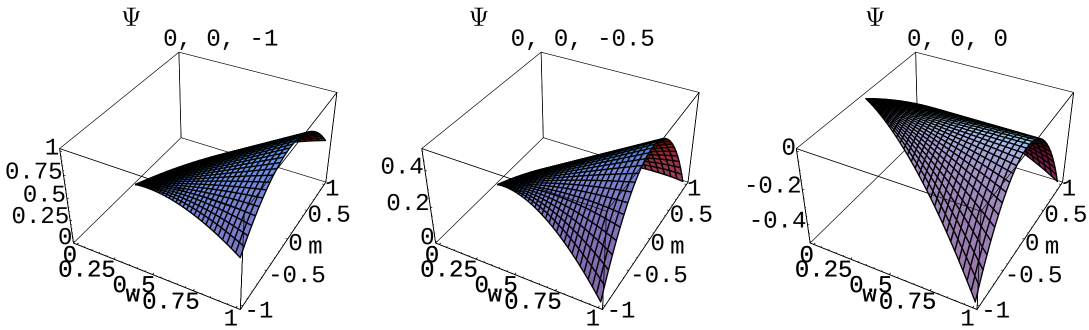

Figure 2.3: The function $\Psi_{\beta,h,l}$ for $h = 0$ and $l \in \{-1, -0.5, 0\}$.

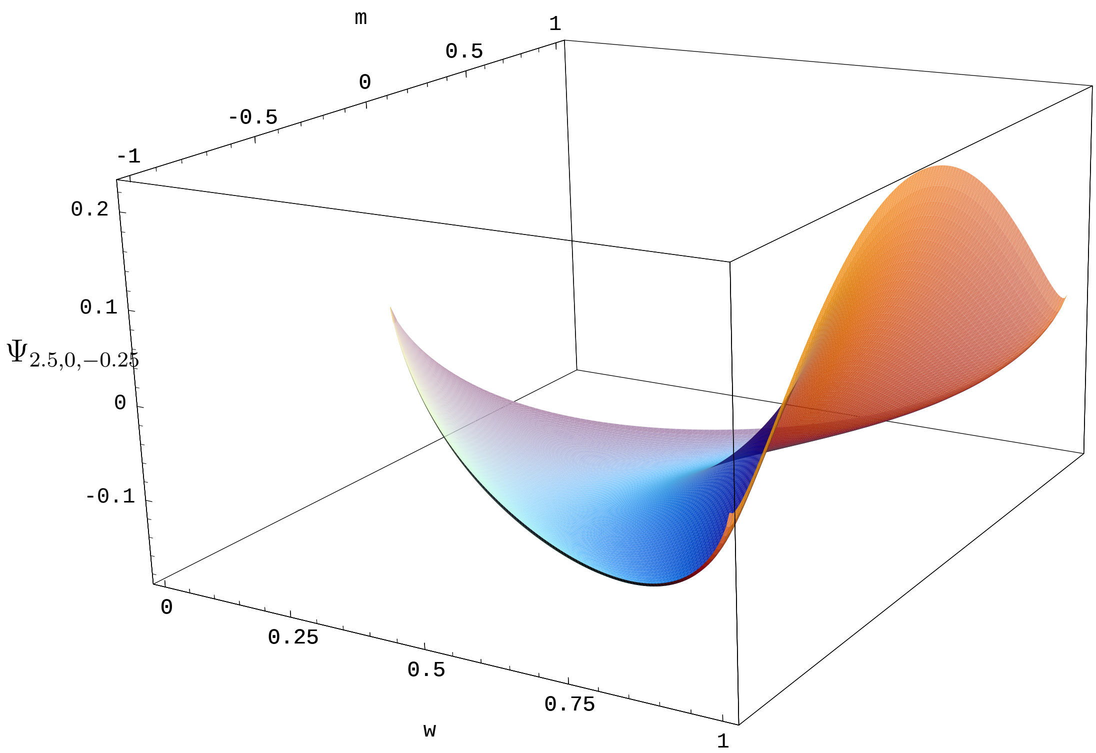

Figure 2.4: The function $\Psi_{2.5,0,-0.25}$

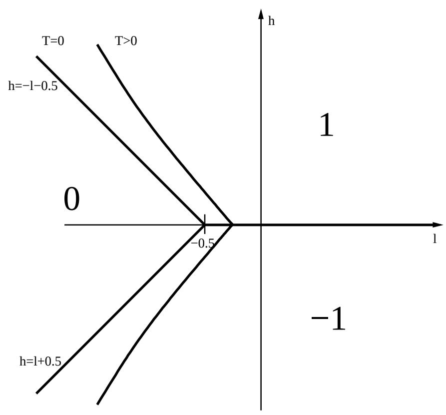

Figure 2.5: Phase diagram of the Blume-Capel model

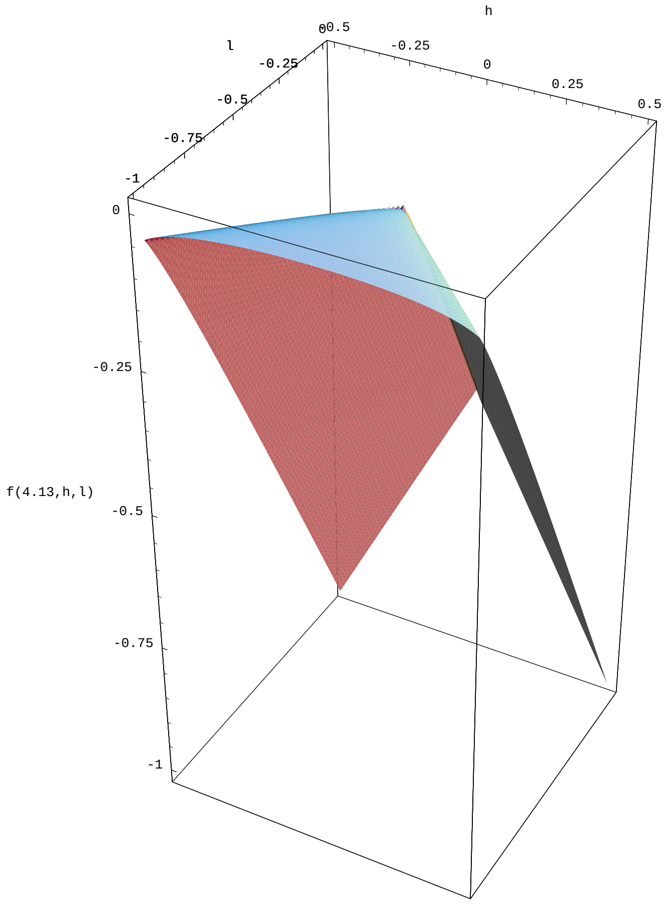

Figure 2.6: Free energy of the Blume-Capel model for $\beta = 4.13$, $h \in [-0.8, 0.8]$, $l \in [-1, 0]$

Chapter 3

Discrete entropy and its continuous approximation

In this chapter we present technical details concerning one part of the transition from discrete to continuous description. An important role is here played by the discrete entropy $S_{r,n}$ and a lot boils down to its estimate by the continuous entropy S_r defined bellow.

Definition 3.0.1 (Discrete entropy) *Let $r, n \in \mathbb{N}$, then we define the set*

$$\mathbb{P}_{r,n} = \left\{ p = (p_1, p_2, \ldots, p_r) : \; p_i \in \tfrac{1}{n}\{0, 1, \ldots, n\}, \; i = 1, 2, \ldots, r \;, \; \sum_{i=1}^{r} p_i = 1 \right\} \tag{3.1}$$

and the discrete entropy $S_{r,n} : \mathbb{P}_{r,n} \to \mathbb{R}$ by the formula

$$S_{r,n}(p_1, p_2, \ldots, p_r) = \frac{1}{n} \log \frac{n!}{(p_1 n)! \; (p_2 n)! \; \cdots \; (p_r n)!}. \tag{3.2}$$

Definition 3.0.2 (Continuous entropy) *Let $r \in \mathbb{N}$, then we define the continuous entropy $S_r : [0, 1]^r \to \mathbb{R}$*

$$S_r(p_1, p_2, \ldots, p_r) \stackrel{\text{df}}{=} \begin{cases} \sum_{i=1}^{r} -p_i \log p_i & 0 < p_i < 1, \; i = 1, .., r \\ 0 & \text{elsewhere.} \end{cases} \tag{3.3}$$

3.1 Stirling's formula

To get our desired estimate between the discrete and continuous entropy, we adopt the Stirling's formula from [Ro]. For the sake of this thesis we use $\mathbb{N}$ to denote the set of natural numbers excluding zero.

Theorem 3.1.1 (Stirling's formula) *Let $n \in \mathbb{N}$, then*

$$n! = \sqrt{2\pi n} \; n^n \; e^{-n} \; e^{r_n}, \tag{3.4}$$

where r_n satisfies double inequality $\frac{1}{12n+1} \leq r_n \leq \frac{1}{12n}$.

Lemma 3.1.2 *Let $r, n \in \mathbb{N}$, $r \geq 2$, $n \geq 8$, and $p = (p_1, p_2, \ldots, p_r) \in \mathbb{P}_{r,n}$, then*

$$|n\ S_{r,n}(p) - n\ S_r(p)| \leq r \log n \tag{3.5}$$

Proof. First let $p_i \neq 0$. Then we can simply plug Stirling's formula (3.4) into the definition of $S_{r,n}$ and we get

$$nS_{r,n}(p) = nS_r(p) - \frac{r-1}{2}\log 2\pi - \frac{1}{2}\sum_{i=1}^{r}\log p_i n + \frac{1}{2}\log n + r_n - \sum_{i=1}^{r} r_{p_i n}. \tag{3.6}$$

Then we use $|r_k| \leq \frac{1}{12k}$ and $|\log p_i n| \leq \log n$ to get

$$|nS_{r,n}(p) - nS_r(p)| \leq \frac{r-1}{2}\log 2\pi + \frac{r+1}{12} + \frac{r+1}{2}\log n. \tag{3.7}$$

For $n \geq 8$ we can use a more rough estimate $|nS_{r,n}(p) - nS_r(p)| \leq r \log n$, which is easier to handle.

Now if there are any $p_i = 0$, let us define $\tilde{r} = r - j$, where j is the number of p_i's which are zero. Then directly from the definition $S_{r,n}(p_1, p_2, \ldots, p_r) = S_{\tilde{r},n}(p_{i_1}, p_{i_2}, \ldots, p_{i_{\tilde{r}}})$, where we just omitted the zero variables. The same holds true for S_r. Thus we can use the estimates above and get $\tilde{r} \log n$ which is still smaller than $r \log n$. In the case when all but one p_i are zero, $S_{r,n}(p) = S_r(p) = 0$. □

Now we would like to say that the functions $S_{r,n}$ converge uniformly to S_r. To be able to talk about convergence, we have define them on the same set. It is natural to choose

$$\mathbb{P}_r \stackrel{\text{df}}{=} \{p \in [0,1]^r, \sum_{i=1}^{r} p_i = 1\} \tag{3.8}$$

and extend the definition of $S_{r,n}$ to $\mathbb{P}_r$. This can be done, off course, in many ways. For example, by taking gamma functions instead of factorials in the original definition. However, it will be useful to keep the range of $S_{r,n}$ to equal $S_{r,n}(\mathbb{P}_{r,n})$. For $p \in \mathbb{P}_r$ we define $S_{r,n}$ as a step function $S_{r,n}(p) = S_{r,n}(\kappa_{r,n}(p))$, where $\kappa_{r,n}$ is a map from $\mathbb{P}_r$ into $\mathbb{P}_{r,n}$ such that

$$|\kappa_{r,n}(p) - p| = \min_{q \in \mathbb{P}_{r,n}} |q - p|. \tag{3.9}$$

Here as well as in the further text $|q| = \max_{i \in \{1,\ldots,r\}} |q_i|$ is the ℓ^∞ norm from $\mathbb{R}^r$. In case, there are several q's minimizing the RHS above, we choose the smallest one in the lexicographic order. The important and easily verified property of the function $\kappa_{r,n}$ is that

$$|\kappa_{r,n}(p) - p| \leq \frac{1}{n}. \tag{3.10}$$

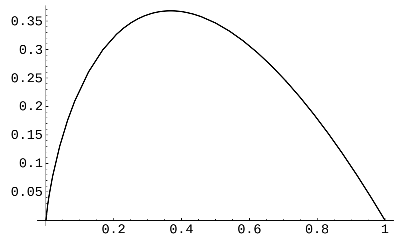

Figure 3.1: The function $\alpha(t) = -t \log t$.

3.2 Uniform bound

Now, let us pay attention to function $\alpha(t) = -t \log t, t \in [0,1], 0 \cdot \log 0 \stackrel{\text{df}}{=} 0$. The function $\alpha(\cdot)$ is continuous, concave and non-negative in the whole domain, differentiable in $(0,1)$, strictly increasing in $[0, \frac{1}{e}]$, and $\alpha'(\cdot)$ is strictly decreasing in $(0,1)$. Moreover, $S_r(p) = \sum_{i=1}^{r} \alpha(p_i)$.

Lemma 3.2.1 *Let $x, y \in [0,1]$, $|x-y| \leq a \leq \frac{1}{e}$, then $|\alpha(x) - \alpha(y)| \leq \alpha(a) = -a \log a$.*

Proof. Suppose $x < y$. We divide the proof into three cases: $a \leq x < y$, $x < a < y$, and $x < y \leq a$. In the first case there exist $\xi > a$ and $\tilde{\xi} \in (0,a)$ such that $|\alpha(y) - \alpha(x)| = \alpha'(\xi)|x-y| \leq \alpha'(\tilde{\xi})|x-y| = \alpha(a) - \alpha(0) = \alpha(a)$. This is due to the Lagrange mean value theorem and the property of α' that it is decreasing.

When $x < y \leq a \leq \frac{1}{e}$, then from the positivity of α and the monotonicity of α in $[0, \frac{1}{e}]$ we have $0 < \alpha(y) - \alpha(x) \leq \alpha(y) \leq \alpha(a)$.

In the last case $x < a < y$ we divide $[x,y]$ into $[x,a]$ and $[a,y]$. Then we use both of the previous ideas. First we take $|\alpha(y) - \alpha(a)| = \alpha'(\xi)|y-a| \leq \alpha'(\tilde{\xi})|(x-(y-a)) - x| = \alpha(x) - \alpha(x-y+a)$, where $x-y+a \geq 0$, $\xi \in (a,y)$, $\tilde{\xi} \in (x-y+a, x)$. Now simply using the triangle inequality we get $|\alpha(y) - \alpha(x)| \leq |\alpha(y) - \alpha(a)| + \alpha(a) - \alpha(x) \leq \alpha(a) - \alpha(x-y+a) \leq \alpha(a)$, which finishes the proof. □

A direct consequence of this lemma is that for $n \geq 3$ and $p, q \in [0,1]^r$ such that $|p-q| \leq \frac{1}{n}$ one has

$$|nS_r(p) - nS_r(q)| \leq r \log n. \tag{3.11}$$

Finally, we have

$$|nS_{r,n}(p) - nS_r(p)| \leq |nS_{r,n}\big(\kappa(p)\big) - nS_r\big(\kappa(p)\big)| + |nS_r\big(\kappa(p)\big) - nS_r(p)| \leq 2\,r \log n, \tag{3.12}$$

which gives us a uniform convergence $n \to \infty \Rightarrow S_{r,n} \rightrightarrows S_r$ on $\mathbb{P}_r$.

3.3 Exchanging limit and minimum in a sequence of functions

Lemma 3.3.1 *Let K be an arbitrary set and let $f : K \to \mathbb{R}$ be such that there exists $x_0 \in K$ satisfying*

$$f(x_0) = \min_{x \in K} f(x). \tag{3.13}$$

Further, let $\{f_n\}_{n=1}^{\infty}$ be a sequence of functions $f_n : K \to \mathbb{R}$ and let there exist a sequence of points $\{x_n\}_{n=1}^{\infty} \subset K$ such that

$$f_n(x_n) = \min_{x \in K} f_n(x). \tag{3.14}$$

If $f_n \rightrightarrows f$ then there exists the limit $\lim_{n\to\infty} f_n(x_n)$ and it equals $f(x_0)$.

Proof. We start with the upper bound. Uniform convergence implies point-wise convergence, $\forall \varepsilon > 0\ \exists n_1 \in \mathbb{N}\ : n > n_1 \Rightarrow f(x_0) > f_n(x_0) - \varepsilon \geq f_n(x_n) - \varepsilon$. The second inequality is a direct consequence of the assumption (3.14).

The lower bound will be obtained in a similar way. The only difference is that here we really need the uniform convergence. From $f_n \rightrightarrows f$ we have $\forall \varepsilon > 0\ \exists n_2 \in \mathbb{N}\ : n > n_2 \Rightarrow f_n(x_n) > f(x_n) - \varepsilon \geq f(x_0) - \varepsilon$. The second inequality is again a direct consequence of our assumption, this time (3.13). The claim is now obtained by setting $n_0 = \max\{n_1, n_2\}$. □

This lemma tells us that for reasonable sequences of functions we can swap the limit operation and the operation of taking the minimum. We will use it to prove the following useful lemma.

Lemma 3.3.2 *Let $r \in \mathbb{N}$. Then the following limit exists and*

$$\lim_{n\to\infty} \min_{p \in \mathbb{P}_{r,n}} -S_{r,n}(p) = \min_{p \in \mathbb{P}_r} -S_r(p) \tag{3.15}$$

Proof. For $r = 1$, we have $\mathbb{P}_{1,n} = \mathbb{P}_1 = \{1\}$ and $S_{1,n}(1) = S_1(1) = 0$. For $r \geq 2$ we use the fact that $\min_{p\in\mathbb{P}_{r,n}} -S_{r,n}(p) = \min_{p\in\mathbb{P}_r} -S_r(p)$. It follows from the definition of the extension of $S_{r,n}$ to $\mathbb{P}_r$. Further, we use the uniform convergence $-S_{r,n} \rightrightarrows -S_r$ on $\mathbb{P}_r$, combined with the previous lemma. □

Chapter 4

Lebowitz-Penrose theorem for the extended Blume-Capel model

In the second chapter we discussed the r-model in the case of the meanfield approximation and we showed that the free energy of the meanfield model is equal to the minimum of $\Psi_{\beta,h}$ over the compact set $\mathbb{M}_r$.

Now, we consider Kac r-models. These are models based on r-models but with slowly decaying and finite range interaction potentials. An interesting behaviour can be observed if we decrease the interaction strength while extending the range of interaction and simultaneously keeping the total energy per one site fixed. Then we will show that the free energy is as close as desired to the minimum of $\Psi_{\beta,h}$ over $\mathbb{M}_r$.

4.1 Kac potentials

Definition 4.1.1 (Kac potentials) *Let $J : \mathbb{R}^d \to \mathbb{R}$ be a twice differentiable real-valued function such that*

- *J is supported on the* unite ball *in $\mathbb{R}^d$,*[1] *i.e.* $|u| \geq 1 \Rightarrow J(u) = 0$
- $\int_{\mathbb{R}^d} J(u)du = 1$.

For $\gamma > 0$ we define the Kac potential $J_\gamma : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ setting

$$J_\gamma(u, v) \stackrel{\text{df}}{=} \gamma^d J\Big(\gamma\ (v - u)\Big).$$

Remark 4.1.2 *From the definition above we get*

[1] Since we consider consider the space $\mathbb{R}^d$ to be equipped with the ℓ^∞ norm $|u| = \max_{i\in\{1,\ldots,d\}}|u_i|$, the unit ball is actually the set $[-1, 1]^d$.

1. *translation invariance*
   $J_\gamma(u+t, v+t) = J_\gamma(u,v)$ *for all* $u, v, t \in \mathbb{R}^d$,

2. *normalization condition*
   $\int_{\mathbb{R}^d} J_\gamma(u,v)\,dv = \int_{\mathbb{R}^d} J(t)\,dt = 1$ *for all* $u \in \mathbb{R}^d$,

3. $J_\gamma(u,\cdot)$ *is supported on a ball with the center at* u *and a radius* γ.

Notice that the parameter γ controls both the strength and the range of the interaction.

Before we proceed, let us recall that configuration $\sigma \in \mathbf{\Omega}$ is a mapping $\mathbb{Z}^d \to \Omega_0 = \{\omega_1, \omega_2, \dots, \omega_r\}$. When computing the partition function, we always consider a finite $\Lambda \subset \mathbb{Z}^d$ and talk about configurations on Λ and boundary conditions on Λ^c. These are respectively restrictions of σ to Λ and $\tilde{\sigma}$ to Λ^c.

Now, we define the Kac r-models.

Definition 4.1.3 (Kac r-model Hamiltonian) *Let* $\gamma > 0$, $r \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, $\Lambda \in \mathscr{P}_f(\mathbb{Z}^d)$, *and* $\sigma \in \mathbf{\Omega}$. *The Hamiltonian of the Kac* r*-model with a parameter* γ *is defined by*

$$H_h(\sigma)_{\gamma,\Lambda} = -\frac{1}{2}\sum_{x\in\Lambda}\sum_{y\in\Lambda}\mathbb{I}_{x\neq y}J_\gamma(x,y)\sigma(x)\sigma(y) - \sum_{i=1}^{r-1} h_i \sum_{x\in\Lambda}\sigma^i(x) - \sum_{x\in\Lambda}\sum_{y\in\Lambda^c} J_\gamma(x,y)\sigma(x)\sigma(y), \quad (4.1)$$

where $\mathbb{I}_{x\neq y}$ is the characteristic function of the set $\{(x,y) \in \mathbb{R}^d \times \mathbb{R}^d : x \neq y\}$. For $\beta > 0$ and $\tilde{\sigma} \in \mathbf{\Omega}$ we have the partition function of the Kac r-model with boundary condition $\tilde{\sigma}$

$$Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda} = \sum_{\sigma\in\mathbf{\Omega}(\tilde{\sigma})_\Lambda} e^{-\beta H_h(\sigma)_{\gamma,\Lambda}}. \quad (4.2)$$

We will show, that in the limit $\gamma \to 0$, the free energy of the Kac r-model converges to the free energy of meanfield approximation. Such a statement is called the Lebowitz-Penrose theorem according to its original version for the Ising model.

Theorem 4.1.4 (The Lebowitz-Penrose theorem for the Kac r-model) *Let* $\beta > 0$, $r \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, $\tilde{\sigma} \in \mathbf{\Omega}$, *and* $\{\Lambda_n\}_{i=1}^\infty \subset \mathscr{P}_f(\mathbb{Z}^d)$ *be a van Hove sequence. Further, let* $\Psi_{\beta,h}$ *be the function defined in* (2.23) *and* $Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda}$ *be the partition function of the Kac* r*-model. Then*

$$\lim_{\gamma\to 0}\lim_{n\to\infty} -\frac{1}{\beta|\Lambda_n|}\log Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda_n} = \min_{m\in\mathbb{M}_r}\Psi_{\beta,h}(m). \quad (4.3)$$

The proof consist of several steps. First we introduce the free energy functional to approximate both the RHS and LHS of 4.3. Then we sketch the approximation steps and formulate theorems, each one in a stand-alone section. In the following section we will connect these two approximations together using the lower bound on the free energy functional and in the last section we complete the proof of the Lebowitz-Penrose theorem. Finally the next to last section is devoted to technical lemmas used throughout the proof.

4.2 Free energy functional

Introducing the free energy functional involves a transition form the lattice variables ($x, y \in \mathbb{Z}^d$) to real variables ($u, v \in \mathbb{R}^d$). We need a symbol to denote the subsets of $\mathbb{R}^d$, which would fulfil a similar role as the set $\Lambda \subset \mathbb{Z}^d$ in the lattice description. With a small abuse of notation we choose Λ for this purpose and from now on, if not explicitly specified otherwise, Λ will be a Borel subset of $\mathbb{R}^d$. Nevertheless, in the context of Hamiltonian $H(\sigma)_{\gamma,\Lambda}$, the partition function $Z(\beta, h \,|\, \tilde{\sigma})_{\gamma,\Lambda}$ and configuration space $\mathbf{\Omega}(\tilde{\sigma})_\Lambda$ we keep Λ which stands for $\Lambda \cap \mathbb{Z}^d$. We will strictly use $u, v \in \mathbb{R}^d$ and $x, y \in \mathbb{Z}^d$.

By introducing the free energy function we reach out from the microscopical scale of statistical mechanics to the mesoscopic sale of a continuous description. There a configuration at each point is considered to be a local average of underlying microscopical configurations and hence we get functions of real variables which can attain any (but usually we restrict to bounded) real values. More details are included in the last but one chapter in the context of the van der Waals theory. Here it suffices to say that the free energy functional will be defined on a suitable set of measurable functions:

Definition 4.2.1 *Let r and d be fixed positive integers. Then we define*

$$\mathcal{M} = \{\mathsf{m} : \mathbb{R}^d \to \mathbb{M}_r;\ \mathsf{m}_i \in L^\infty(\mathbb{R}^d), i = 1, \ldots, r-1\}. \tag{4.4}$$

Definition 4.2.2 (Energy, Entropy and Free energy functionals) *Let $\gamma, \beta > 0$, $h \in \mathbb{R}^{r-1}$, $\Lambda \subset \mathbb{R}^d$ be a Borel set with a finite Lebesgue measure. We introduce functionals $\mathcal{U}_h(\cdot)_{\gamma,\Lambda}$, $\mathcal{S}(\cdot)_{\gamma,\Lambda}$, and $\mathcal{F}_{\beta,h}(\cdot)_{\gamma,\Lambda}$: $\mathcal{M} \to \mathbb{R}$. They are defined, for any $\mathsf{m} \in \mathcal{M}$ as follows,*

Energy functional

$$\begin{aligned}\mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda} \stackrel{\text{df}}{=} & -\frac{1}{2}\int_\Lambda \int_\Lambda J_\gamma(u,v)\mathsf{m}_1(u)\mathsf{m}_1(v)dudv \\ & -\sum_{i=1}^{r-1} h_i \int_\Lambda \mathsf{m}_i(u)du - \int_\Lambda \int_{\Lambda^c} J_\gamma(u,v)\mathsf{m}_1(u)\mathsf{m}_1(v)dudv,\end{aligned} \tag{4.5}$$

Entropy functional

$$\mathcal{S}(\mathsf{m})_\Lambda \stackrel{\text{df}}{=} \int_\Lambda S_r(L^{-1}(\mathsf{m}(u)))du, \tag{4.6}$$

Free energy functional

$$\mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} \stackrel{\text{df}}{=} \mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda} - \frac{1}{\beta}\mathcal{S}(\mathsf{m})_{\Lambda}. \tag{4.7}$$

Now, let us point out the relation between $\mathcal{F}_{\beta,h}$ and $\Psi_{\beta,h}$.

Remark 4.2.3 (Relation between $\mathcal{F}_{\beta,h}$ and $\Psi_{\beta,h}$) *Let $\gamma, \beta > 0$, $h \in \mathbb{R}^{r-1}$, $\Lambda \subset \mathbb{R}^d$ be a Borel set with a finite Lebesgue measure, and $\mathsf{m} \in \mathcal{M}$. Then,*

$$\mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} = \int_\Lambda \Psi_{\beta,h}(\mathsf{m}(u))du + \frac{1}{4}\int_\Lambda\int_\Lambda J_\gamma(u,v)[\mathsf{m}_1(u) - \mathsf{m}_1(v)]^2 dvdu$$
$$+ \frac{1}{2}\int_\Lambda\int_{\Lambda^c} J_\gamma(u,v)[\mathsf{m}_1(u) - \mathsf{m}_1(v)]^2 dvdu - \frac{1}{2}\int_\Lambda\int_{\Lambda^c} J_\gamma(u,v)\mathsf{m}_1^2(v)dvdu. \tag{4.8}$$

Proof. Expanding $[\mathsf{m}_1(u) - \mathsf{m}_1(v)]^2$ on the RHS and using the Fubini theorem, we get

$$\int_\Lambda \Psi_{\beta,h}(\mathsf{m}(u))du + \frac{1}{2}\int_\Lambda \mathsf{m}_1^2(u)\int_\Lambda J_\gamma(u,v)dvdu$$
$$- \frac{1}{2}\int_\Lambda\int_\Lambda J_\gamma(u,v)\mathsf{m}_1(u)\mathsf{m}_1(v)dvdu - \int_\Lambda\int_{\Lambda^c} J_\gamma(u,v)\mathsf{m}_1(u)\mathsf{m}_1(v)dvdu$$
$$\frac{1}{2}\int_\Lambda \mathsf{m}_1^2(u)\int_{\Lambda^c} J_\gamma(u,v)dvdu + \frac{1}{2}\int_\Lambda\int_{\Lambda^c} J_\gamma(u,v)\mathsf{m}_1^2(v)dvdu$$
$$- \frac{1}{2}\int_\Lambda\int_{\Lambda^c} J_\gamma(u,v)\mathsf{m}_1^2(v)dvdu. \tag{4.9}$$

The last two terms cancel. The second term and first term on the third line produce $\frac{1}{2}\int_\Lambda \mathsf{m}_1^2(u)du$ which cancels the same term in $\int_\Lambda \Psi_{\beta,h}(\mathsf{m}(u))du$. Only terms containing the external fields and entropy survive and together with the second line it yields exactly the definition of $\mathcal{F}_{\beta,h}(\mathsf{m})$. □

The next definition is analogous to the definition of configuration space with boundary condition.

Definition 4.2.4 *Let $\tilde{\mathsf{m}} \in \mathcal{M}$ and Λ be a subset of $\mathbb{R}^d$. Then we define*

$$\mathcal{M}_\Lambda(\tilde{\mathsf{m}}) = \{\mathsf{m} \in \mathcal{M}; x \in \Lambda^c \Rightarrow \mathsf{m}(x) = \tilde{\mathsf{m}}(x)\}. \tag{4.10}$$

Now we approximate the RHS of (4.3) by the free energy functional.

Theorem 4.2.5 *Let $\gamma, \beta > 0$, $h \in \mathbb{R}^{r-1}$, $\tilde{\mathsf{m}} \in \mathcal{M}$, and let $\Lambda \subset \mathbb{R}^d$ be a cube with the length of the edge $\sqrt[d]{|\Lambda|} \geq 2\gamma^{-1}$. Then,*

$$\left| \inf_{\mathsf{m}\in\mathcal{M}_\Lambda(\tilde{\mathsf{m}})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} - |\Lambda| \min_{m\in\mathbb{M}_r} \Psi_{\beta,h}(m) \right| \leq 2\,\|L\|^2\,\gamma^{-1}\,|\partial\Lambda|. \tag{4.11}$$

Proof. Let $\mathsf{m} \in \mathcal{M}_\Lambda(\tilde{\mathsf{m}})$. We will use the evaluation of $\mathcal{F}_{\beta,h}$ via the function $\Psi_{\beta,h}$ from the previous remark. Denoting $I = \int_\Lambda \int_{\Lambda^c} J_\gamma(u,v)dudv$, we get

$$\mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} \geq \min_{m\in\mathbb{M}_r} \Psi_{\beta,h}(m)|\Lambda| - \frac{1}{2}\|L\|^2 I, \tag{4.12}$$

$$\mathcal{F}_{\beta,h}(\mathsf{m}^*)_{\gamma,\Lambda} \leq \min_{m\in\mathbb{M}_r} \Psi_{\beta,h}(m)|\Lambda| + 2\|L\|^2 I, \tag{4.13}$$

where $m^* \in \mathbb{M}_r$ is any minimizer of $\Psi_{\beta,h}$ and $\mathsf{m}^*(u) = m^*$ for $u \in \Lambda$, $\mathsf{m}^*(u) = \tilde{\mathsf{m}}(u)$ for $u \in \Lambda^c$. Finally, if the length of the edge of Λ is bigger than $2\gamma^{-1}$ we have

$$I = \int_\Lambda \int_{\Lambda^c} J_\gamma(u,v)dudv \leq \gamma^{-1}|\partial\Lambda|, \tag{4.14}$$

which is easy to verify. □

4.3 Coarse graining

Our aim in this section will be to approximate $\log Z$ on the LHS of (4.3) by the free energy functional. As a preparatory step we will discuss the coarse graining procedure. Before we do so, we introduce several notions.

Definition 4.3.1 (Elementary ℓ-cube) *Let $\ell \in \mathbb{N}$ and $x \in (\ell \cdot \mathbb{Z})^d$, then*

$$C_x^{(\ell)} \stackrel{\text{df}}{=} \left\{ u \in \mathbb{R}^d, x_j \leq u_j < x_j + \ell, j = 1, \ldots, d \right\} \tag{4.15}$$

For $u \in \mathbb{R}^d$ we define

$$C_u^{(\ell)} \stackrel{\text{df}}{=} C_{\lfloor \frac{u}{\ell} \rfloor \ell}^{(\ell)}, \tag{4.16}$$

where $\lfloor u_i \rfloor$ is the lower integer part of u_i and $\lfloor u \rfloor = (\lfloor u_1 \rfloor, \lfloor u_2 \rfloor, \ldots, \lfloor u_d \rfloor)$.

An ℓ-cube will be a union of elementary ℓ-cubes which form a cube in the usual meaning.

Definition 4.3.2 (ℓ-cube) *We say that a cube $\Lambda \subset \mathbb{R}^d$ is an ℓ-cube, if there exists $\mathcal{A} \subset (\ell \cdot \mathbb{Z})^d$ such that*

$$\Lambda = \bigcup_{x\in\mathcal{A}} C_x^{(\ell)}. \tag{4.17}$$

Then, off course, $\mathcal{A} = \Lambda \cap (\ell \cdot \mathbb{Z})^d$.

Definition 4.3.3 (Coarse graining operation) *Let Λ be an ℓ-cube and $f : \mathbb{Z}^d \to \mathbb{R}$. We define the coarse-grained function $f^{(\ell)} : \mathbb{R}^d \to \mathbb{R}$ by*

$$f^{(\ell)}(u) \stackrel{\text{df}}{=} \frac{1}{|C_u^{(\ell)}|} \sum_{x\in C_u^{(\ell)}\cap\mathbb{Z}^d} f(x). \tag{4.18}$$

For a vector function $f = (f_1, f_2, \ldots, f_r) : \mathbb{Z}^d \to \mathbb{R}^r$ we put

$$f^{(\ell)}(u) \stackrel{\text{df}}{=} (f_1^{(\ell)}, f_2^{(\ell)}, \ldots, f_r^{(\ell)})\,(u). \tag{4.19}$$

A direct consequence of this definition is the fact that the function $f^{(\ell)}$ is defined on $\mathbb{R}^d$ and it is constant on every elementary ℓ-cube. We will use this property very often when computing the estimates of $|f - f^{(\ell)}|$ or when replacing sums over ℓ-cubes by an integral $\sum_{x \in \Lambda \cap (\ell \cdot \mathbb{Z})^d} f(x) = \int_\Lambda f^{(\ell)}(u) du$. [2]

Definition 4.3.4 (Set of coarse grained configurations) *Let $\ell \in \mathbb{N}$, Λ be an ℓ-cube, and $\tilde{\sigma} \in \boldsymbol{\Omega}$. Then we define*

$$\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma}) = \{\mathsf{m} : \mathbb{R}^d \to \mathbb{M}_{r,\ell^d},\ \mathsf{m} \text{ constant on each elementary } \ell\text{-cube}, \\ u \in \Lambda^c \Rightarrow \mathsf{m}(u) = (\tilde{\sigma}, \tilde{\sigma}^2, \dots, \tilde{\sigma}^{r-1})^{(\ell)}(u)\}. \quad (4.20)$$

The set $\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$ is simply an image of the set $\{(\sigma, \sigma^2, \dots, \sigma^{r-1}) : \sigma \in \boldsymbol{\Omega}(\tilde{\sigma})_\Lambda\}$ under the coarse graining operation. We use this fact and split $\boldsymbol{\Omega}(\tilde{\sigma})_\Lambda$ into classes of equivalence according to the functions from $\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$.

Definition 4.3.5 *Let $\ell \in \mathbb{N}$, Λ be an ℓ-cube, $\tilde{\sigma} \in \boldsymbol{\Omega}$, and $\mathsf{m} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$. Then we define*

$$\boldsymbol{\Omega}_{\mathsf{m}}^{(\ell)}(\tilde{\sigma})_\Lambda = \left\{\sigma \in \boldsymbol{\Omega}(\tilde{\sigma})_\Lambda : (\sigma, \sigma^2, \dots, \sigma^{r-1})^{(\ell)} = \mathsf{m}\right\}. \quad (4.21)$$

Now, we can rewrite the partition function

$$Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda} = \sum_{\mathsf{m} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \sum_{\sigma \in \boldsymbol{\Omega}_{\mathsf{m}}^{(\ell)}(\tilde{\sigma})_\Lambda} e^{-\beta H_h(\sigma)_{\gamma,\Lambda}}. \quad (4.22)$$

For a fixed $\mathsf{m} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$, we approximate $H_h(\sigma)_{\gamma,\Lambda}$ by $\mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda}$ and, consequently, the second sum by $|\boldsymbol{\Omega}_{\mathsf{m}}^{(\ell)}(\tilde{\sigma})_\Lambda| e^{-\beta \mathcal{U}(\mathsf{m})_{\gamma,\Lambda}}$.

The cardinality of the set above can be evaluated in terms of the finite volume entropy S_{r,ℓ^d}: [3]

$$\log |\boldsymbol{\Omega}_{\mathsf{m}}^{(\ell)}(\tilde{\sigma})_\Lambda| = \sum_{x \in \Lambda \cap \mathbb{Z}^d} \ell^d S_{r,\ell^d}\big(L^{-1}\mathsf{m}(x\,\ell)\big) = \int_\Lambda \mathcal{S}_{r,\ell^d}\big(L^{-1}\mathsf{m}(u)\big)\, du. \quad (4.23)$$

This can be further approximated by $\mathcal{S}(\mathsf{m})_{\gamma,\Lambda}$. Putting these two approximations together, we get

$$Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda} \sim \sum_{\mathsf{m} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} e^{-\beta \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda}}. \quad (4.24)$$

The sum on the RHS consists of non negative numbers. Thus we can bound it from below by the maximal summand and from above by the maximal summand

[2] This holds true also for the coarse graining from Definition 4.4.1.

[3] Likewise in (2.31).

multiplied by the cardinality of the set we sum over. Then we take logarithm of both sides and divide them by $\beta|\Lambda|$. We write down the upper bound

$$\frac{1}{\beta|\Lambda|}\log Z(\beta,h\,|\tilde{\sigma})_{\gamma,\Lambda} \lesssim -\min_{\mathsf{m}\in\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \frac{1}{|\Lambda|}\mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} + \frac{\log|\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})|}{|\Lambda|}. \tag{4.25}$$

The lower bound is simply $-\min_{\mathsf{m}\in\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \frac{1}{|\Lambda|}\mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda}$ and to get our desired estimate

$$\frac{1}{\beta|\Lambda|}\log Z(\beta,h\,|\tilde{\sigma})_{\gamma,\Lambda} \sim -\min_{\mathsf{m}\in\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \frac{1}{|\Lambda|}\mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda}, \tag{4.26}$$

we only need to show that $\frac{\log|\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})|}{|\Lambda|} \to 0$. To be precise, we formulate the second theorem of this chapter.

Theorem 4.3.6 *Let $\gamma \in (0,1)$, $\ell \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, Λ be an ℓ-cube, and $\tilde{\sigma} \in \mathbf{\Omega}$. If $2\,\ell \le \gamma^{-1}$, then there exists a constant $C(d,\Omega_0,|J|_\infty,|\nabla J|_\infty) \in \mathbb{R}$ such that*

$$\Big|\min_{\mathsf{m}\in\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} + \frac{1}{\beta}\log Z(\beta,h\,|\tilde{\sigma})_{\gamma,\Lambda}\Big| \le \varepsilon_\beta(\gamma,\ell)\ |\Lambda|, \tag{4.27}$$

$$\varepsilon_\beta(\gamma,\ell) = C\,\gamma\,\ell + \frac{r}{\beta}\frac{\log \ell^d}{\ell^d} + (r-1)\frac{\log(\ell^d+1)}{\ell^d}. \tag{4.28}$$

Proof. The proof has been sketched above the theorem and its intrinsic idea is the same as in the proof of the Theorem 2.3.2 (meanfield). We want to replace the sum over $\mathbf{\Omega}(\tilde{\sigma})_\Lambda$ (which grows exponentially with $|\Lambda|$: $|\mathbf{\Omega}(\tilde{\sigma})_\Lambda| = |\Omega_0|^{|\Lambda|}$) with a sum over a set which grows slower with the volume of Λ. Slower in the sense that the logarithm of the set divided by $|\Lambda|$ tends to zero for $|\Lambda| \to \infty$ (for example polynomial growth). Because the summands in partition function are non negative, we can take the lower bound of the sum to be the the maximal summand and the upper bound to be the maximal summand multiplied by the cardinality of the set we sum over. Finally we take a logarithm of the bounds divided by $|\Lambda_n|$ and let $|\Lambda_n| \to \infty$. The limit free energy is then simply a logarithm of the limit of the maximal summands.

In the meanfield case we were able to find the set discussed above. Namely, the set $\mathbb{M}_{r,|\Lambda|}$. The Hamiltonian was constant on $\mathbf{\Omega}_m(\tilde{\sigma})_\Lambda$'s which formed a disjoint decomposition $\mathbf{\Omega}(\tilde{\sigma})_\Lambda = \dot{\bigcup}_{m\in\mathbb{M}_{r,|\Lambda|}} \mathbf{\Omega}_m(\tilde{\sigma})_\Lambda$, and provided us with the equation (2.26). Then everything went smoothly according to the schema above.

Here the situation is more complicated. We don't have such a decomposition of $\mathbf{\Omega}(\tilde{\sigma})_\Lambda$ where the Kac r-model Hamiltonian would be constant. However, we will artificially create one. We achieve that by coarse graining $\mathbf{\Omega}(\tilde{\sigma})_\Lambda$ and replacing the Hamiltonian with energy functional. First we define equivalence "$\sim$" on $\mathbf{\Omega}(\tilde{\sigma})_\Lambda$:

$$\sigma,\overline{\sigma} \in \mathbf{\Omega}(\tilde{\sigma})_\Lambda,\ \sigma \sim \overline{\sigma}\ \textit{if}\ \sigma^{(\ell)} = \overline{\sigma}^{(\ell)}. \tag{4.29}$$

Then the set $\mathbf{\Omega}(\tilde{\sigma})_\Lambda$ splits up into classes of equivalence $\mathbf{\Omega}^{(\ell)}_{\mathsf{m}}(\tilde{\sigma})_\Lambda$, where $\mathsf{m} \in \mathcal{M}^{(\ell)}_\Lambda(\tilde{\sigma})$. The set $\mathcal{M}^{(\ell)}_\Lambda(\tilde{\sigma})$ will play the the same role $\mathbb{M}_{r,|\Lambda|}$ did in the meanfield case. For any $\ell \in \mathbb{N}$ we have

$$\mathbf{\Omega}(\tilde{\sigma})_\Lambda = \dot{\bigcup}_{\mathsf{m}\in\mathcal{M}^{(\ell)}_\Lambda(\tilde{\sigma})} \mathbf{\Omega}^{(\ell)}_{\mathsf{m}}(\tilde{\sigma})_\Lambda. \tag{4.30}$$

Using this decomposition, we split the partition sum over $\mathbf{\Omega}(\tilde{\sigma})_\Lambda$ into the double sum (4.22). Within $\mathbf{\Omega}^{(\ell)}_{\mathsf{m}}(\tilde{\sigma})_\Lambda$ we perform coarse graining and replace $H_h(\sigma)_{\gamma,\Lambda}$ by $\mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda}$. In order to do so, we have to be able to control their difference. For $\sigma \in \mathbf{\Omega}^{(\ell)}_{\mathsf{m}}(\tilde{\sigma})$, $\gamma \in (0,1)$, and $2\,\ell \le \gamma^{-1}$ we get the bound

$$|H_h(\sigma)_{\gamma,\Lambda} - \mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda}| \le C\,\gamma\,\ell\,|\Lambda| \tag{4.31}$$

from the Lemma 4.5.1. So far we suppressed one significant fact. The set $\mathcal{M}^{(\ell)}_\Lambda(\tilde{\sigma})$ grows exponentially with $|\Lambda|$. This is the point where the difference between the Kac and meanfield r-models arises and the coarse graining parameter ℓ comes into play. We are able to estimate $|\mathcal{M}^{(\ell)}_\Lambda(\tilde{\sigma})|$ from above with $\left[(\ell^d+1)^{r-1}\right]^{\frac{|\Lambda|}{\ell^d}}$ which yields $\frac{1}{|\Lambda|}\log|\mathcal{M}^{(\ell)}_\Lambda(\tilde{\sigma})| \le \frac{r-1}{\ell^d+1}$. To make the error from (4.25) to vanish we have to take the limit $\ell \to \infty$. This is one of the reasons why we do not get the expression for the free energy of the Kac r-model for finite γ, but after taking its limit to zero. The parameter ℓ will be later linked up with γ and for $\gamma \to 0$ it will tend to infinity.

The only thing we have to do now, to make the procedure above the theorem to be correct, is to write down carefully inequalities instead of $\sim$. Two of them we already provided. The last one comes from the Lemma 3.1.2:

$$\Big|\int_\Lambda S_{r,\ell^d}\Big(L^{-1}\big(\mathsf{m}(u)\big)\Big)du - \mathcal{S}(\mathsf{m})\Big| \le r\frac{\log \ell^d}{\ell^d}. \tag{4.32}$$

Finally, putting the three estimates together finishes the proof. □

The theorem 4.3.6 is not only important as one of the main parts of the proof of the Lebowitz-Penrose theorem. Moreover, it is a key step in the transition from the lattice description based on the partition function to the continuous description based on the free energy functional and a variational principle to look for its minimum. Here we considered only a finite set of *test functions* $\mathsf{m} \in \mathcal{M}^{(\ell)}_\Lambda(\tilde{\sigma})$. In the following section, as another part of the proof, we show that we can extend the test space to the whole *continuous configuration space* $\mathcal{M}_\Lambda(\tilde{\mathsf{m}})$ with a suitable choice of the boundary condition $\tilde{\mathsf{m}} \in \mathcal{M}$.

4.4 The lower bound on free energy functional

In the previous two sections we expressed the LHS and RHS of (4.3) in terms of the free energy functional. In the first case we used the infimum of $\mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda}$ over

$\mathcal{M}_\Lambda(\tilde{\mathsf{m}})$ and in the other one its minimum over $\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$. Notice especially, that in the equation (4.11) we can arbitrarily choose the "boundary condition" $\tilde{\mathsf{m}} \in \mathcal{M}$.

If we want to prove the Lebowitz-Penrose theorem, we are likely to find inequalities between the infimum and the minimum of the free energy functional. We choose $\tilde{\mathsf{m}} = (\tilde{\sigma}, \tilde{\sigma}^2, \ldots, \tilde{\sigma}^{r-1})^{(\ell)}$. Then the functions from $\mathcal{M}_\Lambda(\tilde{\mathsf{m}})$ and $\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$ differ only inside Λ and directly from the definitions we get $\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma}) \subset \mathcal{M}_\Lambda(\tilde{\mathsf{m}})$ for any $\ell \in \mathbb{N}$. This implies

$$\inf_{\mathsf{m} \in \mathcal{M}_\Lambda(\tilde{\mathsf{m}})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} \leq \min_{\mathsf{m} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda}. \tag{4.33}$$

The opposite inequality does not generally hold for finite ℓ and we will look for its approximation. First we construct a map π^ℓ from $\mathcal{M}_\Lambda(\tilde{\mathsf{m}})$ to $\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$ and find an estimate of the form

$$\mathcal{F}_{\beta,h}\big(\pi_\ell(\mathsf{m})\big)_{\gamma,\Lambda} \leq \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} + \text{error} \tag{4.34}$$

Then by taking infimum of the inequality over $\mathcal{M}_\Lambda(\tilde{\mathsf{m}})$ we get our desired relation

$$\min_{\mathsf{m} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} \leq \inf_{\mathsf{m} \in \mathcal{M}_\Lambda(\tilde{\mathsf{m}})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} + \text{error} \tag{4.35}$$

with an error term that vanishes in the limit $\gamma \to 0$.

Let us begin with the construction of π_ℓ. The first step will be the coarse graining of the set $\mathcal{M}_\Lambda(\tilde{\mathsf{m}})$. It is an analog to the Definition 4.3.3.

Definition 4.4.1 (Coarse graining) *Let $f : \mathbb{R}^d \to \mathbb{R}$, $f \in L^\infty(\mathbb{R}^d)$. We define the coarse grained function $f^{(\ell)} \in L^\infty(\mathbb{R}^d)$:*

$$f^{(\ell)}(u) \stackrel{\text{df}}{=} \frac{1}{|C_u^{(\ell)}|} \int_{C_u^{(\ell)}} f(v)dv. \tag{4.36}$$

For a vector function $f = (f_1, f_2, \ldots, f_r) : \mathbb{R}^d \to \mathbb{R}^r$, $f_i \in L^\infty(\mathbb{R}^d)$, $i = 1, \ldots, r$

$$f^{(\ell)}(u) \stackrel{\text{df}}{=} (f_1^{(\ell)}, f_2^{(\ell)}, \ldots, f_r^{(\ell)})\,(u). \tag{4.37}$$

And finally, for functions $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, $f \in L^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ we define

$$f^{(\ell)}(u,v) \stackrel{\text{df}}{=} \frac{1}{|C_u^{(\ell)}|} \frac{1}{|C_v^{(\ell)}|} \int_{C_u^{(\ell)}} \int_{C_v^{(\ell)}} f(\tilde{u}, \tilde{v}) d\tilde{v} d\tilde{u}. \tag{4.38}$$

The last definition will be used in Section 4.5 for *coarse graining of* the *Kac potential* $J_\gamma(\cdot,\cdot)$.

After coarse graining we get functions which are constant on elementary ℓ-cubes, but they can still take any values from $\mathbb{M}_r$. We need them to attain values only from $\mathbb{M}_{r,\ell^d}$. In the equation (3.9) we introduced the map $\kappa_{r,n} : \mathbb{P}_r \to \mathbb{P}_{r,n}$. Recall that $\mathbb{M}_r = L(\mathbb{P}_r)$ and $\mathbb{M}_{r,n} = L(\mathbb{P}_{r,n})$. This offers us a straightforward way how to construct the map $(\,\cdot\,)^{[n]} : \mathbb{M}_r \to \mathbb{M}_{r,n}$:

$$(\,\cdot\,)^{[n]} \stackrel{\text{df}}{=} L \circ \kappa_{r,n} \circ L^{-1}. \tag{4.39}$$

For functions we define $(\cdot)^{[n]}$ point wise, i.e. $\mathsf{m}^{[n]}(u) = \mathsf{m}(u)^{[n]}$. From the property (3.10) of $\kappa_{r,n}$ we get a uniform bound

$$|m^{[n]} - m| \leq ||L||\; |\kappa_{r,n}(L^{-1}m) - L^{-1}m| \leq \frac{||L||}{n}. \tag{4.40}$$

Now we have two maps $(\,\cdot\,)^{(\ell)}$ and $(\,\cdot\,)^{[n]}$ that can be applied on functions from $\mathcal{M}$. The map $(\,\cdot\,)^{(\ell)}$ produces functions constant on ℓ-cubes and the other one changes their range to $\mathbb{M}_{r,n}$. We join them together to get our desired map $\pi^\ell :\ \mathcal{M}_\Lambda(\tilde{\mathsf{m}}) \to \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$, $\pi^\ell(\,\cdot\,) \stackrel{\text{df}}{=} (\,\cdot\,)^{(\ell)[\ell^d]}$. To make this definition correct we have to make sure that that the range of $\mathsf{m}^{(\ell)}$ is $\mathbb{M}_r$. This will be shown in the proof of the following remark.

Remark 4.4.2 *Let $\gamma, \beta > 0$, $\ell \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, Λ be an ℓ-cube, $\tilde{\sigma} \in \mathbf{\Omega}$, and $\tilde{\mathsf{m}} = (\tilde{\sigma}, \tilde{\sigma}^2, \ldots, \tilde{\sigma}^{r-1})^{(\ell)}$. If $\ell^d \geq e\,\|L\|$ and $2\,\ell \leq \gamma^{-1}$ then there exists a constant $K(d, \Omega_0, |\nabla J|_\infty) \in \mathbb{R}$ such that*

$$\Big| \min_{\mathsf{m}\in\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} - \inf_{\mathsf{m}\in\mathcal{M}_\Lambda(\tilde{\mathsf{m}})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} \Big| \leq \tilde{\varepsilon}_{\beta,h}(\gamma, \ell, \ell^d)|\Lambda|, \tag{4.41}$$

$$\tilde{\varepsilon}_{\beta,h}(\gamma, \ell, n) = K\,\gamma\,\ell + \frac{\|L\|}{n}\Big(3\,\|L\| + \sum_{i=1}^{r-1} |h_i| + \frac{r}{\beta} \log \frac{n}{\|L\|}\Big). \tag{4.42}$$

This remark is a simple corollary of the equation (4.33), the paragraph above and the Theorem 4.4.3.

Proof. First of all, we make sure that for $\mathsf{m} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\mathsf{m}})$ also $\mathsf{m}^{(\ell)} \in \mathcal{M}_\Lambda(\tilde{\mathsf{m}})$. This is easy to verify, because outside Λ the function doesn't change at all and inside Λ we only have to make sure that $\mathsf{m}^{(\ell)}(u) \in \mathbb{M}_r$ which is equivalent to $L^{-1}\mathsf{m}^{(\ell)}(u) \in \mathbb{P}_r$. But we have

$$L_{ij}^{-1}\mathsf{m}_j^{(\ell)}(u) = L_{ij}^{-1}\frac{1}{|C_u^{(\ell)}|}\int_{C_u^{(\ell)}} \mathsf{m}_j(v)dv = \frac{1}{|C_u^{(\ell)}|}\int_{C_u^{(\ell)}} L_{ij}^{-1}\mathsf{m}_j(v)dv\,, \tag{4.43}$$

$$L_{ij}^{-1}\mathsf{m}_j(u) \in [0,1] \Rightarrow \frac{1}{|C_u^{(\ell)}|}\int_{C_u^{(\ell)}} L_{ij}^{-1}\mathsf{m}_j(v)dv \in [0,1], \tag{4.44}$$

$$\sum_{i=1}^{r} L_{ij}^{-1}\mathsf{m}_j^{(\ell)}(u) = \frac{1}{|C_u^{(\ell)}|}\int_{C_u^{(\ell)}} \sum_{i=1}^{r} L_{ij}^{-1}\mathsf{m}_j(v)dv = 1, \tag{4.45}$$

which implies $L^{-1}\mathsf{m}^{(\ell)}(u) \in \mathbb{P}_r$.

Because $\mathsf{m}^{(\ell)} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\mathsf{m}})$ we can apply the map $(\cdot)^{[\ell^d]}$ on it and from the Theorem 4.4.3 we get

$$\mathcal{F}_{\beta,h}(\mathsf{m}^{(\ell)[\ell^d]})_{\gamma,\Lambda} \le \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} + \tilde{\varepsilon}_{\beta,h}(\gamma,\ell,\ell^d)|\Lambda|. \tag{4.46}$$

Moreover, $\mathsf{m}^{(\ell)[\ell^d]} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$ and by taking infimum of the previous inequality over $\mathcal{M}_\Lambda(\tilde{\mathsf{m}})$ we get

$$\min_{\mathsf{m}\in\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} \le \inf_{\mathsf{m}\in\mathcal{M}_\Lambda(\tilde{\mathsf{m}})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} + \tilde{\varepsilon}_{\beta,h}(\gamma,\ell,\ell^d)|\Lambda|. \tag{4.47}$$

To complete the proof we recall the equation 4.33. □

Theorem 4.4.3 (Lower bound of the free energy functional) *Let $\gamma, \beta > 0$, $n, \ell \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, Λ be an ℓ-cube, and $\mathsf{m} \in \mathcal{M}$. If $n \ge e\,\|L\|$ and $2\,\ell \le \gamma^{-1}$ then there exists a constant $K(d, \Omega_0, |\nabla J|_\infty) \in \mathbb{R}$ such that*

$$\mathcal{F}_{\beta,h}(\mathsf{m}^{(\ell)[n]})_{\gamma,\Lambda} \le \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} + \tilde{\varepsilon}_{\beta,h}(\gamma,\ell,n)|\Lambda|, \tag{4.48}$$

$$\tilde{\varepsilon}_{\beta,h}(\gamma,\ell,n) = K\,\gamma\,\ell + \frac{\|L\|}{n}\Big(3\,\|L\| + \sum_{i=1}^{r-1}|h_i| + \frac{r}{\beta}\log\frac{n}{\|L\|}\Big). \tag{4.49}$$

The first term of the error comes from the coarse graining $(\cdot)^{(\ell)}$ and belongs to the two point interaction terms $m_1(u)m_1(v)$. The remaining terms come from the $(\cdot)^{[n]}$ operation and they belong to the two point interaction terms, terms with external fields, and the entropy term, respectively.

Proof. We will start with the coarse graining $(\cdot)^{(\ell)}$. Saying that Λ is an ℓ-cube means that it is a cube and there exists $\mathcal{A} \in (\ell\cdot\mathbb{Z})^d$ such that $\Lambda = \bigcup_{x\in\mathcal{A}} C_x^{(\ell)}$. Recall α defined in Section 3.2, choose $i \in \{1,\dots,r-1\}$ and $x \in \mathcal{A}$. Because $-\alpha$ is a convex function we can use the Jensen's inequality

$$-\alpha\big(\mathsf{m}_i^{(\ell)}(x)\big) = -\alpha\Big(\frac{1}{|C_x^{(\ell)}|}\int_{C_x^{(\ell)}} \mathsf{m}_i(v)dv\Big) \le -\frac{1}{|C_x^{(\ell)}|}\int_{C_x^{(\ell)}} \alpha\big(\mathsf{m}_i(v)\big)dv. \tag{4.50}$$

Now we use the fact that $\mathsf{m}_i^{(\ell)}$ is constant on any $C_x^{(\ell)}$, multiply the previous inequality by $|C_x^{(\ell)}|$ and sum over all $x \in \mathcal{A}$. We get

$$-\int_\Lambda \alpha\big(\mathsf{m}_i^{(\ell)}(v)\big)dv \le -\int_\Lambda \alpha\big(\mathsf{m}_i(v)\big)dv, \tag{4.51}$$

which implies $-\mathcal{S}(\mathsf{m}^{(\ell)}) \le -\mathcal{S}(\mathsf{m})$.

Terms with the external fields are easy to handle because $\int_\Lambda \mathsf{m}^{(\ell)}(u)du = \int_\Lambda \mathsf{m}(u)du$.

Further, if $2\,\ell \le \gamma^{-1}$, it follows from Lemma 4.5.2 that $|\mathcal{U}_{\beta,h}(\mathsf{m}^{(\ell)})_{\gamma,\Lambda} - \mathcal{U}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda}| \le K\,\gamma\,\ell\,|\Lambda|$. We put the estimates together and obtain

$$\mathcal{F}_{\beta,h}(\mathsf{m}^{(\ell)})_{\gamma,\Lambda} \le \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} + K\,\gamma\,\ell\,|\Lambda|. \tag{4.52}$$

For the rest of the proof, let us use $\overline{m}$ instead of $\mathsf{m}^{(\ell)}$. One may also think of $\overline{m}$ being an arbitrary element of $\mathcal{M}$ because the following steps hold for any $\overline{m} \in \mathcal{M}$. We know that $\overline{m}(u), \overline{m}^{\,[n]}(u) \in \mathbb{M}_r$. Then $|\overline{m}_i| \le \|L\|$,$|\overline{m}_i^{[n]}| \le \|L\|$. We use it together with (4.40) to get

$$|\mathsf{m}_1^{[n]}(u)\mathsf{m}_1^{[n]}(v) - \mathsf{m}_1(u)\mathsf{m}_1(v)| \le \frac{\|L\|}{n}\big(|\mathsf{m}_1^{[n]}(u)| + |\mathsf{m}_1(v)|\big) \le 2\,\frac{\|L\|^2}{n}. \tag{4.53}$$

Consequently,

$$\begin{aligned} \Big|\int_\Lambda\int_\Lambda J_\gamma(u,v)\mathsf{m}_1^{[n]}(u)\mathsf{m}_1^{[n]}(v)dudv - \int_\Lambda\int_\Lambda J_\gamma(u,v)\mathsf{m}_1(u)\mathsf{m}_1(v)dudv\Big| \\ \le 2\,\frac{\|L\|^2}{n}\int_\Lambda\int_\Lambda J_\gamma(u,v)dudv \le 2\,\frac{\|L\|^2}{n}|\Lambda|, \end{aligned} \tag{4.54}$$

where we used $\int_\Lambda J_\gamma(u,v)du \le 1$. Similarly, we get the same estimate for the boundary term using $\int_{\Lambda^c} J_\gamma(u,v)du \le 1$. Now, we take a look at the terms with the external fields and, directly from (4.40), we get

$$\Big|\, h_i\int_\Lambda \overline{m}_i^{[n]}(u)du - h_i\int_\Lambda \overline{m}_i(u)du\,\Big| \le |h_i|\,\frac{\|L\|}{n}|\Lambda|. \tag{4.55}$$

Finally, we take care of the entropy term. If $\frac{\|L\|}{n} \le \frac{1}{e}$, we can use Lemma 3.2.1 and together with 4.40 we get

$$\Big|\alpha\big(\overline{m}^{\,[n]}(u)\big) - \alpha\big(\overline{m}(u)\big)\Big| \le \frac{\|L\|}{n}\log\frac{n}{\|L\|}. \tag{4.56}$$

This inequality provides us immediately with the entropy bound

$$|\mathcal{S}\big(\overline{m}^{\,[n]}\big) - \mathcal{S}\big(\overline{m}\big)| \le r|\Lambda|\frac{\|L\|}{n}\log\frac{n}{\|L\|}. \tag{4.57}$$

We collect the inequalities concerning $(\cdot)^{[n]}$ and get

$$|\mathcal{F}_{\beta,h}(\overline{m}^{\,[n]}) - \mathcal{F}_{\beta,h}(\overline{m})| \le \frac{\|L\|}{n}\Big(3\,\|L\| + \sum_{i=1}^{r-1}|h_i| + \frac{r}{\beta}\log\frac{n}{|\Lambda|}\Big)|\Lambda|. \tag{4.58}$$

Now, we put this bound together with (4.52), which finishes the proof. □

4.5 Supplementary lemmas

Lemma 4.5.1 *Let* $\gamma \in (0,1)$, $\ell \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, Λ *be an* ℓ*-cube,* $\tilde{\sigma} \in \mathbf{\Omega}$, $\mathsf{m} \in \mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})$, $\sigma \in \mathbf{\Omega}_{\mathsf{m}}^{(\ell)}(\tilde{\sigma})$, *and let* $2\,\ell \leq \gamma^{-1}$. *Then there exists a constant* $C \in \mathbb{R}$ *such that*

$$|H_h(\sigma)_{\gamma,\Lambda} - \mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda}| \leq C\,\gamma\,\ell\,|\Lambda|. \tag{4.59}$$

Moreover,

$$C \leq (3 \cdot 4^d\,|\nabla J|_1 + |J|_\infty)\,\omega_{max}^2, \tag{4.60}$$

where $\omega_{max} = \max_{\omega\in\Omega_0}|\omega|$ *and* J *is the function from* $\mathcal{C}^1(\mathbb{R}^d)$ *which was used in the definition of the Kac potentials.*

Lemma 4.5.2 *Let* $\gamma > 0$, $\ell \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, Λ *be an* ℓ*-cube,* $\mathsf{m} \in \mathcal{M}$, *and* $2\,\ell \leq \gamma^{-1}$. *Then there exists a constant* $K \in \mathbb{R}$ *such that*

$$|\mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda} - \mathcal{U}_h(\mathsf{m}^{(\ell)})_{\gamma,\Lambda}| \leq K\,\gamma\,\ell\,|\Lambda|. \tag{4.61}$$

Moreover,

$$K \leq 3 \cdot 4^d\,|\nabla J|_1 \|L\|^2. \tag{4.62}$$

Lemma 4.5.3 *Let* $\gamma > 0$, $\ell \in \mathbb{N}$, $u, v \in \mathbb{R}^d$, $J_\gamma^{(\ell)}(\cdot,\cdot) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ *be a Kac potential. Then*

$$|J_\gamma(u,v) - J_\gamma^{(\ell)}(u,v)| \leq 2\,\ell\;\gamma^d\,\gamma\,|\nabla J|_1\;\mathbb{I}_{|u-v|<\gamma^{-1}+2\,\ell},^{4} \tag{4.63}$$

where $|\nabla J|_1 = \max_{u\in[-1,1]^d} \sum_{i=1,\ldots,d} |\partial_i J|(u)$.

This estimate plays a key role in the proof of the two lemmas above, which in turn play a key role in the transition from the partition function to the variation principle for the free energy functional. In order to easily remember the bound we disclose that the first two coefficients come from the Lagrange mean value theorem and they stand for the maximal distance of elements of $C_u^{(\ell)}$ plus the maximum distance of elements of $C_v^{(\ell)}$ multiplied by the gradient of $J_\gamma(0,\cdot)$. The fact that $J_\gamma(0,\cdot)$ has a finite support with radius γ^{-1} affects the bound significantly and is represented by the characteristic function of the set $\{(u,v) \in \mathbb{R}^d \times \mathbb{R}^d : \; |u-v| < \gamma^{-1} + 2\,\ell\}$.

Now we prove the lemmas.

[4] For $J_\gamma^{(\ell)}(\cdot,\cdot)$ see the Definition 4.4.1.

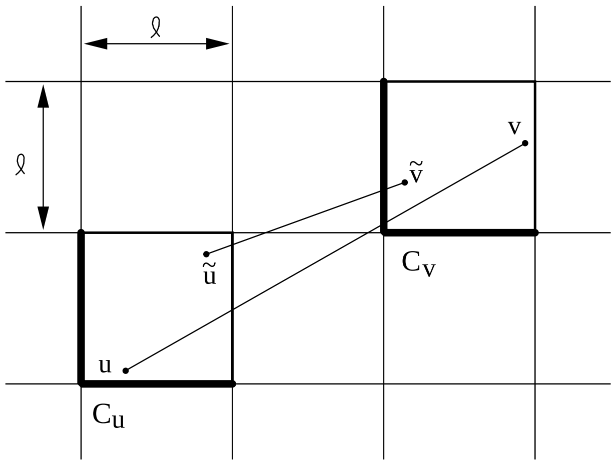

Figure 4.1: Elementary ℓ-cubes C_u and C_v $(d = 2)$

Proof of the Lemma 4.5.1

From the definition of $\mathbf{\Omega}_{\mathsf{m}}^{(\ell)}(\tilde{\sigma})$, it follows that $\sum_{x \in \Lambda \cap \mathbb{Z}^d} \sigma^i(x) = \int_\Lambda \mathsf{m}_i(u)du$ and thus we have

$$|H_h(\sigma)_{\gamma,\Lambda} - \mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda}| = |H_0(\sigma)_{\gamma,\Lambda} - \mathcal{U}_0(\mathsf{m})_{\gamma,\Lambda}| \leq \frac{1}{2} I_1 + I_2. \tag{4.64}$$

Here

$$I_1 = \Big| \sum_{x \in \Lambda} \sum_{y \in \Lambda} \mathbb{I}_{x \neq y} J_\gamma(x,y)\sigma(x)\sigma(y) - \int_\Lambda \int_\Lambda J_\gamma(u,v)\mathsf{m}_1(u)\mathsf{m}_1(v)dudv \Big| \leq I_3 + I_4, \tag{4.65}$$

$$I_3 = \omega_{max}^2 \sum_{x \in \Lambda} \sum_{y \in \Lambda} \mathbb{I}_{x=y} J_\gamma(x,y) \leq \omega_{max}^2 \gamma^d |J|_\infty |\Lambda| \leq \omega_{max}^2 |J|_\infty |\Lambda|, \tag{4.66}$$

$$I_4 = \Big| \sum_{x \in \Lambda} \sum_{y \in \Lambda} J_\gamma(x,y)\sigma(x)\sigma(y) - \int_\Lambda \int_\Lambda J_\gamma(u,v)\mathsf{m}(u)\mathsf{m}(v)dudv \Big|, \tag{4.67}$$

$$I_2 = \Big| \sum_{x \in \Lambda} \sum_{y \in \Lambda^c} J_\gamma(x,y)\sigma(x)\sigma(y) - \int_\Lambda \int_{\Lambda^c} J_\gamma(u,v)\mathsf{m}(u)\mathsf{m}(v)dudv \Big|. \tag{4.68}$$

From the definition of $\mathbf{\Omega}_{\mathsf{m}}^{(\ell)}(\tilde{\sigma})$ we also have $\mathsf{m}_1 = \sigma^{(\ell)}$ and thus [5]

$$\int_\Lambda \int_\Lambda J_\gamma(u,v)\mathsf{m}_1(u)\mathsf{m}_1(v)dudv = \sum_{x \in \Lambda} \sum_{y \in \Lambda} J_\gamma^{(\ell)}(x,y)\sigma(x)\sigma(y). \tag{4.69}$$

Then

$$|I_4| \leq \omega_{max}^2 \sum_{x \in \Lambda} \sum_{y \in \Lambda} |J_\gamma(x,y) - J_\gamma^{(\ell)}(x,y)| \tag{4.70}$$

[5] For $J_\gamma^{(\ell)}(\cdot,\cdot)$ see the Definition 4.4.1.

and similarly,

$$|I_2| \leq \omega_{max}^2 \sum_{x\in\Lambda} \sum_{y\in\Lambda^c} |J_\gamma(x,y) - J_\gamma^{(\ell)}(x,y)|. \tag{4.71}$$

From Lemma 4.5.3 we get

$$\sum_{x\in\Lambda} \sum_{y\in\mathbb{Z}^d} |J_\gamma(x,y) - J_\gamma^{(\ell)}(x,y)| \leq 2\,\ell\,\gamma^d\,\gamma|\nabla J|_1 \sum_{x\in\Lambda} \sum_{y\in\mathbb{Z}^d} \mathbb{I}_{|x-y|\leq\gamma^{-1}+2\,\ell}. \tag{4.72}$$

Further we compute

$$\sum_{x\in\Lambda} \sum_{y\in\mathbb{Z}^d} \mathbb{I}_{|x-y|<\gamma^{-1}+2d\,\ell} \leq |\Lambda| \big[2(\gamma^{-1}+2\ell)\big]^d \leq |\Lambda|\,4^d\,\gamma^{-d}, \tag{4.73}$$

where we just used the assumption $2\,\ell \leq \gamma^{-1}$.

Altogether, we have

$$\sum_{x\in\Lambda} \sum_{y\in\mathbb{Z}^d} |J_\gamma(x,y) - J_\gamma^{(\ell)}(x,y)| \leq C_1\,\gamma\,\ell\,|\Lambda|, \tag{4.74}$$

$$C_1 = 2\cdot 4^d\,|\nabla J|_1. \tag{4.75}$$

This estimate provides us with upper bound of the same form $\omega_{max}^2\,C_1\,\gamma\,\ell\,|\Lambda|$ on both $|I_2|$ and $|I_4|$. If we add the bound on $|I_3|$, we receive the final inequality. □

Proof of the Lemma 4.5.2

This proof is very similar to the previous one. From the definition of $(\cdot)^{(\ell)}$, it immediately follows that $\int_\Lambda \mathsf{m}^{(\ell)}(u)du = \int_\Lambda \mathsf{m}(u)du$ and because

$$\int_\Lambda \int_\Lambda J_\gamma(u,v)\mathsf{m}_1^{(\ell)}(u)\mathsf{m}_1^{(\ell)}(v)dudv = \int_\Lambda \int_\Lambda J_\gamma^{(\ell)}(u,v)\mathsf{m}_1(u)\mathsf{m}_1(v)dudv, \tag{4.76}$$

we have

$$|\mathcal{U}_h(\mathsf{m})_{\gamma,\Lambda} - \mathcal{U}_h(\mathsf{m}^{(\ell)})_{\gamma,\Lambda}| \leq \frac{1}{2}I_1 + I_2, \tag{4.77}$$

where

$$I_1 = \|L\|^2 \int_\Lambda \int_\Lambda |J_\gamma(u,v) - J_\gamma^{(\ell)}(u,v)|dudv, \tag{4.78}$$

$$I_2 = \|L\|^2 \int_\Lambda \int_{\Lambda^c} |J_\gamma(u,v) - J_\gamma^{(\ell)}(u,v)|dudv. \tag{4.79}$$

We use again Lemma 4.5.3 and for $2\,\ell \leq \gamma^{-1}$ we get, similarly to the equation (4.74), the bound

$$\int_\Lambda \int_{\mathbb{R}^d} |J_\gamma(u,v) - J_\gamma^{(\ell)}(u,v)|dudv \leq 2\cdot 4^d\,|\nabla J|_1\,\gamma\,\ell\,|\Lambda|. \tag{4.80}$$

□

Proof of the Lemma 4.5.3

From the definition of $J^{(\ell)}(u,v)$, [6] we have

$$|J_\gamma(u,v) - J_\gamma^{(\ell)}(u,v)| \leq \tfrac{1}{|C_u^{(\ell)}|\,|C_v^{(\ell)}|} \int_{C_u^{(\ell)}} \int_{C_v^{(\ell)}} |J_\gamma(u,v) - J_\gamma(\tilde{u},\tilde{v})| d\tilde{u} d\tilde{v} \qquad (4.81)$$

and we need an estimate on $|J_\gamma(u,v) - J_\gamma(\tilde{u},\tilde{v})|$ where $u, \tilde{u} \in C_u^{(\ell)}$ and $v, \tilde{v} \in C_v^{(\ell)}$. Then $|u-\tilde{u}| \leq \ell$, $|v-\tilde{v}| \leq \ell$, and because $J_\gamma(u,v) = \gamma^d J\big(\gamma(v-u)\big)$, where $J \in \mathcal{C}^1(\mathbb{R}^d)$, it follows from the Lagrange mean value theorem that

$$|J_\gamma(u,v) - J_\gamma(\tilde{u},\tilde{v})| \leq \gamma^d \gamma \left|\nabla J\right|_1 |v-u-(\tilde{v}-\tilde{u})| \leq 2\,\ell\,\gamma^d\,\gamma \left|\nabla J\right|_1. \qquad (4.82)$$

From the formula for $J_\gamma(\cdot,\cdot)$, we also see that, if $\gamma|u-v| \geq 1$ and $\gamma|\tilde{u}-\tilde{v}| \geq 1$, the difference is zero because both $J_\gamma(u,v)$ and $J_\gamma(\tilde{u},\tilde{v})$ are zero. From Figure 4.1 (or triangle inequality) we can see that $|\tilde{u}-\tilde{v}| > |u-v| - 2\,\ell$. Finally, if we take $|u-v| \geq \gamma^{-1} + 2\,\ell$ then $|\tilde{u}-\tilde{v}| > \gamma^{-1}$ and the difference is zero. □

4.6 Proof of the Lebowitz-Penrose theorem

In this section we collect the results of previous sections and complete the proof of the Lebowitz-Penrose theorem. Let us first make a brief recapitulation of achieved results.

For $\beta > 0$, $\gamma \in (0,1)$, $\ell \in \mathbb{N}$, $h \in \mathbb{R}^{r-1}$, $\tilde{\sigma} \in \mathbf{\Omega}$, $\tilde{\mathsf{m}} = (\tilde{\sigma}, \tilde{\sigma}^2, \ldots, \tilde{\sigma}^{r-1})^{(\ell)}$, Λ an ℓ-cube with the length of the edge $\sqrt[d]{|\Lambda|} \geq 2\gamma^{-1/2}$, $2\ell \geq \gamma^{-1/2}$, and $\ell^d \geq e\|L\|$, we get from Theorem 4.3.6, Remark 4.4.2, and Theorem 4.2.5, in the respective order,

$$\Big| -\frac{1}{\beta} \log Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda} - \min_{\mathsf{m}\in\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda}\Big| \leq \varepsilon_\beta(\gamma,\ell)\;|\Lambda|, \qquad (4.83)$$

$$\Big| \min_{\mathsf{m}\in\mathcal{M}_\Lambda^{(\ell)}(\tilde{\sigma})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} - \inf_{\mathsf{m}\in\mathcal{M}_\Lambda(\tilde{\mathsf{m}})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda}\Big| \leq \tilde{\varepsilon}_{\beta,h}(\gamma,\ell,\ell^d)\;|\Lambda|, \qquad (4.84)$$

$$\Big| \inf_{\mathsf{m}\in\mathcal{M}_\Lambda(\tilde{\mathsf{m}})} \mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} - |\Lambda| \min_{m\in\mathbb{M}_r} \Psi_{\beta,h}(m)\Big| \leq 2\left\|L\right\|^2 \gamma^{-1}\,|\partial\Lambda|. \qquad (4.85)$$

We combine the inequalities to get

$$\Big| -\frac{1}{\beta|\Lambda|} \log Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda} - \min_{m\in\mathbb{M}_r} \Psi_{\beta,h}(m)\Big| \leq \varepsilon_\beta(\gamma,\ell) + \tilde{\varepsilon}_{\beta,h}(\gamma,\ell,\ell^d) + 2\left\|L\right\|^2 \gamma^{-1}\,\frac{|\partial\Lambda|}{|\Lambda|}. \qquad (4.86)$$

Now we choose a sequence of ℓ-cubes $\{\Lambda_n\}_{n=1}^\infty \subset \mathscr{P}_f(\mathbb{Z}^d)$ such that $|\Lambda_n| \to \infty$ for $n \to \infty$. Such a sequence is van Hove and by the Lemma 2.1.1 the limit of

[6] See the Definition 4.4.1.

$-\frac{1}{\beta|\Lambda_n|} \log Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda_n}$ exists. Because $|\Lambda_n| \to \infty$ there must exist $n_0 \in \mathbb{N}$ such that $\sqrt[d]{|\Lambda_n|} \geq 2\,\gamma^{-1/2}$ for all $n \geq n_0$ and we get

$$\Big|\lim_{n\to\infty} -\frac{1}{\beta|\Lambda_n|} \log Z(\beta, h\,|\tilde{\sigma})_{\gamma,\Lambda_n} - \min_{m\in\mathbb{M}_r} \Psi_{\beta,h}(m)\Big| \leq \varepsilon_\beta(\gamma,\ell) + \tilde{\varepsilon}_{\beta,h}(\gamma,\ell,\ell^d). \quad (4.87)$$

The limit also does not depend on the choice of the sequence and thus the estimate above holds true for any van Hove sequence.

Finally, let $\gamma_0 = \min\left\{\frac{1}{1+\sqrt[d]{e\|L\|}}, \frac{1}{4d}\right\}$, $\gamma \in (0, \gamma_0)$ and $\ell_\gamma = \lfloor\gamma^{-1/2}\rfloor$. Then $\gamma \in (0,1)$, $\ell_\gamma \geq e\|L\|$, and $2\ell_\gamma \leq \gamma^{-1}$. For such γ and ℓ_γ, all the above mentioned conditions are satisfied so that (4.87) holds true and we can make the limit $\gamma \to 0$. Let us demonstrate on the key terms that both $\varepsilon(\gamma,\ell_\gamma)$ and $\tilde{\varepsilon}(\gamma,\ell_\gamma,\ell_\gamma^d)$ tend to zero if $\gamma \to 0$.

Remark 4.6.1

$$0 \leq \gamma\,\ell_\gamma = \gamma\lfloor\gamma^{-1/2}\rfloor \leq \gamma\,\gamma^{-1/2} = \gamma^{1/2} \to 0, \quad (4.88)$$

$$0 \leq \frac{1}{\ell_\gamma} = \frac{1}{\lfloor\gamma^{-1/2}\rfloor} \leq \frac{1}{\gamma^{-1/2}-1} = \frac{\gamma^{1/2}}{1-\gamma^{1/2}} \to 0, \quad (4.89)$$

$$0 \leq \frac{\log \ell_\gamma}{\ell_\gamma} = \frac{\log\lfloor\gamma^{-1/2}\rfloor}{\lfloor\gamma^{-1/2}\rfloor} \leq \frac{\log\gamma^{-1/2}}{\gamma^{-1/2}-1} = \frac{1}{1-\gamma^{1/2}}\frac{\log\gamma^{-1/2}}{\gamma^{-1/2}} \to 0. \quad (4.90)$$

Now, *the proof is complete.*

Chapter 5

Van der Waals theory

In the last chapter we have moved up to the mesoscopic level, where the elementary variables are averages of spins over microscopical regions and, finally, established the link between discrete and continuous description. An interpretation of the values of mesoscopic configurations as averages of microscopical values essentially establishes the relation with underlying microscopic level.

The mesoscopic theory is, in fact, based entirely upon a free energy functional, which specifies the free energy of all possible mesoscopic states and thus all the thermodynamical properties of the system. We restrict ourselves to the definition of basic notions and establishing a link to the free energy functional derived within the proof of Lebowitz-Penrose theorem. However, we want to stress again that the microscopic origin is not explicitly considered in the van der Waals theory and the free energy functional is there regarded as a primitive notion and a starting point of a self consistent theory.

5.1 Basic notions

The starting notion is the specification of all the possible states of the system, whose ensemble, the phase space, reflects the nature of the system. In the mesoscopic theory the states of systems are specified by measurable functions m, defined on some spatial domain, a region Λ or the whole $\mathbb{R}^d$. Thus for example for magnetic systems m has a meaning of a magnetization density at the point r. For simplicity we suppose m to be bounded, in suitable units $\mathsf{m}(u) \in [-1,1]^{r-1}$. The reader may refer to the Chapter 4 for a specific example of how such a continuum description may arise from a lattice spin systems. The considered configurations are functions from $L^\infty(\mathbb{R}^d, [-1,1]^{r-1})$ which is the phase space of the mesoscopic theory.

We consider here the mesoscopic theory as a coarse grained version of a microscopic model. As a result, a loss of information occurs but on the other hand, it leads to a gain of a simpler structure which allows a deeper analysis. It describes *collective properties* of the system and neglects all statistical fluctuations. Thus $\mathsf{m}(u)$ is a *local average* of spins in some microscopically large region around the point u. Such a region must be in mesoscopical units regarded as infinitesimal and in the end not distinguished from a point.

The basic notion in the theory is a free energy functional F specifying the free energy of of the configurations m. As a rule we will use the symbol $\mathcal{F}$ to denote the excess free energy functional. It differs from the previous one by an additive constant, chosen in such a way that the minimum of the latter is zero: this is why it is called an "excess free energy". Notice that, in the infinite volume, the additive constant may become infinite and, indeed, the free energy functional F is usually defined only in bounded spatial domains.

In order to introduce thermodynamics we postulate a variational principle (the second law of thermodynamics) that an equilibrium is attained once the free energy functional is minimal over the space of all permissible states of the system.

5.2 Ginzburg-Landau free energy functional

The Ginzburg-Landau excess free energy functional

$$\mathcal{F}^{gl}(\mathsf{m}) = \int_{\mathbb{R}^d} w\big(\mathsf{m}(u)\big) + C|\nabla \mathsf{m}(u)|^2 dr, \tag{5.1}$$

where C is an positive constant, is a prototype of the free energy functional in the van der Waals theory. The most studied example is the one with $w(s) = (s^2-1)^2$. In general we suppose that w is a smooth function whose minimal value is taken to be zero, according to the interpretation of the functional as a free energy excess (energy modulo an additive constant). The "magnetization" m is required to be differentiable and such that the integral above is well defined. Since the interest is in minimization problems, often the domain of definition is extended allowing for the functional to have also the value $+\infty$. We regard the "magnetization" m to be generic non-equilibrium profile and $\mathcal{F}^{gl}(\mathsf{m})$ be its "distance" from the equilibrium: the smaller $\mathcal{F}^{gl}(\mathsf{m})$, the closer to equilibrium.

Ginzburg and Landau had in mind two mechanisms to penalize departures from equilibrium: the first one is ruled by a mean field free energy density described in w. Any value of $\mathsf{m}(u)$ which is not a minimizer of w contributes to the total free energy proportionally to the space volume where it is occurs. This term therefore favours profiles supported by the minimizers of w. In order to describe a phase transition, there must be also a penalty for changing the minimizer which, in the Ginzburg-Landau functional, is the last term in (5.1). Thus the global minimizers of $\mathcal{F}^{gl}$ are functions m constantly equal to a minimizer of w and their free energy is zero. They are therefore interpreted as the pure phases. All the other profiles have a non zero free energy and are therefore non equilibrium profiles.

5.3 A link to the r-model

The analysis as described in Chapter 4 indicates another candidate for the free energy functional, namely the expression (4.8) from which we simply drop the last term because it does not have any relevant meaning here. It does neither correspond to the mean-field minimizer nor to the penalty for changing the minimizer. For the readers convenience we rewrite it here:

$$F_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} = \int_\Lambda \Psi_{\beta,h}(\mathsf{m}(u))du + \frac{1}{4}\int_\Lambda\int_\Lambda J_\gamma(u,v)[\mathsf{m}_1(u)-\mathsf{m}_1(v)]^2 dvdu + \frac{1}{2}\int_\Lambda\int_{\Lambda^c} J_\gamma(u,v)[\mathsf{m}_1(u)-\mathsf{m}_1(v)]^2 dvdu. \quad (5.2)$$

To establish a valid excess free energy functional with zero ground state we subtract from the first term its minimum, i.e. we define a function $\varphi_{\beta,h}(m) = \Psi_{\beta,h}(m) - \min_{\tilde{m}\in\mathbb{M}_r}\Psi_{\beta,h}(\tilde{m})$. Further we choose $\Lambda = \mathbb{R}^d$ and define the *r-model excess free energy functional*

$$\mathcal{F}_{\beta,h}(\mathsf{m})_{\gamma,\Lambda} = \int_{\mathbb{R}^d} \varphi_{\beta,h}(\mathsf{m}(u))du + \frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} J_\gamma(u,v)[\mathsf{m}_1(u)-\mathsf{m}_1(v)]^2 dvdu.$$

This is the final result of our effort to find a link between the lattice models (r-model) with the configurations residing on a discrete subsets of $\mathbb{Z}^d$ to a model with configurations being measurable functions $\mathsf{m} \in \mathcal{M}$ residing on [1] $\mathbb{R}^d$ and interpreting the value $\mathsf{m}(u)$, $u \in \mathbb{R}^d$ as a local average of "magnetization" over microscopical region around u. Notice that the main steps that allow us to interpret the functional above, as a "van der Waals theory counterpart" of the partition function of the r-model, involve coarse graining procedure and are subject to the Remark 4.2.3, Theorem 4.3.6, and Remark 4.4.2.

5.4 Instantons

After coarse graining of the lattice model we have lost the information about the microscopical structure of the system. However, the main advantage of the derived mesoscopical theory should be its simpler structure and presence of newly available tools for its analysis.

If we restrict ourselves to the assumption of planar symmetry, we can reduce to a one dimensional problem that should be accessible for study in a great detail. In particular, we are interested in the minimizing profile (an instanton) which monotonically connects several phases. In the case of Ising model there are fundamental results like existence, uniqueness, regularity, exponential decay form one phase to the other, etc. proved in [Pr]. A challenging task is to prove similar results for the Blume-Capel model, where an intrinsic dependence of such results on the "new"

[1] The set $\mathcal{M}$ was defined in (4.4).

external field l (or h_2 in the notation of a general r-model) comes into the play. This will be subject of further research.

Chapter 6

Conclusion

I was able to establish a direct link from statistical mechanics of an extended Blume-Capel model (r-model) to its formulation within the mesoscopic van der Waals theory.

Further I succeeded in the proof of the Lebowitz-Penrose theorem for the r-model, a large class of models including the Ising and Blume-Capel (so far the theorem had been known to hold true for the Ising model).

However, there still remain open questions concerning instantons in the Blume-Capel model, which require further research. The motivation and direction can be drawn by the fourth and fifth chapter of [Pr] where all the important question about existence, uniqueness, regularity and decay of the instantons are proved in the case of Ising model.

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