RSG: Mathematics of Multiscale Materials

One Dimensional Gradient Models

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1 Introduction

Our project focuses on the study of a gradient field model: in particular we consider a 1-dimensional model on a lattice box $\Lambda \subset \mathbb{Z}$ and consider the thermodynamic limit as $\Lambda \to \mathbb{Z}$. The model is determined by a Gibbs distribution which weights possible configurations according to how nearby particles interact; the model is introduced formally in section 1.2, but first we provide a motivation from material science.

1.1 Modelling Defects in Crystal Structures

The physical motivation for the work in this report is the following problem, in which we want to model a material which is made up of many interacting atoms. We would like to be able to study the effects that defects have on the atomic structure of the material, and whether microscopic defects can have macroscopic effect. Figure 1 gives examples of the possible defects that may occur in such a material, and descriptions can be found in [7].

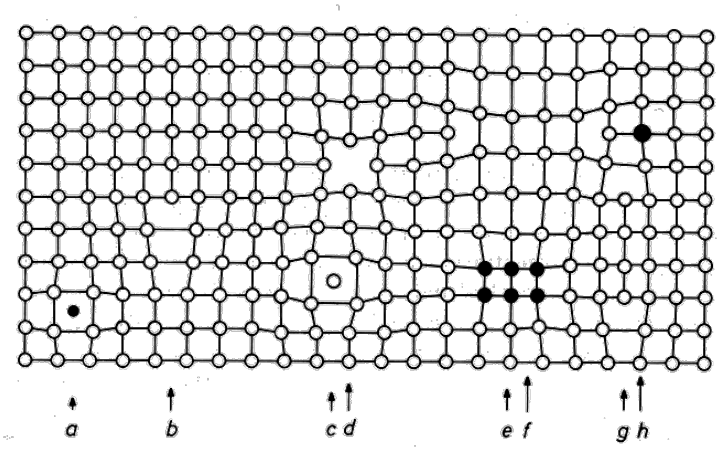


Figure 1: Possible defects that can occur in a crystal. Image courtesy of Helmut Föll, [7].

Studying such materials in realistic dimensions (i.e. $d = 2, 3$) is typically hard, so we turn to a toy model in 1-dimension which we hope captures some of the features of the material. To justify this approach we consider the model to be made up of many layers of particles, so that taking a cross section through the material results in a collection of 1-dimensional systems stacked on top of one another, Figure 2. In our model we consider just one of these layers, and model it by considering the particles as the sites of a lattice segment displaced according to interactions and distorting forces.

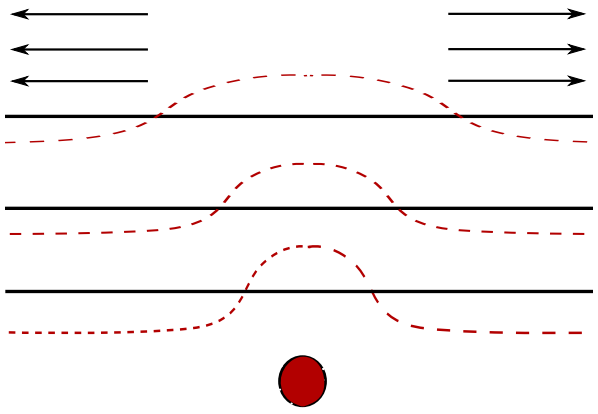


Figure 2: A force field is induced by a defect in the material, and is seen to effect the behaviour of surrounding layers of particles.

The 1-dimensional gradient Gibbs model takes into account the interactions between particles in one layer of the material which we model by configurations of particles in a box $\Lambda \subset \mathbb{Z}$, where interactions

between particles can have arbitrary distance (though we concentrate on the cases of nearest and next nearest neighbour potentials). We are interested in describing the behaviour of the model as we take the thermodynamic limit and send $\Lambda \to \mathbb{Z}$. We also assume that the material is under stress, which is expressed via a tilt boundary condition, as shown by the arrows in Figure 2. When $x > 0$ this tilt can be interpreted as a stretch that is applied pulling the particles apart, whilst when $x < 0$ the tilt plays the role of a squeezing force.

For the most part of this project we concentrate on the case in which there is no defect in the material, though in section 4.4 we take such extra forces into account. We briefly comment, however, on what forms these forces could take.

- Trivial force. In this case we do not add a force term, and consider the material to be defect free.
- Force field on a sub-box. In this case we define a box $\Delta \subset \Lambda$ with the interpretation of being the region which can be effected by the defect. The force only acts directly on those sites contained in Δ, and is 0 on $\Lambda \backslash \Delta$. A particularly simple case would be to assume the force to be homogeneous inside Δ, so that all the atoms are acted on in an identical manner. A more realistic model would be inhomogeneous, so that the particles behave differently under the force, for instance the force could be stronger near the middle of Δ, with the interpretation that these atoms are closer to the defect.
- Decaying force field. The force is inhomogeneous, and has a strong effect on points in a particular region with the interpretation that this is the neighbourhood of the defect (though no specific sub-box need be defined); the force continuous to be non-trivial away from this region, though its strength is decaying.

Clearly the final case is the most realistic, though we believe it is sufficient to consider inhomogeneous forces on a sub-box. To justify this we note that a force on the whole of Λ can be approximated by applying cut-offs to the force, so we consider its effect only on a box $\Delta \subset \Lambda$. We recover the original case by taking the limit $\Delta \to \Lambda$; if we can analyse the sub-box case, and if the decay of the force is sufficiently fast, then we expect the relevant thermodynamic function (in our case the free energy) will converge, [13].

With our motivation described, we now continue to define the model in technical detail. We save the description of how to add forcing terms, however, until section 4.4.

1.2 The Gradient Gibbs Distribution

Our project considers gradient models on the 1-dimensional lattice $\mathbb{Z}$, where configurations are weighted according to a Gibbs distribution; in particular we define the finite state space Gibbs distributions, and analyse the limiting behaviour by studying the free energy. In this section we introduce the basic technical notions and definitions which will be used throughout the report.

Let $\Lambda = \Lambda_N = \{0, 1, \dots, N\} \subset \mathbb{Z}$ denote a finite box. Our attention will focus on the case where we equip Λ with periodic boundary conditions, and often refer to it as the 1-dimensional torus on $N+1$ points. The configuration space Ω_N on Λ is taken to be the space of real-valued height fields $\Omega_N = \mathbb{R}^\Lambda$, and the weight of a configuration $u \in \Omega_N$ is determined by a Hamiltonian, $H(u) = H_N(u)$. In particular, we consider Hamiltonian functions which can be expressed as sums over 'k-th neighbour' gradient potentials

$$H_N(u) = \sum_{k=1}^{K} \sum_{\substack{i,j \in \Lambda \\ |i-j|=k}} V_k\left(\frac{u_i - u_j}{|i-j|}\right), \tag{1}$$

where $K \leq N$ is the greatest interaction distance, and we assume periodic boundary conditions. For the purposes of our report we will consider only the cases of $K = 1, 2$, and in particular will focus initially on the pure cases of $V_1 \not\equiv 0$, $V_2 \equiv 0$, and $V_1 \equiv 0$, $V_2 \not\equiv 0$.

Remark 1. The archetypal potential used to model real world interactions between atoms is the Lennard–Jones potential. The reason for its prevalence in the literature is that is has a simple form but approximates interactions well. In section 4 we consider mixed Gaussian potentials which may be used to approximate the Lennard–Jones potential, see Figure 3.

Traditional statistical mechanics would then proceed by analysing the Gibbs distribution,

$$\gamma_N^\beta(u) \propto \exp\big(-\beta H(u)\big), \qquad u \in \Omega_N,$$

where $\beta > 0$ is the inverse temperature. What makes the gradient model tractable (and gives it its name) is the reinterpretation of the model as a configuration of gradients over bonds. Let $\mathcal{B}(\Lambda) = \{b_i = (i, i+1) : i \in$

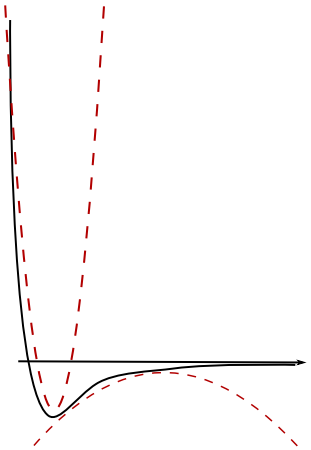


Figure 3: Approximate Lennard–Jones by taking a positive nearest neighbour potential and a negative next nearest neighbour potential.

$\Lambda\}$ denote the bond set of Λ_N, again endowed with periodic boundary conditions so that $b_N = (N, 0) \in \mathcal{B}(\Lambda)$. Given a configuration $u \in \Omega_N$ we obtain a bond configuration $\eta = \eta_u \in \mathbb{R}^{\mathcal{B}(\Lambda)}$ by letting $\eta(b_i) = u_{i+1} - u_i$, be the gradient across bond b_i. Maintaining the interpretation that the value $\eta(b_i)$ is the gradient across bond b_i, the periodic boundary conditions on Λ enforce the requirement that

$$\sum_{i=0}^{N} \eta(b_i) = 0, \tag{2}$$

implying that the mean gradient must be 0: this condition is heuristically justified since the mean gradient of the bonds is $|\Lambda|^{-1}(u_0 - u_0) = 0$. Henceforth we refer to (2) as the *loop condition*. Now given a configuration η of bonds satisfying (2), if we fix the position of one site, $u_0 = 0$ for instance, then η uniquely determines a site configuration in Ω_N. It follows that the models are equivalent up to translation invariance, and henceforth consider the gradient model to be described by a Gibbs distribution on the space of bond configurations satisfying the loop condition. In the case of pure nearest neighbour interactions, $V_k \equiv 0$, $k \geq 2$, this correspondence means we can replace the configuration space with

$$\Omega_N = \{\eta_i = \eta(b_i) \in \mathbb{R} : b_i \in \mathcal{B}(\Lambda)\} = \mathbb{R}^{\mathcal{B}(\Lambda)}. \tag{3}$$

This correspondence generalises to more general potentials, for instance when $V_2 \not\equiv 0$ we add to $\mathcal{B}(\Lambda)$ the set of edges joining next nearest neighbours. Now given a bond configuration space Ω_N and a suitably defined Hamiltonian H_N, the gradient Gibbs distribution $\mu_N \in \mathcal{M}^1(\Omega_N)$ is defined as

$$\mu_N(d\eta) = \frac{1}{Z_N^\beta} e^{-\beta H_N(\eta)} d\eta_N, \tag{4}$$

where $\beta > 0$, $d\eta_N$ is the uniform measure on Ω_N, and Z_N^β is the partition function (or normalising constant).

To model physical systems, we endow the gradient model with a tilt, $x \in \mathbb{R}$, which corresponds to stretching or compressing Λ: if we consider the case that Λ has free boundary conditions as done by Blanc, Le Bris, Legoll and Patz [3], this is implemented by restricting attention to configurations for which the mean bond gradient is x, i.e. $u_N - u_0 = Nx$. However, since we consider the model on the torus there is no way to add a tilt with this interpretation, since we already have the loop condition. Instead we add the tilt to each term in the potential, and see it as a stretching factor; that is we consider the tilted Hamiltonian in which we replace $V_k(\cdot)$ by $V_k(\cdot + x)$. Hence, in the case of pure nearest neighbour interactions, we consider the Gibbs distribution $\mu_N^x \in \mathcal{M}^1(\Omega_N)$

$$\mu_N^x(d\eta) = \frac{1}{Z_{N,x}^\beta} \exp\left(-\beta \sum_{b \in \mathcal{B}(\Lambda)} V\big(\eta(b) + x\big)\right) d\eta_N, \tag{5}$$

and denote H_N^x for the tilted Hamiltonian. For the gradient model to be of interest it is important that we can show the existence of some form of limiting distribution on the space Ω of bond configurations on $\mathbb{Z}$; in [9] it is shown that for pure nearest neighbour interactions with convex potential $V = V_1$, there is a

measure μ^x to which a subsequence of μ_N^x converges weakly. In section 2.2 we confirm that convexity can be replaced by a weaker requirement.

The emphasis of our project is to analyse the behaviour of the free energy as $|\Lambda| \to \infty$, namely $f\colon \mathbb{R} \to \mathbb{R}$ given by

$$f(x) = \lim_{N\to\infty} -\frac{1}{\beta|\Lambda|} \log Z_{N,x}^{\beta}. \tag{6}$$

In section 2 we extend the results in [9, 11] to show the existence of the free energy for a class of non-convex potentials, before applying the results to particular examples and obtaining bounds on f. Section 3 concentrates on pure next nearest neighbour interactions; following the large deviations approach of Blanc et al. we see that subject to the same conditions as in [3], the free energy exists and can be expressed as the solution to a variational problem. Finally in section 4 we examine the case of quadratic potentials, a simplification which enables the study of mixed interactions and in particular reveals an explicit formula for the free energy with tractable convergence analysis. We conclude the section by studying the effect a simple form of external force has on the free energy.

2 Pure Nearest Neighbour Interaction

In this section we consider Hamiltonians of the form (1) with $V_k \equiv 0$ for $k \geq 2$, and study the existence of the free energy (6), before analysing examples for particular choices of the potential $V = V_1$. Throughout, to avoid cumbersome notation and equations we absorb the inverse temperature $\beta > 0$ into the potential (see Remark (6)), so that $V = V^\beta$ (though we will not adhere to this convention in later sections, where this factor plays a more important role).

We also remark at this stage that whilst the literature we reference uses the term surface tension σ we continue to refer to the free energy f.

In [9], Funaki and Spohn provide a theory for nearest neighbour gradient models where the potential satisfies the following conditions

$$V \in C^2(\mathbb{R}), \tag{7}$$
$$V(-\eta) = V(\eta) \quad \forall \eta \in \mathbb{R}, \tag{8}$$
$$c_- \leq V''(\eta) \leq c_+, \, \forall \eta \in \mathbb{R}, \text{ for some } c_-, c_+ > 0. \tag{9}$$

In particular under these conditions, Funaki and Spohn use the Brascamp-Lieb inequality to prove tightness of the sequence $\{\mu_N^x\}_{N\in\mathbb{N}}$, which ensures the existence of the limiting distribution μ^x (where we understand this as the weak limit of a subsequence in $\{\mu_N^x\}_{N\in\mathbb{N}}$). Having estabished this they proceed to show the existence and convexity of the free energy, as well as describing results for $\nabla f(x)$.

Remark 2. We take as our starting point the following question, asked in [9] p.5: what effect does relaxing the conditions (7)-(9) have on the shape of f? For instance, are there flat regions that correspond to a macroscopic phase transition, or could it have cusps which correspond to a roughening transition?

Our aim is to address this question for the special 1-dimensional models under weaker conditions on the potential. In doing this we find a tractable expression for the free energy, which we apply to some concrete examples of potentials.

2.1 Outline of the Method

Throughout this section we assume the potential satisfies the restrictions introduced by Guo, Papanicalao and Varadhan [11], which require that V satisfies

$$V \in C^1(\mathbb{R}), \tag{10}$$
$$M(\lambda) \coloneqq \int_{\mathbb{R}} e^{\lambda\eta - V(\eta)} d\eta < \infty, \quad \forall \lambda \in \mathbb{R}, \tag{11}$$
$$\int_{\mathbb{R}} e^{\tau|V'(\eta)| - V(\eta)} d\eta < \infty, \quad \forall \tau \in \mathbb{R}. \tag{12}$$

In addition to this we also require (8); this class of potentials contains those considered in [9]. We assume that a limiting measure μ^x exists for all $x \in \mathbb{R}$, and will prove this in a special case in section 2.2. Our main aim will be to show that under the conditions above the free energy exists, and has a representation which can be computed explicitly in some cases, whilst in others it can be applied to obtain bounds.

Remark 3. For condition (11) on the moment generating function M to hold, we require that in the tail, $\lim_{\eta\to\pm\infty} \lambda\eta - V(\eta) = -\infty$, so V needs to have superlinear growth for $\eta \gg 1$, and for $\eta \ll -1$, the decay must be slower than linear. If V is a symmetric polynomial satisfying (11) then we note that (12) holds since the derivative has lower order than V.

For $\lambda \in \mathbb{R}$ we define the Cramér transform $\hat{\nu}_\lambda \in \mathcal{M}^1(\mathbb{R})$ of the distribution with density $\hat{\nu}(\eta) = \frac{1}{\widehat{Z}} e^{-V(\eta)}$ to be

$$\hat{\nu}_\lambda(d\eta) \coloneqq \widehat{Z}_\lambda^{-1} \exp\left(\lambda\eta - V(\eta)\right) d\eta \tag{13}$$

where $\widehat{Z}_\lambda$ is the corresponding partition function. We also define $x(\lambda)$, the expected value of a bond under $\hat{\nu}_\lambda$

$$\begin{aligned} x(\lambda) &\coloneqq \mathbb{E}_{\hat{\nu}_\lambda}[\eta] \\ &= \frac{d}{d\lambda} \log \widehat{Z}_\lambda. \end{aligned}$$

We remark that $x \in C^1(\mathbb{R})$ if V satisfies (11) and (12); in addition, the derivative is the variance of the bond value under $\hat{\nu}_\lambda$, and as such is strictly positive

$$x'(\lambda) = \mathbb{E}_{\hat{\nu}_\lambda}[(\eta - \mathbb{E}_{\hat{\nu}_\lambda}(\eta))^2] > 0. \tag{14}$$

It follows that $x(\lambda)$ is strictly increasing, and as it is also continuous it has a well defined inverse, denoted $\lambda = \lambda(x)$.

In the following we draw together results from [9] and [11] to show that the free energy exists, is differentiable, and satisfies

$$f'(x) = \lambda(x). \tag{15}$$

The following result demonstrates that in the limit the gradients across the bonds are i.i.d. with distribution described by the Cramér measure. This is central to the arguments in both this section, and in section 3.

Lemma 2.1. *For potentials $V : \mathbb{R} \to \mathbb{R}$ satisfying (10)-(12), then given that a limit measure μ^x exists, it is given by*

$$\mu^x(d\eta) = \prod_{b \in \mathcal{B}(\mathbb{Z})} \hat{\nu}_{\lambda(x)}(d\eta(b)), \qquad \eta \in \Omega. \tag{16}$$

Proof. We follow an argument given by Adams, [1]. We note that the measure μ^x can also be seen as the limit of a sequence of image measures $\mu_N^{\nabla,\psi_x} = \mu_N^{\psi_x} \circ \nabla^{-1}$, where $\mu_N^{\psi_x}$ measures height configurations on Λ_N with boundary condition $\psi_x(y) = xy$, and $\nabla : \Lambda_N \to \mathcal{B}(\Lambda_N)$ maps height configurations to bond configurations, [8] pp.152-153. Note that ∇ is not invertible, however $\mu_{\Lambda_N}^{\psi_u} \circ \nabla^{-1}$ is still well defined because the preimage $\nabla^{-1}(\eta)$ consists of height configurations that all have the same mass under $\mu_N^{\psi_x}$, thus there is no ambiguity.

Denoting $b_i = (i, i+1) \in \mathcal{B}(\Lambda)$, we define the height function of a configuration $\eta \in \Omega_N$ to be

$$\phi_\eta(y) \coloneqq \sum_{i=1}^{y} \eta(b_i), \qquad y \in \Lambda_N,$$

so that $\nabla(\phi_\eta) = \eta$. Now if $(\eta(b_i))_{i=0}^N$ are i.i.d. with distribution $\nu(\cdot) \propto \exp(-V(\cdot))$, we see that the measure obtained by conditioning on the final height satisfies $\nu^{\otimes N}(\cdot\,|\phi(N) = xN) = \mu_N^{\psi_x} \circ \nabla^{-1}$, where equality is in law. Hence the limit μ^x is the weak limit of this sequence of conditioned measures.

In Theorem 3.5 of [11], Guo et al. show that in the limit, the conditioned probability measure above can be expressed as a product measure of the relevant Cramér transformed measures; in particular letting $\lambda = \lambda(x)$, they show that this limit is an infinite product of $\hat{\nu}_\lambda$. Now we are done since

$$\mu^x(\cdot) = \lim_{N\to\infty} \mu_N^{\nabla,\psi_x}(\cdot) = \lim_{N\to\infty} \nu^{\otimes N}(\,\cdot\,|\phi(N) = xN) = \prod_{i\in\mathbb{Z}} \hat{\nu}_\lambda(\cdot). \qquad \square$$

Normally, independence of bond values sets the nearest neighbour model apart and makes it much easier to work with. One of the main difficulties in our setting is the fact that the loop condition means that the bond values are no longer independent, rather the bonds are weakly dependent on one another in a global sense. However, (16) implies that in the limit independence is recovered. We note also that the conditions of Lemma 2.1 do not require V to be symmetric, or convex; however for the limit to exist we do require tightness of the sequence $(\mu_N)_{N\in\mathbb{N}}$.

We now state our main result for nearest neighbour interactions.

Lemma 2.2. *Let $V : \mathbb{R} \to \mathbb{R}$ satisfy* (8), (10)- (12) *and assume that a limiting gradient Gibbs measure, μ^x, exists for all tilts $x \in \mathbb{R}$. Then the free energy $f(x)$ exists, is differentiable, and satisfies*

$$f'(x) = \lambda(x). \tag{17}$$

Proof. Let f_N denote the free energy for the gradient model on Λ_N

$$f_N(x) = -\frac{1}{\beta|\Lambda_N|} \log Z_N^x.$$

In [9], Lemma 3.1 (ii) gives the identity

$$f_N'(x) = \mathbb{E}_{\mu_N^x}[V'(\eta_0 + x)],$$

where η_0 represents a specific bond. (Whilst this is proven in the context of conditions (7)-(9), it does not require the convexity assumption or more regularity than $V \in C^1$, therefore it holds in our case). Taking

the limit $N \to \infty$ of this expression requires some explanation as the same result by Funaki and Spohn does rely on convexity of the potential.

Firstly we split the expression using indicators with $M > 0$

$$f'_N(x) = \mathbb{E}_{\mu_N^x}[V'(\eta_0 + x)1_{(|\eta|<M)}] + \mathbb{E}_{\mu_N^x}[V'(\eta_0 + x)1_{(|\eta|>M)}].$$

where the second term in this expression decays as $M \to \infty$, because the probability of a bond taking large values decays exponentially. To keep this outline clear and concise, we do not deal explicitly with this error term here.

Now continuity of V' means that if $K := [-C, C]$ then $C_{K,M} := \sup_{x\in K,\eta\in[-M,M]^N} |V'(\eta + x)|$ is attained, which allows us to obtain the following uniform bound for $x \in K$

$$\begin{aligned}
|\mathbb{E}_{\mu_N^x}[V'(\eta_0 + x)1_{(|\eta|<M)}]| &= \left| \frac{\int_{[-M,M]^N} V'(\eta_0 + x) \exp\Big(-\sum_{b\in T_N^*} V(\eta_b + x)\Big) d\eta_N}{\int_{\mathbb{R}^N} \exp\Big(-\sum_{b\in T_N^*} V(\eta_b + x)\Big) d\eta_N} \right| \\
&= \left| \frac{\int_{[-M,M]^N} V'(\eta_0 + x) \exp\Big(-\sum_{b\in T_N^*} V(\eta_b + x)\Big) d\eta_N}{\int_{[-M,M]^N} \exp\Big(-\sum_{b\in T_N^*} V(\eta_b + x)\Big) d\eta_N + e_M} \right| \\
&\leq C_{K,M}
\end{aligned}$$

where $e_M = \int_{([-M,M]^N)^c} \exp\Big(-\sum_{b\in T_N^*} V(\eta_b + x)\Big) d\eta_N$ is a positive error term. We know that when $|x| < C$, $V'(\eta_0 + x)1_{(|\eta|<M)}$ is bounded and continuous, hence $\mu_N^x \to \mu^x$ weakly implies that

$$\mathbb{E}_{\mu_N^x}[V'(\eta_0 + x)1_{(|\eta|<M)}] \to \mathbb{E}_{\mu^x}[V'(\eta_0 + x)1_{(|\eta|<M)}] \text{ as } N \to \infty,$$

where the convergence is pointwise. This convergence with the uniform bound allows us to apply the Lebesgue dominated convergence theorem to the following expression

$$f_N(\bar{x}) - f_N(x) = \int_0^1 (\bar{x} - x) \frac{df_N}{dx}(t\bar{x} + (1 - t)x) dt$$

where $\bar{x} = x + h$ for $h \in \mathbb{R}$, to obtain

$$f(\bar{x}) - f(x) = \int_0^1 (\bar{x} - x) \mathbb{E}_{\mu^{t\bar{x}+(1-t)x}}[V'(\eta_0 + x)1_{(|\eta|<M)}] dt.$$

This gives us the existence of the limit (6). Now dividing by $(\bar{x} - x)$ and taking $h \to 0$ gives

$$f'(x) = \mathbb{E}_{\mu^x}[V'(\eta + x)] \tag{18}$$

for the limit measure μ^x. Since the expectation on the right-hand side of (18) is for a single bond, then using the factorisation obtained in Lemma 2.1 we obtain

$$f'(x) = \mathbb{E}_{\hat{\nu}_\lambda}[V'(\eta + x)].$$

where $\lambda = \lambda(x)$. Finally, we use integration by parts to evaluate the expectation

$$\begin{aligned}
f'(x) &= \frac{1}{\widehat{Z}_\lambda} \int_{\mathbb{R}} V'(\eta + x) e^{-V(\eta+x)} e^{\lambda\eta} d\eta \\
&= -\frac{e^{\lambda\eta - V'(\eta+x)}}{\widehat{Z}_\lambda}\Bigg|_{-\infty}^{\infty} + \frac{\lambda}{\widehat{Z}_\lambda} \int_{\mathbb{R}} e^{\lambda\eta - V(\eta+x)} d\eta \\
&= \lambda,
\end{aligned}$$

where we require (11) to ensure that the first term vanishes, as we saw in Remark 3. □

This method can be used to deduce the existence of the free energy for potentials satisfying the requirements of Lemma 2.2; in section 2.3.3 we will see that in particular this holds for the double-well potential, an example of a non-convex potential with asymptotic growth. In addition to existence, we have the following corollary.

Corollary 2.3. *Under the conditions of Lemma 2.2, $f \in C^2(\mathbb{R})$ and is strictly convex.*

Proof. From the discussion before equation (14) we know that $x(\lambda) \in C^1(\mathbb{R})$ and hence that $\lambda(x) \in C^1(\mathbb{R})$. From Lemma 2.2 it follows that f'' exists and is given by $f''(x) = \lambda'(x)$. Recalling that a function is (strictly) convex if its second derivative is (strictly) positive, then from (14) we know $x'(\lambda) > 0$ for all $\lambda \in \mathbb{R}$ and since $\lambda(x)$ is the inverse

$$f''(x) = \lambda'(x) > 0, \qquad \forall x \in \mathbb{R}. \qquad \square$$

Remark 4. Finally, another result that we glean from [9], which is worth mentioning at this stage, is the following representation of the free energy as a Legendre Transform

$$f(x) = \sup_{\lambda \in \mathbb{R}} \{\lambda x - \log M(\lambda)\}.$$

This agrees with Theorem 3.3.

We now return to the question in Remark 2 concerning the shape of the free energy. In response to Funaki and Spohn, we have demonstrated that there is a broader class of potentials for which we are able to analyse free energy, and in particular have seen that within this class f is strictly convex, which indicates a lack of a phase transition.

In section 2.3 we will apply the results above to concrete examples of potentials, in one case identifying an explicit formula for the free energy, whilst in others obtaining bounds. Before doing this, however, we address the technical 'elephant in the room': the existence of the limiting measure, μ^x.

2.2 Tightness for Non-Convex Potentials

Recall that we are looking to find a measure which (in some way) defines the limit of the sequence $\{\mu_N^x\}$ of finite volume gradient Gibbs measures. By Prokhorov's theorem, if we can prove that the sequence $\{\mu_N^x\}$ is tight (with reference to the suitable topological space) then there is a subsequence $\{\mu_{N_k}^x\}_{k=1}^{\infty}$, and a measure μ^x such that the subsequence converges weakly, $\lim_{k\to\infty} \mu_{N_k}^x = \mu^x$. Whilst the definition of f does not directly require a limiting measure to exist, the proof of Lemma 2.2 relies heavily on such existence, in that we use the factorisation (16) of μ^x. Throughout this section we talk of 'showing tightness for the potential V', by which we mean showing tightness for the relevant sequence of Gibbs distributions. Our aim is to show that if a potential is bounded by Gaussian potentials then it is tight. That is we enforce the following condition: there exist constants $c_1, c_2, c_3, c_4 > 0$ such that

$$-c_1 + c_2\eta^2 \leq V(\eta) \leq c_3 + c_4\eta^2. \tag{19}$$

Remark 5. Whilst we prove tightness for potentials satisfying this condition, we conjecture that it holds for any potential with sufficient growth at the tails, since tightness requires configurations with large gradients to have low probability mass. Given the result of Lemma 2.4, we conjecture that any potential with faster than Gaussian growth also produces a tight sequence of measures. This assumption will be made use of when we consider the double well potential in section 2.3. For the sake of completeness we also note that it is generally thought that super-linear growth is sufficient to guarantee tightness, thus the class of potentials (10)-(12) is valid in terms of existence of a limiting gradient Gibbs measure.

Note that choosing V to satisfy the upper and lower bounds in (19), then the partition functions are Gaussian integrals, and are finite. Hence there are constants $K_1, K_2 \in \mathbb{R}$ such that for any potential V satisfying (19)

$$K_1 \leq \liminf_{N\to\infty} \frac{1}{N} \log Z_{N,x} \leq \limsup_{N\to\infty} \frac{1}{N} \log Z_{N,x} \leq K_2. \tag{20}$$

So it suffices to prove tightness for any V satisfying this condition.

Lemma 2.4. *Let $V : \mathbb{R} \to \mathbb{R}$ satisfy (20), then there exist $\epsilon, K > 0$ such that*

$$\mu_N^x \left(\frac{1}{N} \sum_{b \in \Lambda_N} \eta(b)^2 \geq K \right) \leq e^{-\epsilon N}, \tag{21}$$

and subsequently $\{\mu_N^x\}_{N\in\mathbb{N}}$ is tight.

Proof. Before proving that (21) holds, we show that this condition is sufficient for tightness. For a given bond b', translation invariance of μ_N^x allows us to rewrite $\mu_N^x(|\eta_{b'}| \geq L)$ as:

$$\mu_N^x(|\eta_{b'}| \geq L) = E_{\mu_N^x}\left[1_{|\eta_{b'}|\geq L}\right] = E_{\mu_N^x}\left[\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L}\right],$$

where 1_A is the indicator function of an event A. Now for any $\delta > 0$

$$E_{\mu_N^x}\left[\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L}\right] = E_{\mu_N^x}\left[1_{\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L}>\delta}\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L}\right] + E_{\mu_N^x}\left[1_{\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L}\leq\delta}\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L}\right].$$

Since $\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L} \leq 1$ and $1_{|\eta_{b'}|\geq L}1_{|\eta_{b'}|\geq L} \leq 1_{|\eta_{b'}|\geq L}\eta_{b'}^2/L^2$ we have that

$$E_{\mu_N^x}\left[\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L}\right] \leq \delta + \mu_N^x\left[\frac{1}{N}\sum_{b\in\Lambda_N} 1_{|\eta_{b'}|\geq L} > \delta\right] \leq \delta + \mu_N^x\left[\frac{1}{N}\sum_{b\in T_N}\eta_{b'}^2 \geq \delta L^2\right].$$

It follows that

$$\mu_N^x(|\eta_{b'}| \geq L) \leq \delta + \mu_N^x\left[\frac{1}{N}\sum_{b\in T_N}\eta_{b'}^2 \geq \delta L^2\right],$$

and setting $\delta = K/L^2$

$$\mu_N^x(|\eta_{b'}| \geq L) \leq \frac{K}{L^2} + e^{-\epsilon N}. \tag{22}$$

By adjusting L, one sees that the right handside can be chosen to be arbitrarily small (dependent on N). We now return to show (21). For $0 < \delta < c_2/2$, define

$$H_N^{x,\delta}(u) = H_N^x(u) - \delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2.$$

Given

$$\int e^{-H_N^x(u)+\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2} = Z_{N,x}\int\frac{1}{Z_{N,x}}e^{-H_N^x(u)+\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2} = Z_{N,x}E_{\mu_N^x}\left[e^{\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2}\right],$$

it follows that

$$E_{\mu_N^x}\left[e^{\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2}\right] = \frac{Z_{N,x}^\delta}{Z_{N,x}}.$$

Combining this with (19) and (20) we obtain,

$$\limsup_{N\to\infty}\frac{1}{N}\log E_{\mu_N^x}\left[e^{\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2}\right] \leq K_3(\delta)$$

where $K_3(\delta) < \infty$. Now, using the Markov inequality

$$\mu_N^x\left[\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2 \geq \delta K\right] = \mu_N^x\left[e^{\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2} \geq e^{\delta K}\right] \leq \frac{E_{\mu_N^x}\left[e^{\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2}\right]}{e^{\delta K}}$$

from which it follows that

$$\limsup_{N\to\infty}\frac{1}{N}\log\mu_N^x\left[\delta\frac{1}{N}\sum_{b\in\Lambda_N}\eta(b)^2 \geq \delta K\right] \leq -(K\delta - K_3(\delta)).$$

(21) follows by choosing K and ϵ such that $K > \delta^{-1}K_3(\delta)$, and $\epsilon = K\delta - K_3(\delta)$ □

Having confirmed that tightness holds for our class of potentials, we conclude our study of nearest neighbour interactions by applying our theory to some concrete examples. We note, however, that tightness is widely accepted to hold within a broader class of potentials, and so we relax condition (19).

2.3 Examples

In the preceeding sections we saw that for nearest neighbour interactions satisfying conditions (8), (10)-(12) that for any tilt $x \in \mathbb{R}$ then a limit measure μ^x exists along a subsequence of $\{\mu_N^x\}$, and that the free energy f exists, is twice differentiable and convex. We now apply our findings to several examples of potentials within our framework; we will see that the restrictions we apply allow us to work with potentials that could not be studied under the conditions given in [9].

2.3.1 Gaussian Potential

As a first example we take a Gaussian potential, for which an explicit closed formula for the free energy is known, [9]. The potential is given by

$$V(\eta) = \frac{c}{2}\eta^2, \qquad c > 0. \tag{23}$$

For this choice of potential the partition function $\widehat{Z}_\lambda$ introduced in (13) can be computed explicitly as a Gaussian integral

$$\widehat{Z}_\lambda = \int_{\mathbb{R}} e^{\lambda\eta - \frac{c}{2}\eta^2} d\eta = \sqrt{\frac{2\pi}{c}} e^{\lambda^2/2c}.$$

Then by the definition of $x(\lambda)$, taking logs and differentiating gives $x(\lambda) = \lambda/c$, it follows that $\lambda(x) = cx$ and hence

$$f(x) = \frac{c}{2}x^2. \tag{24}$$

2.3.2 Superposition of Gaussian Potentials

Throughout we have stressed that our methods do not depend on the potential being convex, we now make use of this in defining the following superposed Gaussian potential. Fix $\kappa_1, \kappa_2 > 0$, and $p \in [0,1]$ the potential $V : \mathbb{R} \to \mathbb{R}$ is defined by

$$\exp\big(-V(\eta)\big) = p\exp\left(-\frac{\kappa_1}{2}\eta^2\right) + (1-p)\exp\left(-\frac{\kappa_2}{2}\eta^2\right). \tag{25}$$

Here $\kappa_1, \kappa_2 > 0$ are stiffness parameters and it is generally assumed that $\kappa_1 \gg \kappa_2$, so that the Gaussian described by κ_1 is highly concentrated and describes the behaviour of ordered bonds, whilst the Gaussian described by κ_2 is disperse and describes disorder in the system. The weight parameter, p, is chosen to be biased towards either order or disorder. The measure can be reformulated so that with probability p (respectively $1-p$) the distribution is conditioned to behave according to the density $\exp(-\frac{\kappa_1}{2}\eta^2)$ (respectively $\exp(-\frac{\kappa_2}{2}\eta^2)$).

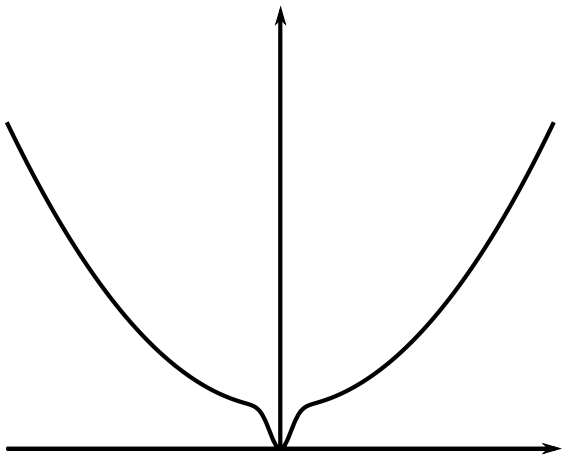


Figure 4: Superposition of two Gaussian potentials.

The potential (25) (as shown in figure 4) is studied in [2] for lattice boxes $\Lambda \subset \mathbb{Z}^d$, $d \geq 2$, endowed with periodic boundary conditions. Biskup and Kotecký show that for $d = 2$, with tilt $x = 0$ if $\kappa_1/\kappa_2 \gg 1$ then a critical probability p_t at which the model exhibits a phase transition, in the sense that there exist two distinct gradient Gibbs measures. In particular they determine p_t by the equation $p_t/(1-p_t) = (\kappa_1/\kappa_2)^{1/4}$, [2] Theorem 2.5. Further they observe that a 'roughening' transition occurs at p_t, in line with Remark 2.

In our 1-dimensional setting it can be confirmed that the potential described by (25) satisfies conditions the conditions of Lemma 2.2. Using the same Gaussian integral evaluation we used for the potential (23),

we can easily compute the partition function $\widehat{Z}_\lambda$ for the superposed Gaussian potential

$$\begin{aligned}\widehat{Z}_\lambda &= \int_{\mathbb{R}} e^{\lambda\eta}\left(p\exp\left(-\frac{\kappa_1}{2}\eta^2\right)+(1-p)\exp\left(-\frac{\kappa_2}{2}\eta^2\right)\right)d\eta \\ &= p\int_{\mathbb{R}}\exp\left(\lambda\eta-\frac{\kappa_1}{2}\eta^2\right)d\eta+(1-p)\int_{\mathbb{R}}\exp\left(\lambda\eta-\frac{\kappa_2}{2}\eta^2\right)d\eta \\ &= p\sqrt{\frac{2\pi}{\kappa_1}}e^{\lambda^2/2\kappa_1}+(1-p)\sqrt{\frac{2\pi}{\kappa_2}}e^{\lambda^2/2\kappa_2}\end{aligned}$$

Again drawing comparison with the simple Gaussian potential, we identify $x(\lambda)$ by taking logs and differentiating

$$\begin{aligned}x(\lambda) &= \frac{d}{d\lambda}\log\left(p\sqrt{\frac{2\pi}{\kappa_1}}e^{\lambda^2/2\kappa_1}+(1-p)\sqrt{\frac{2\pi}{\kappa_2}}e^{\lambda^2/2\kappa_2}\right) \\ &= \left(\frac{\kappa_2 a+\kappa_1 b}{\kappa_1\kappa_2(a+b)}\right)\lambda\end{aligned}$$

where $a \coloneqq pe^{\frac{\lambda^2}{2\kappa_1}}\sqrt{\frac{2\pi}{\kappa_1}}$ and $b \coloneqq (1-p)e^{\frac{\lambda^2}{2\kappa_2}}\sqrt{\frac{2\pi}{\kappa_2}}$, and we define

$$C(\lambda) \coloneqq \left(\frac{\kappa_2 a+\kappa_1 b}{\kappa_1\kappa_2(a+b)}\right),$$

so that $x(\lambda) = C(\lambda)\lambda$. If we choose the stiffness parameters so that $\kappa_1, \kappa_2 > 1$ then $(\kappa_1\kappa_2)^{-1} < C(\lambda) < 1$; from this we obtain bounds on the free energy by

$$\begin{aligned}\frac{\lambda}{\kappa_1\kappa_2} < x(\lambda) < \lambda &\implies x < \lambda(x) < \kappa_1\kappa_2 u \\ &\implies \int_0^x s\,ds < f(x) < \kappa_1\kappa_2\int_0^x s\,ds \\ &\implies \frac{x^2}{2} < f(x) < \kappa_1\kappa_2\frac{x^2}{2}.\end{aligned}$$

Similarly when $\kappa_1, \kappa_2 < 1$ we have

$$\kappa_1\kappa_2\frac{x^2}{2} < f(x) < \frac{x^2}{2}.$$

Whilst we have not been able to obtain a formula for f, our method has enabled us to find bounds which show that f is $O(x^2)$.

2.3.3 Double Well Potential

As a final example we consider the double well potential

$$V(\eta) \coloneqq \frac{c}{2}(\eta^2-1)^2. \tag{26}$$

Again, it is easily confirmed that V (as shown in figure 5) satisfies the requirements of Lemma 2.2; whilst our proof of tightness in section 2.2 does not cover the double well potential, in line with Remark 5 since it has tails of order $O(\eta^4)$ we assume that tightness does in fact hold. Applying Lemma 2.2 we note that the free energy exists and is strictly convex. Whilst we have not found an explicit formula for the free energy, the fact that it is strictly convex is interesting in itself, since one would not expect this of a potential that has two energy minima.

For such a potential one would expect to find two distinct equilibrium configurations, one of which favours $+1$-valued bonds, whilst the other has a majority of -1-valued bonds, in turn corresponding to the existence of two distinct Gibbs measures, and the occurrence of a phase transition. However, the strict convexity of the surface tension corresponds to a strict energy minimum of the system, which would appear to contradict this reasoning, and indicates (though does not prove) a lack of phase transition.

This rather counterintuitive situation is commonplace in 1-dimension, and can be partially explained by comparison to other models. Noting that the potential V has energy minima at ± 1 and has ground states of pure $+1$ and pure -1 configurations, it is somewhat natural to relate it to the 1-dimensional Ising model, which is known not to exhibit a phase transition even though the model does in higher dimensions.

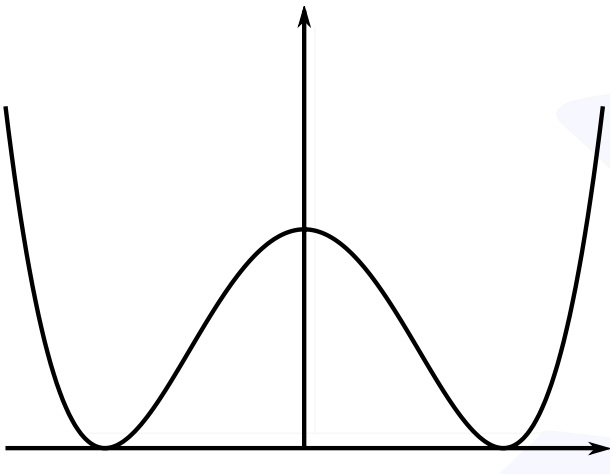


Figure 5: The double well potential.

A second comparison is to a random walk; viewing configurations as height fields, the model is known to have a random walk representation, described by the potential (26). If the random walk is seen to have long range dependence, then this would indicate the possibility of phase transition since the first step chosen would then bias all our remaining steps; the double well would then result in two possible Gibbs states, corresponding to whether we had first stepped according to the left or right well. However, the symmetry of the double well potential indicates that the walk will be recurrent, and the tails of the distribution decay sufficiently fast as to stop long range dependency. As a result we see that the model fluctuates wildly, in particular the variance of the height field at the origin is $O(N)$. This lack of long range interaction justifies the lack of a phase transition. On the other hand, as we increase dimension, we would see this behaviour does not continue to hold: the variance above drops to $O(\log N)$ for $d = 2$, and drops further as d is increased; so whilst the phase transition is not observed in 1 dimension, we would not expect this to hold in higher dimensions.

As a final justification, consider the case of zero tilt (purely fore ease of understanding), $x = 0$. The loop condition asserts that the mean value taken by a bond is 0, and since the double well concentrates mass around bonds taking ± 1 values, this is saying that we expect there to be equally as many $+1$ bond as their are -1. Taking the thermodynamic limit, one expects to preserve this balance between positive and negative bonds, which is to say that there is a unique limiting Gibbs measure in which we have phase coexistence, rather than the expected distinct Gibbs measures corresponding to the two possible phases.

Remark 6. The inverse temperature β is taken into account by the constants that have been used in the definitions of these potentials. Classically in statistical mechanics the free energy would be calculated in terms of β, because temperature related phase transitions are often studied. However, as we have concentrated on how properties of the potential affect existence and convexity of the free energy, we have neglected to deal explicitly with this parameter. In the next section we will see how β fits into the setting of the free energy more explicitly.

3 Next Nearest Neighbour Interactions

In this section we move away from studying nearest neighbour interactions, and instead consider pure next nearest potentials, $V_1 \equiv 0$, $V_2 \not\equiv 0$. We take a complementary approach to that taken in section 2, and follow the work of Blanc et al., [3]. In that paper, they prove an asymptotic statement about the free energy in the case of nearest neighbour interactions on a line segment. They consider the same gradient model as we described in section 1.2, however do not apply periodic boundary conditions; further they simultaneously take the thermodynamic and scaling limits. That is they rescale the box Λ_N onto the unit interval $[0, 1]$, so that their potential is of the form

$$H_N(u) = \sum_{i=1}^{N} V\left(\frac{u_i - u_{i-1}}{h}\right), \qquad h = \frac{1}{N}.$$

In this setting they show the following.

Theorem 3.1 (Blanc et al., [3])**.** *Assume the potential V satisfies*

$$\forall \lambda \in \mathbb{R}, \quad \int_{\mathbb{R}} \exp(\lambda y - \beta V(y)) dy < \infty,$$

and $\exp(-\beta V) \in H^1(\mathbb{R}\backslash 0)$. Then the limit behaviour of f_N is given by the Legendre transform

$$\lim_{N\to\infty} \left(f_N(x) + \frac{1}{\beta} \log \frac{z}{N} \right) = F_\infty(x),$$

where

$$F_\infty(x) := \frac{1}{\beta} \sup_{\xi} \left(\xi x - \log \left[z^{-1} \int_{\mathbb{R}} \exp(\xi y - \beta V(y)) dy \right] \right), \tag{27}$$

and $z = \int_{\mathbb{R}} \exp\left(-\beta V(y)\right) dy$.

We note that in their setting the limit $\lim_{N\to\infty} F_N$ does not actually exist, a quirk which arises as a result of the box rescaling. The theorem relies strongly on the fact that for nearest neighbour interactions, the Hamiltonian can be rewritten as a sum over weighted bonds; under this framework the bond weights are independent of one another, which is imperative for the subsequent application of well known large deviations results. The essential difference between the approach taken in this section, and the work of section 2 is that we work the loop condition into the integrand of the partition function, as opposed to considering it as a condition on the measure; this allows us to bypass the results of Guo et al. for conditioned measures, and facilitates the large deviations approach.

Remark 7. Whilst we follow the methods of Blanc et al. we remain true to the description of the gradient model given in section 1.2 and continue to consider $\Lambda_N \subset \mathbb{Z}$ with unit spacing, i.e. we fix $h = 1$ and do not take a scaling limit, with the result that the free energy exists; our results however will strongly echo those of [3].

In the spirit of this report, we aim to prove an analogous result to Theorem 3.1 for the thermodynamic limit, and in particular extend the result to pure next nearest neighbour interactions on the torus. To introduce this approach and because it serves as an auxiliary result, we first redo the main calculation used by Blanc et al. in Theorem 3.1 for nearest neighbour interactions.

3.1 Nearest Neighbour Interactions on the Torus

As an initial exercise we confirm that Theorem 3.1 continues to hold when we bestow the lattice segment $\Lambda = \Lambda_N = \{0, 1, \ldots, N\}$ with periodic boundary conditions and consider the thermodynamic limit.

Recall that the tilted Hamiltonian, with tilt $x \in \mathbb{R}$, for nearest neighbour interactions on $\Lambda = \Lambda_N$ is

$$H_N(u_1, \ldots, u_N) = \sum_{i=0}^{N} V\left(u_i - u_{i-1} + x\right), \tag{28}$$

and that the free energy for the finite box is given to be

$$f_N(x) = -\frac{1}{\beta|\Lambda|} \log Z_N, \tag{29}$$

where $|\Lambda| = N+1$, and Z_N is the partition function

$$Z_N = \int_{\mathbb{R}^N} \exp\Big(-\beta H_N(u_1, \dots, u_N)\Big) du_1, \dots, du_N.$$

For a configuration $u \in \Lambda^{\mathbb{R}}$ consider the induced bond configuration $y \in \mathcal{B}(\Lambda)^{\mathbb{R}}$ given by

$$y_i = \frac{u_i - u_{i-1}}{h}, \qquad 0 \le i \le N,$$

under periodic boundaries: $u_{N+1} = u_0$, $u_{-1} = u_N$. Here h represents the interatomic spacing, which we take to be $h = 1$ to obtain the thermodynamic limit; we also fix $u_0 = 0$ by translation invariance.

The loop condition (2) allows us to free a variable, since given knowledge of $y_0, \dots, y_{N-1}$, the final bond gradient is uniquely determined. In particular

$$y_N + x = x - \sum_{i=0}^{N-1} y_i. \tag{30}$$

In what follows we use the modified bond gradients

$$\tilde{y}_i = y_i + x, \qquad 0 \le i \le N,$$

to shorten the equations. Under this notation, (30) reads:

$$\tilde{y}_N = (N+1)x - \sum_{y_0}^{N-1} \tilde{y}_i.$$

Performing the change of variables (from site evaluations to bonds) and using the equality above we obtain

$$f_N(x) = -\frac{1}{\beta(N+1)} \log \int_{\mathbb{R}^N} \exp\left(-\beta \sum_{i=0}^{N-1} V(\tilde{y}_i) - \beta V\left((N+1)x - \sum_{i=0}^{N-1} \tilde{y}_i\right)\right) d\tilde{y}_0 \dots d\tilde{y}_{N-1},$$

where the Jacobian for the change of variables has determinant equal to 1. To proceed we recognise the integral as a convolution of i.i.d. random variables. More precisely, let μ_{N+1} denote the law of the empirical sum $(N+1)^{-1}\sum_{i=0}^{N} \widetilde{Y}_i$, where the $\widetilde{Y}_i$ are i.i.d. with law $\mu(\cdot) \propto \exp(-\beta V(\cdot))$. The measure μ_{N+1} is be obtained as a convolution of the μ

$$\mu_{N+1}(x) = \frac{N+1}{z^{N+1}} \int_{\mathbb{R}^N} \exp\left(-\beta \sum_{i=0}^{N-1} V\Big(\tilde{y}_i\Big) - \beta V\left((N+1)x - \sum_{i=0}^{N-1} \tilde{y}_i\right)\right) d\tilde{y}_0 \dots d\tilde{y}_{N-1},$$

where z is the normalising constant for μ. We note that this agrees with the result of Guo, Papanicolaou and Varadhan [11], who show that in the limit each of the $\tilde{y}_i$ are i.i.d. with law μ. Substituting into the formula for the free energy

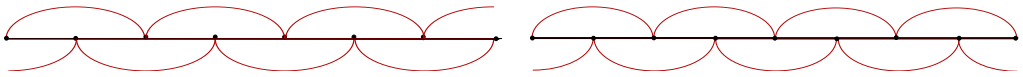
$$\begin{aligned} f_N(x) &= -\frac{1}{\beta(N+1)} \log\left(\mu_{N+1}(x)\frac{z^{N+1}}{N+1}\right) \\ &= -\frac{1}{\beta}\log z - \frac{1}{\beta(N+1)}\log \mu_{N+1}(x) - \frac{1}{\beta(N+1)}\log\frac{1}{N+1} \\ &= -\frac{1}{\beta(N+1)}\log\frac{1}{N+1} - \frac{1}{\beta}\log z - \frac{1}{\beta(N+1)}\log\mu_{N+1}(x). \end{aligned}$$

We are now done since the sequence $(\mu_N)_{N=1}^{\infty}$ satisfies an LDP and Blanc et al. apply large deviation techniques to establish the limiting behaviour. Note the first term converges to 0 as $N \to \infty$. Hence we obtain the following corollary.

Corollary 3.2. *If V satisfies the conditions of Theorem 3.1, then for the gradient Gibbs model with periodic boundary conditions the limit $f = \lim_{N\to\infty} f_N$ is is given to be*

$$f(x) = F_\infty(x) - \frac{1}{\beta}\log z,$$

where F_∞ is given by (27).



(a) Odd case. (b) Even case.

Figure 6: Analysis on torus depends on parity of number of atoms.

Remark 8. Whist we have not made explicit reference to the use of the condition on the potential, we note that it is crucial as it facilitates the large deviations approach; moreover, the moment generating function appears in the definition of F_∞. We also note that this is exactly the same condition as (11), which was required in the previous approach where it was necessary for the use of the log moment generating function and further underlying large deviations reasoning from [11].

The existence of the limit f, unlike in Theorem 3.1, is a result of not rescaling the atomic spacing and not a consequence of considering the model on the torus. We see that giving the box periodic boundaries has not had an effect on the form of the free energy.

3.2 Pure Next Nearest Neighbour Interaction

Still considering Λ to be endowed with periodic boundary conditions we now consider the case where the energy H_N is determined by a next nearest neighbour potential. Incorporating the tilt, that is

$$H_N(u_1, \dots, u_N) = \sum_{i=0}^{N} V\left(\frac{u_{i+1} - u_{i-1}}{2} + x\right), \tag{31}$$

where as before we have periodic labelling of the variables. We observe that for next nearest neighbour interactions on the finite lattice segment $\Lambda_N = \{0, 1, \dots, N\}$ the analysis of the free energy is done in two cases, see Figure 6. If Λ has an even number of vertices, ie. $N = 2M - 1$, then the model decomposes into two independent chains one containing all odd vertices and the other containing the even vertices. Alternatively if $N = 2M$ then we have one chain containing all of the vertices. In both cases we seek to reduce the calculations to those of the nearest neighbour model, with the only difference occurring from the increased distance between interacting particles. In the following we describe the relevant calculations for the two cases, and in particular observe that in the limit the resulting expressions agree.

3.2.1 Cycle Decomposition when $N = 2M - 1$

When the lattice $\Lambda = \Lambda_N$ has an even number of vertices, $N = 2M - 1$, then the next nearest neighbour interactions split the energy into two independent sums: one over the odd vertices, and the other over the evens. To emphasise this we relabel the elements $u \in \mathbb{R}^\Lambda$ as

$$u_{2k+1} =: u_k^{(1)}, \quad u_{2k} =: u_k^{(2)}, \qquad \text{for } k = 0, \dots, M.$$

As in the previous case we fix $u_0^{(1)} = u_0^{(2)} = 0$ and observe that the Hamiltonian factorises as

$$\begin{aligned} H_N(u^{(1)}; u^{(2)}) &= H_N(u^{(1)}) + H_N(u^{(2)}) \\ &= \sum_{i=0}^{M} V\left(\frac{u_i^{(1)} - u_{i-1}^{(1)}}{2} + x\right) + \sum_{i=0}^{M} V\left(\frac{u_i^{(2)} - u_{i-1}^{(2)}}{2} + x\right). \end{aligned}$$

The factorisation can now be used to split the exponential term

$$\exp\big(-\beta H_N(u^{(1)}; u^{(2)})\big) = \exp\big(-\beta H_N(u^{(1)})\big) \exp\big(-\beta H_N(u^{(2)})\big),$$

after which the calculation of the free energy proceeds by Fubini's theorem, and the change of variables described in section 3.1

$$\begin{aligned} f_N(x) = &- \frac{1}{\beta(2M)} \log \int_{\mathbb{R}^M} \exp\left(\sum_{i=0}^{M} V\left(\frac{u_i^{(1)} - u_{i-1}^{(1)}}{2} + x\right)\right) du_1^{(1)} \dots du_M^{(1)} \\ &- \frac{1}{\beta(2M)} \log \int_{\mathbb{R}^M} \exp\left(\sum_{i=0}^{M} V\left(\frac{u_i^{(2)} - u_{i-1}^{(2)}}{2} + x\right)\right) du_1^{(2)} \dots du_M^{(2)}. \end{aligned}$$

As a result of the above factorisation we see that we can consider the two integrals as partition functions $Z_M^{(1)} = Z_M^{(2)} = Z_M$, where Z_M is the same partition function as in section 3.1 but with an extra factor $1/2$ corresponding to the spacing. By defining analogous changes of variables $\tilde{y}_i^{(1)}, \tilde{y}_i^{(2)}$, we obtain

$$\begin{aligned} f_N(x) &= -\frac{1}{\beta M}\log Z_M \\ &= -\frac{1}{\beta M}\log\left(2^M \frac{z^{M+1}}{M+1}\mu_{M+1}\right) \\ &= -\frac{1}{\beta}\log 2 - \frac{(M+1)}{\beta M}\log z - \frac{1}{\beta M}\log\frac{1}{M+1} - \frac{1}{\beta M}\log\mu_{M+1}. \end{aligned}$$

Note that in the limit we see

$$\lim_{N\to\infty} f_N(x) = -\frac{1}{\beta}\log 2 - \frac{1}{\beta}\log z - \lim_{M\to\infty}\frac{1}{\beta M}\log\mu_{M+1}(x).$$

Noting that $M^{-1} = (M+1)^{-1} + (M(M+1))^{-1}$ then

$$\frac{1}{\beta M}\log\mu_{M+1}(x) = \frac{1}{\beta(M+1)}\log\mu_{M+1}(x) + \frac{1}{\beta M(M+1)}\log\mu_{M+1}(x),$$

and by the quotient rule for real sequences

$$\lim_{M\to\infty}\frac{1}{\beta M}\log\mu_{M+1}(x) = \lim_{M\to\infty}\frac{1}{\beta(M+1)}\log\mu_{M+1}(x).$$

In the case of an even number of lattice points, our intuition is correct and the next nearest neighbour interaction behaves as a scaled nearest neighbour interaction.

3.2.2 Looped Cycle when $N = 2M$

When we have an odd number of lattice sites the energy no longer factorises as in the above, but instead we see a 'looped' cycle occurring: where there is dependence between all of the vertices, but nearest neighbours do not directly interact. At a heuristic level we expect this to behave similarly to the previous case, since the 'influence' that a vertex has over its neighbour is diluted as we pass through M other vertices before being affected. In particular as N grows, this influence decreases as the behaviour at each site is dominated by the particles that are close in the loop; at the extreme level in the limit we would in fact observe two independent (infinite) loops, which is the same limiting view as is observed in the even case. We therefore expect the limiting free energies to agree.

Again the computation reduces to being the same as in section 3.1. Now $\Lambda = \Lambda_N = \{0,\dots,N\}$, $N = 2M$ and the energy $H_N : \mathbb{R}^\Lambda \to \mathbb{R}$ is given by (31). Letting $Z_N = Z_{2M}$ be the partition function as before (with spacing 2) then

$$\begin{aligned} f_N(x) &= -\frac{1}{\beta(N+1)}\log Z_N \\ &= -\frac{1}{\beta(2M+1)}\log\left(2^{2M}\frac{z^{2M+1}}{2M+1}\mu_{2M+1}(x)\right) \\ &= -\frac{2M}{\beta(2M+1)}\log 2 - \frac{1}{\beta}\log z - \frac{1}{\beta(2M+1)}\log\frac{1}{2M+1} - \frac{1}{\beta(2M+1)}\log\mu_{2M+1}(x). \end{aligned}$$

Taking the limit in N we see,

$$\lim_{N\to\infty} f_N(x) = -\frac{1}{\beta}\log 2 - \frac{1}{\beta}\log z - \lim_{M\to\infty}\frac{1}{\beta(2M+1)}\log\mu_{2M+1}(x),$$

which we observe agrees with the limit in the even case.

Theorem 3.3. *For a pure next nearest neighbour potential V satisfying the same requirements as in Theorem 3.1 for the gradient model on the torus, the limit of the free energy exists and is given by*

$$f(x) = F_\infty(x) - \frac{1}{\beta}\log 2z, \tag{32}$$

where F_∞ is given by (27).

4 Mixed Gaussian Interactions

The approach taken in the previous section can only take us so far, and it is not readily apparent how we could extend the method to consider the case when we have non-trivial nearest and next nearest interactions, i.e. $V_1, V_2 \not\equiv 0$. In our final section we place stronger restrictions on the choice of potential and assume that they are Gaussian. When the potentials are chosen to have this form the problem can be rephrased as one for linear operators, which can be handled via discrete Fourier analysis, [14]. Since this approach only works for Gaussian potentials, one would be inclined to believe that the method is limited; however by taking second order Taylor expansions of more general potentials, it is possible to find Gaussian approximations. In particular, we may approximate general potentials W_i by Gaussians $V_i = a_i r^2$, $i = 1, 2$, where

$$a_1 = \frac{1}{2} W_1''(x), \qquad a_2 = \frac{1}{2} W_2''(x),$$

which capture the curvature of the potentials W_i at x. We obtain

$$H(\phi) \sim \sum_j a_1 (u_j - u_{j-1} + x)^2 + 4a_2 \left(\frac{u_{j-1} - u_{j+1}}{2} + x \right)^2 . \tag{33}$$

The matrix analysis approach we take is particularly appealing since endowing Λ with periodic boundaries ensures that the relevant matrices are all circulant, a class of matrices for which there is a rich spectral theory. In the following we first consider the gradient model with pure interactions, before turning to the new case of mixed potentials. Finally we comment briefly on Hamiltonians with additional external forces. Before studying our model, however, we briefly review some basic facts from the study of circulant matrices.

Recall that a real $(n \times n)$-matrix $M \in \mathbb{R}^{n \times n}$ is said to be circulant if successive rows are given by a shift of the preceding row; in particular, if there exists $c = (c_0, \dots, c_{n-1}) \in \mathbb{R}^n$ such that

$$M = \begin{pmatrix} c_0 & c_{n-1} & \dots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & \dots & c_2 \\ \dots & c_1 & c_0 & \ddots & \vdots \\ c_{n-2} & & \ddots & \ddots & c_{n-1} \\ c_{n-1} & c_{n-2} & \dots & c_1 & c_0 \end{pmatrix}.$$

We denote this matrix by $M = \mathrm{circ}\{c\} = \mathrm{circ}\{c_0, \dots, c_{n-1}\}$. We will require the following basic results, and point the reader to [5, 10] for further details.

Theorem 4.1. *Let C denote an arbitrary circulant matrix, $C \in \mathbb{R}^{n \times n}$, and denote $\{\omega_j\}_{j=1}^n$ for the n-th roots of unity: $\omega_1 = \exp(2\pi i/n)$, $\omega_j = \omega_1^j$. The eigenvectors $\{y^{(j)}\}_{j=1}^n$ of C are given by*

$$y^{(j)} = \frac{1}{\sqrt{n}} \left(1, \omega_j, \dots, \omega_j^{n-1}\right),$$

and the corresponding eigenvalues are

$$\lambda_j = \sum_{k=0}^{n-1} c_k \omega_j^{n-k}.$$

Moreover, C can be expressed in the form $C = Y^T \Psi Y$, where Y is such that for $1 \le j \le n$, the j-th column is $y^{(j)}$, and $\Psi = diag\,(\lambda_k)$.

Remark 9. Note that the theorem above asserts that all circulant matrices have the same eigenvectors, and the same diagonalisation matrix Y.

Theorem 4.2. *Let $B, C \in \mathbb{R}^{n \times n}$ be circulant matrices with eigenvalues $\{\lambda_j\}_{j=1}^n, \{\mu_j\}_{j=1}^n$ respectively. Then the matrix $B + C$ is circulant and has eigenvalues $\{\lambda_j + \mu_j\}_{j=1}^n$.*

4.1 Spectral Analysis of Pure Interactions

As a first application of the spectral method we revisit the cases of pure nearest neighbour, and pure next nearest neighbour interactions ($V_1 \not\equiv 0$, $V_2 \equiv 0$ and $V_1 \equiv 0$, $V_2 \not\equiv 0$ respectively). In light of Theorem 4.2, the mixed case will then be approachable.

4.1.1 Nearest Neighbour

Consider the model with nearest neighbour potential $V_1(r) = a_1 r^2$; substituting this into (28), we obtain the corresponding Hamiltonian H_1, given by

$$H_1(u_1, \dots, u_N) = a_1 \sum_{k=0}^{N} (u_k - u_{k-1})^2 + a_1(N+1)x^2,$$

where the loop condition ensures that the cross terms vanishes. Noting that the linear operator $\nabla_1 u_k = u_k - u_{k-1}$ has the matrix representation

$$\nabla_1 = \operatorname{circ}\{1, 0, \dots, 0, -1\} \in \mathbb{R}^{(N+1)\times(N+1)},$$

with respect to the standard basis, then we find

$$\begin{aligned} H_1 &= a_1 U^T {\nabla_1}^T \nabla_1 U + a_1(N+1)x^2 \\ &= a_1 U^T M_1 U + a_1(N+1)x^2, \end{aligned} \tag{34}$$

where $U = (u_0, u_1, \dots, u_N) \in \mathbb{R}^{N+1}$ and $M_1 = {\nabla_1}^T \nabla_1 = \operatorname{circ}\{2, -1, 0, \dots, 0, -1\}$. Now applying Theorem 4.1, and evaluating the sum, the eigenvalues of M_1 are found to be

$$\lambda_j^{(1)} = 4\sin^2\left(\frac{\pi j}{N+1}\right), \qquad 0 \le j \le N. \tag{35}$$

Defining $\Psi_1 = \operatorname{diag}\big(\lambda_j^{(1)}\big)$, (34) becomes

$$H_1 = a_1 U^T Y^T \Psi_1 Y U + a_1(N+1)x^2,$$

where Y is as in Theorem 4.1.

4.1.2 Next Nearest Neighbour

Similarly we consider the pure next nearest neighbour interaction with Gaussian potential $V_2(r) = a_2 r^2$, for which the Hamiltonian is

$$H_2(u_1, \dots, u_N) = \frac{a_2}{4} \sum_{k=0}^{N} (u_{k-1} - u_{k+1})^2 + a_2(N+1)x^2.$$

As before, we define the linear operator $\nabla_2 u_k = u_{k-1} - u_{k+1}$ with the representation $\nabla_2 = \operatorname{circ}\{0, -1, 0, \dots, 0, 1\}$. Defining $M_2 = \nabla_2^T \nabla_2^T = \operatorname{circ}\{2, 0, -1, 0, \dots, 0, -1, 0\}$, the Hamiltonian becomes

$$H_2 = \frac{a_2}{4} U^T M_2 U + a_2(N+1)x^2.$$

Applying Theorem 4.1, the eigenvalues of M_2 are found to be

$$\lambda_j^{(2)} = 4\sin^2\left(\frac{2\pi j}{N+1}\right), \qquad 0 \le j \le N, \tag{36}$$

and so

$$H_2 = \frac{a_2}{4} U^T Y^T \Psi_2 Y U + a_2(N+1)x^2, \qquad \text{where } \Psi_2 = \operatorname{diag}\left(\lambda_j^{(2)}\right).$$

Remark 10. We observe that the method described above can be trivially extended for arbitrary range pure potentials $V_k(r) = a_k r^2$. Defining ∇_k, M_k analogously to the above we find that the eigenvalues of M_1 are

$$\lambda_j^{(k)} = 4\sin^2\left(\frac{k\pi j}{N+1}\right), \qquad 0 \le j \le N,$$

and the Hamiltonian can be expressed as

$$H_k = \frac{a_k}{k^2} U^T Y^T \Psi_k Y U + a_k(N+1)x^2, \qquad \text{where } \Psi_k = \operatorname{diag}\left(\lambda_j^{(k)}\right).$$

4.2 Free Energy for Nearest and Next Nearest Neighbour Interactions

We now return to the case of interest where we have nearest and next nearest interactions simultaneously. We work with the Hamiltonian (33), i.e. $H = H_1 + 4H_2$, where H_1, H_2 are as above

$$H = U^T Y^T \left(a_1 \Psi_1 + a_2 \Psi_2\right) YU + (a_1 + 4a_2)(N+1)x^2.$$

Introducing the coordinates $(w_0, \ldots, w_N)^T = Y^T U$, the Hamiltonian is

$$\begin{aligned} H &= W^T \left(a_1 \Psi_1 + a_2 \Psi_2\right) W + (a_1 + 4a_2)(N+1)x^2 \\ &= \sum_{j=0}^{N} \left(a_1 \lambda_j^{(1)} + a_2 \lambda_j^{(2)}\right) w_j^2 + (a_1 + 4a_2)(N+1)x^2. \end{aligned}$$

The Jacobian for the change of variables has determinant equal to 1, and so the partition function is given by

$$\begin{aligned} Z_N &= \int_{\mathbb{R}^N} \exp\left(-\beta H(u_1, \ldots, u_N)\right) \, du_1 \ldots du_N \\ &= \exp\left(-\beta(a_1 + 4a_2)(N+1)x^2\right) \int_{\mathbb{R}^N} \exp\left(-\beta \sum_{j=1}^{N} \left(a_1 \lambda_j^{(1)} + a_2 \lambda_j^{(2)}\right) w_j^2\right) \, dw_1 \ldots dw_N. \end{aligned}$$

Recalling $\int_{\mathbb{R}} \exp(-\alpha x^2)\, dx = \sqrt{\pi/\alpha}$ for $\alpha > 0$ and since $\beta \left(a_1 \lambda_m^{(1)} + a_2 \lambda_m^{(2)}\right) > 0$

$$Z_N = \exp\left(-\beta(a_1 + 4a_2)(N+1)x^2\right) \left(\frac{\pi}{\beta}\right)^{N/2} \prod_{j=1}^{N} \left(a_1 \lambda_m^{(1)} + a_2 \lambda_m^{(2)}\right)^{-1/2}.$$

To compute the free energy we take logarithms, however we must impose a condition on a_1, a_2 to ensure positivity. Substituting in the eigenvalue expressions (35), (36) we obtain the condition

$$\min\{a_1, a_1 + 4a_2\} > 0, \tag{37}$$

which we henceforth assume. We return to the origins of this assumption in section 4.3. Taking logarithms we obtain the following limit.

Theorem 4.3. *The mixed next nearest neighbour interaction model on the torus with potentials $V_1(r) = a_1 r^2$, $V_2(r) = a_2 r^2$, where $\min\{a_1, a_1 + 4a_2\} > 0$, has free energy*

$$f(x) = (a_1 + 4a_2)x^2 - \frac{1}{2\beta} \log \frac{\pi}{\beta} + \frac{1}{2\beta} \lim_{N \to \infty} \sum_{j=1}^{N} \log\left(4a_1 \sin^2(\pi y_j) + 4a_2 \sin^2(2\pi y_j)\right) \Delta y$$

where we set $y_j = \frac{j}{N+1}$ for $0 \le j \le N$ and $\Delta y = \frac{1}{N+1}$.

In order to study the convergence of the free energy, we can realise the summation as a quadrature form

$$Q_N[g] := \sum_{j=1}^{N} g(y_j) \, \Delta y,$$

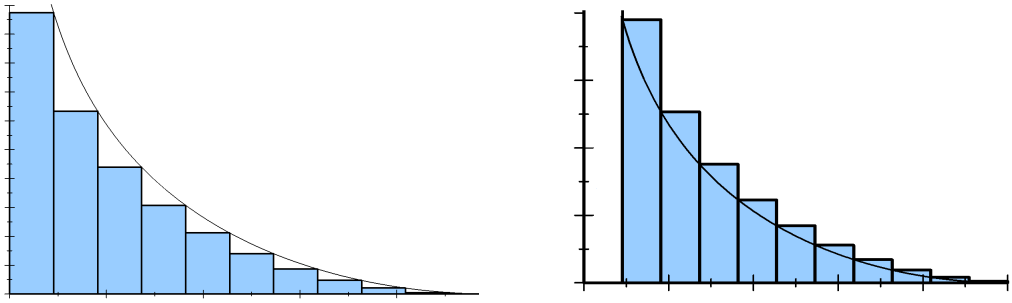
where $g = g_1 + g_2$ with

$$g_1(t) := -\log(\sin(\pi t)) \quad \text{and} \quad g_2(t) := -\log\left(4a_1 + 16a_2 \cos^2(\pi t)\right).$$

Since $g_2 \in C^\infty([0,1])$

$$\lim_{N \to \infty} Q_N[g_2] = \int_0^1 g_2(t)\, dt,$$

viewed as a Riemann sum for a Riemann-integrable function with convergence rate of order $1/N$. For g_1 we offer a more careful analysis for the convergence.



(a) Lower bound. (b) Upper bound.

Figure 7: Lower and upper integral bounds.

Lemma 4.4. *For g_1 defined above, $\int_0^1 g_1(t)\,dt$ is a convergent improper Riemann integral and*

$$\left|\int_0^1 g_1(t)\,dt - Q_N[g_1]\right| \leq C\frac{\log N}{N}$$

for some constant $C > 0$. Hence $\lim_{N\to\infty} Q_N[g_1] = \int_0^1 g_1(t)\,dt = \log 2$.

Proof. Note that g_1 is symmetric about $t = 1/2$ and moreover $g_1(1/2) = 0$, so that $Q_N[g_1] = 2\sum_{j=1}^{\lfloor N/2\rfloor} g_1(y_j)\Delta y$. It follows that we can restrict our attention to the interval $[0, 1/2]$. Looking at Figure 7 it is clear that

$$\int_{x_1}^{1/2} g_1(t)\,dt \leq \frac{1}{2}Q_N[g_1] \leq \int_0^{x_{\lfloor N/2\rfloor}} g_1(t)\,dt.$$

Defining the remainder $R_N[g_1] = \int_0^1 g_1(t)\,d(t) - Q_N[g_1]$, we see that it satisfies

$$\int_{x_{\lfloor N/2\rfloor}}^{1/2} g_1(t)\,dt \leq \frac{1}{2}R_N[g_1] \leq \int_0^{x_1} g_1(t)\,dt.$$

Finally, since $\log(x/2) \leq \log(\sin x) \leq \log x$ for $x \in (0, \pi/2]$, evaluating the integrals we deduce that the dominant rate of convergence is of order $N^{-1}\log N$. It follows that $\int_0^1 g_1(t)\,dt = \lim_{N\to\infty} Q_N[g_1]$. Integration by parts gives $\int_0^1 g_1(t)\,dt = \log 2$. □

Applying the lemma, we may take limits in both quadratures and hence obtain the following result for the free energy.

Theorem 4.5. *For the next nearest neighbour interaction model on the torus with potentials $V_1(r) = a_1 r^2$, $V_2(r) = a_2 r^2$, with $\min\{a_1, a_1 + 4a_2\} > 0$, the free energy is given by*

$$f(x) = (a_1 + 4a_2)x^2 - \frac{1}{2\beta}\log\frac{\pi}{\beta} + \frac{1}{2\beta}\int_0^1 \log\left(4a_1\sin^2(\pi t) + 4a_2\sin^2(2\pi t)\right)dt.$$

Moreover, the rate of convergence is of order $N^{-1}\log N$.

We observe that a strength of this method is that the constant term of the free energy is obtained explicitly. Moreover, taking $a_i = 0$ for either $i = 1, 2$ we obtain the free energy for pure interactions, and note that the expression agrees (up to a constant) with those found in previous sections, (24), (32).

Remark 11. Recall that we can approximate the Lennard-Jones potential via the potential $V = V_1 + V_2$, 1, where it is assumed that the coefficients satisfy $a_1 > 0 > 4a_2$. If in addition $|a_1| > 4|a_2|$, then condition (37) holds. In particular, under restrictions on the coefficients we are able to approximate the free energy of the Lennard-Jones potential.

In line with Remark 10 the result of Theorem 4.5 can be extended to hold for Hamiltonians which can be expressed as sums of pure Gaussian potentials; care must be taken in choosing the coefficients a_j however, to ensure that the logarithm of the partition function is well defined.

4.3 Stability

We now study the stability of the Hamiltonian for the mixed interaction model, which amounts to positive definiteness of the matrix H. We follow the work done in [12, 6] and introduce the ℓ^2-inner product

$$\langle u, v\rangle = \sum_{j=0}^{N} u_j v_j,$$

with induced norm $\|\cdot\|_{\ell^2}$.

Lemma 4.6. *H is positive definite, uniformly for $N \in \mathbb{N}$ if and only if $c = \min\{a_1, a_1 + 4a_2\} > 0$. Moreover for a configuration u on the torus*

$$\inf_{\|\nabla u\|_{\ell^2}=1} \langle Hu, u\rangle \geq c\|\nabla u\|_{\ell^2}, \tag{38}$$

where $\nabla = \nabla_1$ above.

Proof. Following the steps in [12, 6] we have

$$\begin{aligned}\langle Hu, u\rangle &= \textstyle\sum_{j=0}^{N}\left[(a_1+4a_2)\left|\nabla u_j\right|^2 - a_2\left|\Delta u_j\right|^2\right] \\ &= (a_1+4a_2)\left\|\nabla u\right\|_{\ell^2}^2 - a_2\left\|\Delta u\right\|_{\ell^2}^2\end{aligned}$$

where $\Delta u_j = \nabla^2 u_j = -u_{j-1} + 2u_j - u_{j+1}$. In the case $a_2 < 0$ we get (38) and if $a_2 > 0$, we use

$$\begin{aligned}\langle Hu, u\rangle &= \textstyle\sum_{j=0}^{N}\left[a_1\left|\nabla u_j\right|^2 + 4a_2\left|\nabla u_{j+1} + \nabla u_j\right|^2\right] \\ &\geq \textstyle\sum_{j=0}^{N} a_1\left|\nabla u_j\right|^2 \geq c\left\|\nabla u\right\|_{\ell^2}^2\end{aligned}$$

where the next nearest neighbour drops out and we obtain (38). □

This explains the condition (37) in the previous section; the lattice must be stable for the free energy to exist.

4.4 External Force for Nearest Neighbour Interaction

We finally turn to consider the case of an external force, as motivated in Section 1.1. To model this, we add a forcing term to the Hamiltonian

$$H^g_{N,x}(u) \coloneqq H_{N,x}(u) + \sum_{i=0}^{N+1} g_i(u_i) \tag{39}$$

where $H_{N,x}$ is as before, and $\{g_i\}_{i\in\mathbb{Z}}$ represent the strength of the force field on the particle sitting at site $i \in \mathbb{Z}$. A Taylor expansion of the functions g_i enables us to approximate the force in a dead-load form $g_i(u_i) \approx \tilde{g}_i u_i$, which simplifies the Hamiltonian. We assume that interactions between particles in different layers of the material are incorporated into this force field; this is a simplified form of the Frenkel-Kontorova model for vacancies and dislocations, [13]. In the dead-load form, we obtain the Hamiltonian

$$H^g(u) \coloneqq H_x(u) - g \cdot u,$$

where $H_x = H_{N,x}$ is used to simplify notation. Let u_g denote the minimiser of $H^g_x(\cdot)$, i.e. $\nabla H^g_x(u_g) = 0$. A Taylor expansion of $H^g_x(u)$ about u_g yields

$$\begin{aligned}H^g_x(u) &= H^g_x(u_g) + \nabla H^g_x(u_g)\cdot(u-u_g) + H_x(u-u_g) \\ &= H^g_x(u_g) + H_x(u-u_g),\end{aligned}$$

which is exact because we are working with a Gaussian potential. Indeed the second order derivatives are constants and in particular

$$\nabla^2 H^g_x(u_g)\cdot(u-u_g)^2 = H_x(u-u_g).$$

Setting $\psi = u - u_g$ and noting this change of variables has Jacobian with determinant equal to 1, we can write the free energy as

$$\begin{aligned} f_N^g(x) &= -\frac{1}{\beta N} \log \int_{\mathbb{R}^N} \exp\left(-\beta H_x^g(u)\right) \mathrm{d}u \\ &= -\frac{1}{\beta N} \log \int_{\mathbb{R}^N} \exp\left(-\beta H_x^g(u_g) - \beta H_x(u - u_g)\right) \mathrm{d}u \\ &= \frac{1}{\beta N} H_x^g(u_g) - \frac{1}{\beta N} \log \int_{\mathbb{R}^N} \exp\left(-\beta H_x(\psi)\right) \mathrm{d}\psi \\ &= \frac{1}{\beta N} H_x^g(u_g) + f_N(x), \end{aligned}$$

where $f_N(x)$ is the free energy on Λ_N, (29). We see that the external force manifests itself in the free energy as an extra additive term. With sufficient decay on the external force, we expect the limiting free energy to exist. As before, we can extend this calculation to more general potentials by taking a Taylor expansion, and approximating with suitable Gaussian potentials.

Remark 12. We have seen that the techniques employed in this section allow us to approach two problems that we were unable to answer in the previous sections; in particular we saw that so long as we worked in the Gaussian world, we were able to handle mixed potentials $V_1, V_2 \not\equiv 0$, as well as being able to add non-trivial external force terms. However, the set back of the spectral approach is that it is really only applicable under the Gaussian assumption; it is our hope that in future work one would be able to extend the ideas of the previous sections to handle these two problems. In particular, we expect that simple force terms could be incorporated into the Hamiltonian studied in section 3.

The methods employed in section 2 are however restricted to the nearest neighbour case with no extra force term in the Hamiltonian, thus future possible work in this area would consist of further weakening the conditions on the potential for which the free energy exists and can be analysed.

In this report we have restricted ourselves to dimension 1. But considerations like; can conditions on the potential be weakened, and how do we work with mixed interaction models, are very relevant and challenging, and would be worth pursuing in the context of higher dimensions.

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