

Mesoscopic Analysis of Droplets in Lattice Systems with Long-Range Kac Potentials

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Abstract We investigate the geometry of typical equilibrium configurations for a lattice gas in a finite macroscopic domain with attractive, long range Kac potentials. We focus on the case when the system is below the critical temperature and has a fixed number of occupied sites. We connect the properties of typical configurations to the analysis of the constrained minimizers of a mesoscopic non-local free energy functional, which we prove to be the large deviation functional for a density profile in the canonical Gibbs measure with prescribed global density. In the case in which the global density of occupied sites lies between the two equilibrium densities that one would have without a constraint on the particle number, a “droplet” of the high (low) density phase may or may not form in a background of the low (high) density phase. We determine the critical density for droplet formation, and the nature of the droplet, as a function of the temperature and the size of the system, by combining the present large deviation principle with the analysis of the mesoscopic functional given in Nonlinearity 22, 2919–2952 (2009).

Keywords Lattice systems · Kac potential · Critical droplet

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1 Introduction

The mathematical study of the behavior of a lattice gas of particles (or spins) interacting via a long range Kac potential, both in equilibrium and in non-equilibrium, has been the subject of many works: a recent book [7] provides a comprehensive treatment of the subject as it has developed so far.

The long-range Kac potential introduces a third length scale between the microscopic scale of the lattice spacing and the macroscopic scale of the size of the domain. This third scale is referred to as the mesoscopic scale. As we show here, one can determine the geometric nature of “typical” microscopic particle configurations for such systems through the analysis of a mesoscopic free energy functional that serves as a large deviations functional for the system. We do this in a scaling regime that is critical for droplet formation in these models.

The large deviations functional (LDF) with which we work is a functional of “coarse-grained density profiles”, different from the LDF used to study the corresponding problem in two dimensional nearest-neighbor Ising systems: There, the LDF is a function of “contours” associated to the microscopic configuration on a two dimensional lattice. The mesoscopic analysis that we carry out here goes through in any dimension. Before describing our results, we first describe the models with which we work more precisely.

1.1 The Grand Canonical and Canonical Measures for the Model

Let \mathcal{T}_L be the d -dimensional square torus with side length L . Let γ be such that $L\gamma^{-1}$ is an integer and $\Lambda_{L,\gamma}$ denote the part of the lattice $\gamma\mathbb{Z}^d$ contained in \mathcal{T}_L . For the purpose of connecting the microscopic and mesoscopic scales, it will be convenient, as in [1, 7], to regard $\Lambda_{L,\gamma}$ as a subset of \mathcal{T}_L . A *particle configuration* is a function s from $\Lambda_{L,\gamma}$ to $\{-1, 1\}$. The site $x(i) = \gamma i \in \Lambda_{L,\gamma} \subset \mathcal{T}_L$, $i \in \mathbb{Z}^d$ is *occupied* by a particle if $s(x(i)) = 1$, and is *unoccupied* if $s(x(i)) = -1$.

The Hamiltonian $H_{\gamma,L}$ for the system, giving the total interaction energy of a configuration, is

$$H_{\gamma,L}(s) = -\frac{\gamma^d}{2} \sum_{x(i),x(j) \in \Lambda_{L,\gamma}} J(|x(i) - x(j)|)s(x(i))s(x(j)), \tag{1.1}$$

where J is a non-negative smooth function on \mathbb{R}_+ that is bounded, continuous, supported by $[0, 1]$, and strictly monotone decreasing on $[0, 1]$, where $|x(i) - x(j)|$ denotes the distance separating $x(i)$ and $x(j)$ in the torus. We assume the normalization

$$\int_{\mathbb{R}^d} J(|r|)dr = 1. \tag{1.2}$$

This function J is the *interaction potential*. Since its range is of order γ^{-1} in microscopic units, $H_{\gamma,L}$ is a *local mean field* Hamiltonian: A particle at site $x(i) = \gamma i \in \Lambda_{L,\gamma}$ interacts with a local mean field of neighboring particles:

$$\gamma^d \sum_{x(j) \in \Lambda_{L,\gamma}} J(|x(i) - x(j)|)s(x(j)). \tag{1.3}$$

Let $\Omega_{L,\gamma} = \{-1, 1\}^{\Lambda_{L,\gamma}}$ denote the set of all particle configurations. For any $0 \leq N \leq L^d \gamma^{-d}$, the number of sites in $\Lambda_{L,\gamma}$, define

$$\Omega_{L,\gamma,N} := \left\{ s \in \Omega_{L,j} : \sum_{x \in \Lambda_{L,j}} (s(x) + 1)/2 = N \right\}.$$

Then $\Omega_{L,\gamma,N}$ is the space of N -particle configurations.

To simplify the notation going forward, we shall usually drop the subscripts from $H_{\gamma,L}$ and $\Lambda_{L,\gamma}$, referring to them simply as H and Λ respectively.

Given an inverse temperature β , the grand canonical Gibbs measure P_{gc} on $\Omega_{L,\gamma}$ is defined by

$$P_{gc}(\{s\}) = \frac{1}{Z_{gc}} \exp[-\beta H(s)] \quad \text{and} \quad Z_{gc} = \sum_{s \in \Omega} \exp[-\beta H(s)], \tag{1.4}$$

and the canonical Gibbs measure P_{can} on $\Omega_{L,\gamma,N}$ is defined by

$$P_{can,N}(\{s\}) = \frac{1}{Z_{can,N}} \exp[-\beta H(s)] \quad \text{and} \quad Z_{can,N} = \sum_{s \in \Omega_N} \exp[-\beta H(s)]. \tag{1.5}$$

As is well known [7], our system undergoes a phase transition at $\beta = 1$, when γ goes to zero. In particular, the nature of the microscopic configurations that are typical under the Gibbs measure changes at the phase transition. To see this change clearly, it is convenient to introduce the notion of *coarse-grained* configurations, $\sigma_\delta(r)$. We shall give a precise definition in the next subsection. For the moment it suffices to say that $\sigma_\delta(r)$ is obtained by averaging the microscopic configuration s on a box of size γ^δ centered at r , with $\delta < 1$ so $\gamma^\delta \gg \gamma$ for $\gamma \ll 1$.

For $\beta > 1$, γ small and L large, and say $\delta = 1/2$, the grand canonical probability measure is overwhelmingly concentrated on coarse grained configurations σ_δ for which either $\sigma_\delta(r)$ is very close to m_β at most $r \in \mathcal{T}_L$ or else $\sigma_\delta(r)$ is very close to $-m_\beta$ at most $r \in \mathcal{T}_L$, where m_β is the unique positive solution to

$$m_\beta = \tanh(\beta m_\beta). \tag{1.6}$$

If $\sigma_\delta(r) \approx m_\beta$ we say that the system is in the high density, or ‘‘liquid’’ phase at r , and if $\sigma_\delta(r) \approx -m_\beta$ we say that the system is in the low density, or ‘‘vapor’’ phase at r .

Things are more interesting under the canonical measure, under which the average particle density has the sharp value

$$n = \frac{N}{|\Lambda|},$$

where $|\Lambda|$ denotes the number of lattice sites in Λ , namely $\gamma^{-d} L^d$.

The parameter n plays a significant role in our problem, and it sometimes is more convenient to refer to the corresponding parameter

$$m = 2n - 1 = \frac{2N - |\Lambda|}{|\Lambda|}$$

which is the *average magnetization* in the spin interpretation of the model. When

$$-m_\beta < m < m_\beta, \quad \text{or equivalently,} \quad \frac{1 - m_\beta}{2} < n < \frac{1 + m_\beta}{2},$$

then it is not possible for the system to be in one phase or the other over all of \mathcal{T}_L . Instead, as one might expect, typical configurations will be such that $\sigma_\delta(r) \approx +m_\beta$ in some part D of \mathcal{T}_L , while $\sigma_\delta(r) \approx -m_\beta$ in most of the rest of \mathcal{T}_L . If m is much closer to $-m_\beta$ than it is to m_β , we would expect the vapor state to dominate, so that D will cover only a small part of the whole domain. In such a configuration, we say there is a *droplet* of the liquid phase in a background of the vapor phase. The basic question that concerns us here is this:

- For a given $n, \beta > 1$, small γ and large L , do phase droplets form, and if so, what are the sizes and shapes of droplets for typical configurations under $P_{\text{can},N}$?

To answer this question we first have to define precisely the coarse-graining we will use.

1.2 The Coarse-Graining Transformation

To facilitate combinatoric estimates to come, it will be convenient to assume, as in [1, 7] that $\gamma = 2^{-k}$ for some positive integer k , and that L is an integer. As in [1, 7], we regard particle configurations as functions on \mathcal{T}_L , and not only on the lattice Λ . However, to keep clear which variables range over \mathcal{T}_L , and which range over $\Lambda = \Lambda_{L,\gamma}$, we use their convention of writing r to denote a continuous variable in \mathcal{T}_L , and x to denote the discrete variables on $\Lambda_{L,\gamma}$.

The lattice Λ induces a partition $\mathcal{Q}^{\text{fine}}$ of \mathcal{T}_L into (fine) cubes $F(x), x \in \Lambda$ (Fig. 1, left): For any $x \in \Lambda, F(x)$ is the “half open” cube in the “checkerboard partition” of \mathcal{T}_L with x at its “lower-left corner”

$$F(x) = \{r \in \mathcal{T}_L : x_j < r_j \leq x_j + \gamma, j = 1, \dots, d\}.$$

We now regard each $s \in \Omega_{L,\gamma}$ as a function defined on all of \mathcal{T}_L by defining $\sigma(r)$ to be constant on each cube $F(x)$, with the constant value $\sigma(x)$. If, in two dimensions, we colored $F(x)$ black for $\sigma(x) = 1$ and white for $\sigma(x) = 0$, we would see a black and white checkerboard pattern, with black squares indicating occupied sites.

Now consider a second, coarser partition. Fix any positive integer ℓ with $\ell < k$, and let $\mathcal{Q}^{\text{coarse}}$ denote the partition of \mathcal{T}_L into cubes of side length 2^ℓ in microscopic units, so each contains $2^{d\ell}$ microscopic lattice sites, and so that each cube in this partition consists of exactly $2^{d\ell}$ cubes in the fine partition, $\mathcal{Q}^{\text{fine}}$ (Fig. 1 right).

The coarse-graining transformation is the averaging operation that renders any microscopic configuration σ , regarded as a function on \mathcal{T}_L , constant on the cubes of the coarse partition. Doing this averaging in two dimensions would transform the black and white checkerboard pattern we have described above into a regular array of much larger squares, each uniformly colored with a shade of gray. The darkness of the shade of gray would indicate the fraction of the sites that were occupied. The cubes in the coarse partition $\mathcal{Q}^{\text{coarse}}$ have side-length $\gamma^{\ell/k}$, and it is therefore useful to introduce the parameter

$$\delta = \frac{\ell}{k}.$$

Definition 1.1 (Coarse graining transformation on scale δ) Let f be any integrable function on \mathcal{T}_L , and let $\delta = \ell/k$ for some integers $0 < \ell < k$. The coarse grained projection of f on scale δ is the function on \mathcal{T}_L given by

$$\pi^{(\delta)} f(r) = \frac{1}{|C(r)|} \int_{C(r)} f(r') dr', \tag{1.7}$$

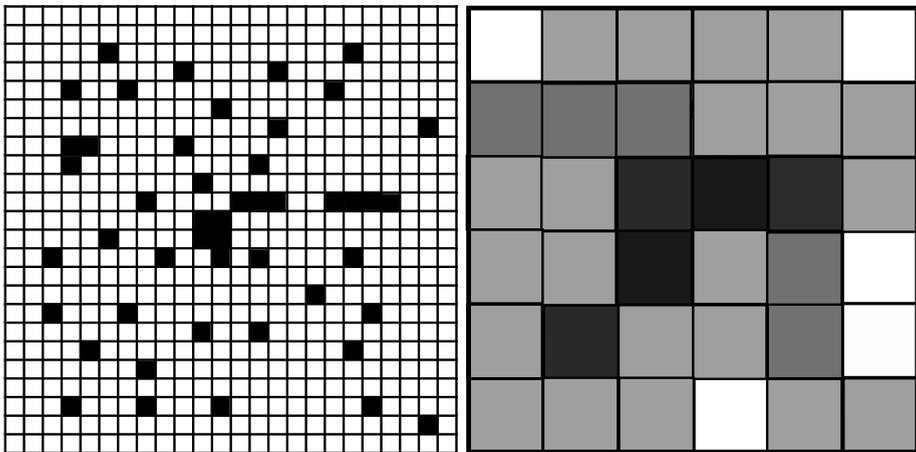


Fig. 1 On the left the partition Q^{fine} and an example of configuration in $d = 2$. On the right the partition Q^{coarse} with $\ell = 2$ and the coarsening of the configuration on the left

where $C(r)$ is the unique cube in the coarse partition Q^{coarse} that contains $r \in \mathcal{T}_L$.

If σ is any particle (spin) configuration in $\Omega_{L,\gamma}$, we define the corresponding coarse grained configuration σ^δ by

$$\sigma_\delta = \pi^{(\delta)} \sigma.$$

Since we consider particle configurations in $\Omega_{L,\gamma}$ as functions, necessarily integrable, on \mathcal{T}_L , the coarse graining transformation may be applied to each $s \in \Omega_{L,\gamma}$.

Definition 1.2 (The coarse grained configuration spaces) For any integer $0 < \ell < k$, and with $\delta = \ell/k$, let $\Omega_{L,\gamma}^{(\delta)}$ be the set of functions $\sigma_\delta = \pi^{(\delta)} \sigma$ for some $\sigma \in \Omega_{L,\gamma}$. That is, $\Omega_{L,\gamma}^{(\delta)}$ is the image of $\Omega_{L,\gamma}$ under the coarse-graining transformation $\pi^{(\delta)}$. Likewise, define $\Omega_{L,\gamma,N}^{(\delta)}$ is the image of $\Omega_{L,\gamma,N}$ under $\pi^{(\delta)}$.

Note that the elements of $\Omega_{L,\gamma,N}^{(\delta)}$ are not only constant on each cube Q^{coarse} , but they can only assume a finite, discrete set of values: for all r ,

$$\frac{1 + \sigma_\delta(r)}{2} \in \{j\gamma^{d(1-\delta)}, j = 0, 1, \dots, \gamma^{-d(1-\delta)}\}.$$

This is because $\sigma_\delta(r)$ is the average over the values ± 1 on each of the $2^{d(k-\ell)} = \gamma^{-d(1-\delta)}$ fine cubes contained in each coarse cube.

For each given $\sigma_\delta \in \Omega_{L,\gamma}^{(\delta)}$ we consider the event

$$E(\sigma_\delta) = \{s \in \Omega_{L,\gamma} \mid \pi^{(\delta)} s = \sigma_\delta\}.$$

Following [7], we define $Z(\sigma_\delta) = \sum_{s \in E(\sigma_\delta)} e^{-\beta H(s)}$.

The grand canonical probability of $E(\sigma_\delta)$ is given by

$$P_{\text{gc}}[E(\sigma_\delta)] = \frac{Z(\sigma_\delta)}{Z_{\text{gc}}}. \tag{1.8}$$

Furthermore, provided $\gamma^{-d} \int_{\mathcal{T}_L} \sigma_\delta(r) dr = N$ so that $E(\sigma_\delta) \subset \Omega_{L,\gamma,N}$, and hence so that $P_{\text{can},N}[E(\sigma_\delta)]$ is defined,

$$P_{\text{can},N}[E(\sigma_\delta)] = \frac{Z(\sigma_\delta)}{Z_{\text{can},N}}. \tag{1.9}$$

1.3 Droplet Profiles

One of our main results may be paraphrased as follows: *If $\beta > 1$, δ small, L large, and $n > (1 - m_\beta)/2$, but*

$$\left(n - \frac{1 - m_\beta}{2} \right) = \mathcal{O}(L^{-\frac{d}{d+1}}),$$

so there is a small excess of particles over what is required for a uniform sea of “vapor”, then, with extremely high probability the coarse-grained profile has a “liquid droplet” of a particular size.

To make this precise we begin with some definitions.

Set $\kappa = (n - (1 - m_\beta)/2)^{1/3} \asymp L^{-\frac{d}{3(d+1)}}$,

$$h_+ = m_\beta - \kappa \quad \text{and} \quad h_- = -m_\beta + \kappa. \tag{1.10}$$

Note that these two values are just below m_β , and just above $-m_\beta$. If a coarse grained configuration σ has $\sigma(r) \geq h_+$, then the configuration is dominated by the “liquid” state at $r \in \mathcal{T}_L$, while if $\sigma(r) \leq h_-$, then the configuration is dominated by the “vapor” state at r . By definition, *our droplet of the liquid state* for the coarse-grained configuration σ is the region in which $\sigma \geq h_+$. For each coarse grained configuration σ , we define the sets:

$$\begin{aligned} A(\sigma) &= \{r \in \mathcal{T}_L : h_- \leq \sigma(r) \leq h_+\}, \\ B(\sigma) &= \{r \in \mathcal{T}_L : \sigma(r) \leq h_-\}, \\ C(\sigma) &= \{r \in \mathcal{T}_L : \sigma(r) \geq h_+\}. \end{aligned} \tag{1.11}$$

As explained below, Lemma 4.6 of [2], together with the large deviation statement we are going to prove, shows that, for the values of β , n and L we consider here, coarse-grained profiles σ for which the set $A(\sigma)$ is not negligible small in measure compared to either $B(\sigma)$ or $C(\sigma)$ are extremely unlikely: The system strongly prefers profiles stay close to one of the two values $\pm m_\beta$ over the vast majority of Λ .

Now, if the profile σ where such that $\sigma(x) \in \{-m_\beta, +m_\beta\}$ for all x , the particle number constraint

$$n = \frac{1}{L^d} \int_{\mathcal{T}_L} \frac{1 + \sigma(r)}{2} dr \tag{1.12}$$

would reduce to

$$n = \frac{1}{2} + \frac{1}{2L^d} (m_\beta |C(\sigma)| - m_\beta |B(\sigma)|) = \frac{1}{2} + m_\beta \left(\frac{|C(\sigma)|}{L^d} - \frac{1}{2} \right),$$

where for any measurable set $X \subset \Lambda$, $|X|$ denotes the Lebesgue measure of X . Solving for $|C(\sigma)|$ we find the value

$$D_0 := \frac{2n - 1 + m_\beta}{2m_\beta} L^d. \tag{1.13}$$

That is, D_0 is the volume of the droplet (liquid) region in a profile that is everywhere either in a pure liquid or pure vapor state, and which satisfies the constraint (1.12). D_0 is called the size of the *equimolar droplet*.

Given any coarse-grained profile σ , define the *volume fraction*

$$\eta(\sigma) = \frac{|C(\sigma)|}{D_0}.$$

Under the canonical probability measure on configurations σ , this becomes a random variable. A more precise version of the statement made in the beginning of this subsection is that in the regime considered here, with high probability η is close to a critical value

$$\eta_c \in 0 \cup [2/(d + 1), 1],$$

and we give a simple variational formula for the value of η_c as a function of β and n in the large L limit; see Theorem 2.2 below.

This gives a fully satisfactory description of the size of droplets in the critical droplet scaling regime, but of course we are also interested in the shape. Indeed, it is not really proper to refer to the set $C(\sigma)$ as a droplet unless the symmetric difference between this set and some “essentially round” shaped set of the same value has small volume. (Recall that our interaction potential J is isotropic.) We shall return to this problem later in the paper once we have the context to discuss it in more precise terms. We now turn to our methodology.

1.4 The Free Energy Functional

The method employed in this paper is to study the canonical probabilities of events defined in terms of coarse-grained profiles entirely through the analysis of a mesoscopic free energy functional \mathcal{F} that we define next. We shall prove a large deviation theorem, Theorem 2.1 below, that allows us to estimate, with precise error bounds, $P_{\text{can},N}[E(\sigma_\delta)]$ in terms of $\mathcal{F}(\sigma_\delta)$. Once Theorem 2.1 is proved, our analysis at the microscopic level is completed. All conclusions about the nature of coarse-grained profiles that one is at all likely to see will be drawn from an analysis of the function \mathcal{F} , that we now introduce:

Definition 1.3 (The GPL free energy functional) Let \mathcal{M} be the set of measurable function σ mapping \mathcal{T}_L into $[-1, 1]$. For any $\sigma \in \mathcal{M}$, The Gates-Penrose-Lebowitz free energy of σ , $\mathcal{F}(\sigma)$ is defined by

$$\begin{aligned} \mathcal{F}(\sigma) &= \frac{1}{\beta} \int_{\mathcal{T}_L} i(\sigma(r))dr - \frac{1}{2} \int_{\mathcal{T}_L} \int_{\mathcal{T}_L} J(|r - r'|)\sigma(r)\sigma(r')drdr' \\ &= \int_{\mathcal{T}_L} f(\sigma(r))dr + \frac{1}{4} \int_{\mathcal{T}_L} \int_{\mathcal{T}_L} J(|r - r'|)[\sigma(r) - \sigma(r')]^2 drdr', \end{aligned} \tag{1.14}$$

where

$$f(m) := \frac{1}{\beta}i(m) - \frac{1}{2}m^2,$$

and

$$i(m) = \frac{1 - m}{2} \log \frac{1 - m}{2} + \frac{1 + m}{2} \log \frac{1 + m}{2}.$$

2 Results

It turns out that the probability measures $P_{\text{can},N}[E(\sigma_\delta)]$ concentrate more and more sharply as N increases on a very special class of coarse-grained configurations, and both the nature of this special class and the quantitative degree of concentration can be analyzed in terms of a Large Deviations Functional (LDF) which is the GPL free energy functional $\mathcal{F}(\sigma_\delta)$.

The key to both the characterization problem and the quantification problem is a constrained variational problem concerning $\mathcal{F}(\sigma_\delta)$, namely to find all *near minimizers* in

$$\inf \left\{ \mathcal{F}(\sigma) : \frac{1}{L^d} \int_{\mathcal{T}_L} \sigma(r) dr = 2n - 1 \right\}.$$

Theorem 2.1 *For any $-1 \leq m \leq 1$, let $N = \lceil \frac{m+1}{2} \gamma^{-d} L^d \rceil$ be the number of occupied sites, recalling that $\gamma^{-d} L^d$ is the total number of lattice sites.*

Let σ^ be a constrained minimizer of \mathcal{F} :*

$$\frac{1}{L^d} \int_{\mathcal{T}_L} \sigma^*(r) dr = m \quad \text{and} \quad \mathcal{F}(\sigma^*) = \inf \left\{ \mathcal{F}(\sigma) : \frac{1}{L^d} \int_{\mathcal{T}_L} \sigma(r) dr = m \right\}. \tag{2.1}$$

For each $0 < \delta < 1$,

$$\left| \log P(\sigma_\delta) + \beta \gamma^{-d} [\mathcal{F}(\sigma_\delta) - \mathcal{F}(\sigma^*)] \right| \leq c \gamma^{-d} L^d [\gamma^\delta + \gamma^{d(1-\delta)}] \log \gamma^{-1}. \tag{2.2}$$

Moreover, let us choose

$$\delta := \frac{d}{d+1},$$

and take $\bar{\delta}$ to be any positive number with $\bar{\delta} < \delta$. Then for any set of \mathcal{A} of coarse-grained configurations in $\Omega_{L,\gamma,N}^{\bar{\delta}}$,

$$\gamma^d \log P(\mathcal{A}) = - \inf_{\sigma \in \mathcal{A}} \beta [\mathcal{F}(\sigma) - \mathcal{F}(\sigma^*)] + L^d \mathcal{O}(\gamma^{\bar{\delta}}). \tag{2.3}$$

Remark 1 The point of the choice $\delta = d/(d+1)$ is that the error term in (2.3) comes from several sources. Some of these errors decrease with δ , while others increase with δ . In the proof it is shown that the choice $\delta = d/(d+1)$ is the best compromise, minimizing the total error, and leading to (2.3).

Analogous results are proved in [1, 7] for the grand canonical measure P_{gc} . Note that when $E(\sigma) \subset \Omega_{L,\gamma,N}$, the difference between $P_{\text{can},N}(E(\sigma))$ and $P_{\text{gc}}(E(\sigma))$ is entirely in the denominators. Thus, all of the estimates in [1, 7] on the numerator in (1.8) apply immediately to the numerator in (1.9).

However, there is somewhat more to be done to estimate the denominator in (1.9) than the denominator in (1.8).

The reason is that in estimating the denominator in (1.8), one shows that the main contribution comes from a small number of configurations that are uniformly close to one of the constant profiles $\sigma = \pm m_\beta$ that are the global minimizers of \mathcal{F} . In the canonical case, we are concerned with profiles that are uniformly close to some profile σ^* that minimizes the constrained variational problem in (2.1).

We do not have *a-priori* information on what these are as we do in the grand canonical case. In particular, we do not know *a-priori* that they are bounded away from ± 1 , where

the derivative of the function f emerging in the definition of \mathcal{F} is infinite. Thus more work has to be done to show that all such configurations have a free energy $\mathcal{F}(\sigma)$ that is very close to $\mathcal{F}(\sigma^*)$. This is the main difference between what we do here, and what was already done in the grand canonical case. The main tool that enables us to deal with this point is Theorem 3.1.

The minimizers for the functional (1.14) for measurable σ satisfying the constraint

$$L^{-d} \int_{\mathcal{I}_L} \sigma(r) dr = m, \tag{2.4}$$

have been studied in [2] under the assumption

$$m = -m_\beta + KL^{-\frac{d}{d+1}}, \tag{2.5}$$

for $K > 0$. This is, as the following result shows, the *critical scaling regime* for droplet formation: Indeed, it turns out that there is a critical value $K_* > 0$ such that for $K < K_*$ there is no droplet formation, while, for $K > K_*$ a droplet will form. As K increases beyond K_* and tends to infinity, the size of the droplet in the minimizer increases to the size of the equimolar droplet (see (1.13)) for the given value of m . Thus, the range of values of m parameterized by (2.5) is precisely the range of values of m for which the droplet size has a non-trivial dependence on m , and this justifies our focus on values of m satisfying (2.5).

Informally speaking, it is proved that [2] that with m satisfying (2.5),

$$\inf \left\{ \mathcal{F}(\sigma) : \frac{1}{L^d} \int_{\mathcal{I}_L} \sigma(r) dr = m \right\} \approx \inf_{\eta \in [0,1]} \Phi(\eta),$$

$$\Phi(\eta) := L^{\frac{d^2-d}{d+1}} S d \omega_d \left(\frac{Kd}{2m_\beta d \omega_d} \right)^{1-\frac{1}{d}} \left[\eta^{1-1/d} + H(K)(1-\eta)^2 \right], \tag{2.6}$$

where

$$H(K) = \frac{2m_\beta^2}{d\chi S} \left(\frac{d}{d\omega_d} \right)^{\frac{1}{d}} \left(\frac{K}{2m_\beta} \right)^{1+\frac{1}{d}}. \tag{2.7}$$

Here S is the planar surface tension, χ is the compressibility and ω_d the volume of the ball in \mathbb{R}^d . (See [2] for the definition of S and χ ; for our purposes now, they are some computable constants associated to the model.) We define $\eta_c \geq 0$ as the absolute minimizer of the function $\Phi(\eta)$.

The precise estimate we use here is (5.13) from [2] which says:

$$\mathcal{F}(\sigma) - \mathcal{F}(\sigma^*) \geq [\Phi(\eta) - \Phi(\eta_c)](1 + o(L^{-\frac{d^2-d}{d+1}})). \tag{2.8}$$

Theorem 2.2 *For any L and any $K > 0$ let m be given by $m = -m_\beta + KL^{-\frac{d}{d+1}}$. For any $\alpha > 0$ and any microscopic configuration σ such that*

$$m = L^{-d} \int_{\mathcal{I}_L} \sigma(r) dr, \tag{2.9}$$

there is a universal constant M such that, for L large enough,

$$\mathcal{F}(\sigma) \geq (1 + \alpha)\mathcal{F}(\sigma^*) \tag{2.10}$$

whenever

$$\frac{(\eta(\sigma) - \eta_c)^2}{M} \geq \alpha. \tag{2.11}$$

Proof For $\eta_c > 0$, we take the quadratic approximation of the function $\varphi(\eta) = \eta^{1-1/d} + H(K)(1 - \eta)^2$ around its minimizer η_c . The inequality (2.10) then follows from (2.8) and the definition of Φ since $\mathcal{F}(\sigma^*) = \Phi(\eta_c)(1 + o(L^{-\frac{d^2-d}{d+1}}))$. If $\eta_c = 0$, then $\varphi(\eta)$ increases even more rapidly than quadratically from its minimum. \square

The following theorem shows that the only coarse-grained profiles one is at all likely to see (for large L) are those with droplets that have a volume fraction η very close to the critical volume fraction η_c for the given values of β and m .

In the final section of the paper, we discuss the shape problem.

Theorem 2.3 *Let m and σ satisfy the hypothesis of Theorem 2.2. Define the event*

$$\mathcal{A}_\varepsilon = \{ \sigma \in \Omega_{L,\gamma}^\ell : |\eta(\sigma) - \eta_c| > \varepsilon \}.$$

Then, for L large enough and $\gamma^{\bar{\delta}} \leq \frac{\varepsilon^2}{6C} \beta \Phi(\eta_c)$, with $\bar{\delta}$ in Theorem 2.1 and M as in Theorem 2.2,

$$\gamma^d \log P(\mathcal{A}_\varepsilon) \leq -\frac{\varepsilon^2}{2M} \beta \Phi(\eta_c). \tag{2.12}$$

Proof By the definition of \mathcal{A}_ε and Theorem 2.2,

$$\inf_{\sigma \in \mathcal{A}} \beta [\mathcal{F}(\sigma) - \mathcal{F}(\sigma^*)] \geq \frac{\varepsilon^2}{M} \beta \mathcal{F}(\sigma^*).$$

By Theorem 2.1 in [2],

$$\mathcal{F}(\sigma^*) = \Phi(\eta_c)(1 + o(L^{-\frac{d^2-d}{d+1}})).$$

Combining this with Theorem 2.1 we obtain

$$\gamma^d \log P(\mathcal{A}_\varepsilon) \leq -\frac{\varepsilon^2}{M} \beta [\Phi(\eta_c) + o(L^{-\frac{d^2-d}{d+1}})] + L^d \mathcal{O}(\gamma^{\bar{\delta}}).$$

For L large enough we have

$$\Phi(\eta_c)(1 + o(L^{-\frac{d^2-d}{d+1}})) \geq \frac{2}{3} \Phi(\eta_c).$$

Hence, by choosing $\bar{\delta}$ such that $\mathcal{O}(\gamma^{\bar{\delta}}) \leq L^{-d} \frac{\varepsilon^2}{6M} \beta \Phi(\eta_c) \approx \varepsilon^2 L^{-\frac{2d}{d+1}}$ (because of the scaling $\Phi(\eta_c) \approx L^{\frac{d^2-d}{d+1}}$ given in (2.6)), we conclude the proof. \square

Remark 2 If $K < K_*$, then $\eta_c = 0$ and there are no droplets. If $K > K_*$, then $\eta_c > 0$ so there is droplet formation. The case $K = K_*$ cannot be decided because there are two absolute minimizers, one corresponding to $\eta_c = 0$ and another to $\eta_c > 0$, which give the same value to $\Phi(\eta)$, see Fig. 2.

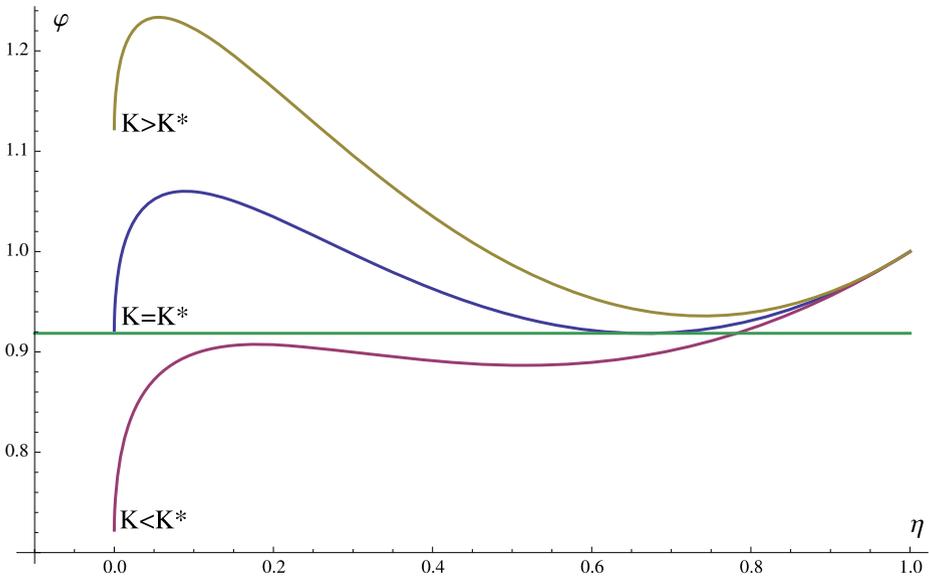


Fig. 2 Plot of the function $\varphi(\eta)$ for three values of K : $K < K_*$ (lower plot, single minimizer $\eta = 0$); $K = K_*$ (middle plot, double minimizer, $\eta = 0$ and $\eta > 0$); $K > K_*$ (upper plot, single minimizer $\eta > 0$)

3 Canonical Large Deviations

This section provides the proof of the canonical ensemble large deviations bounds we use. We closely follow [1, 7] where possible. As noted above, the main difference is in the estimation of the denominator in (1.9).

We now prove a continuity estimate for the functional \mathcal{F} that will show that for any profile σ that is close to a minimizer in the L^∞ norm, $\mathcal{F}(\sigma)$ has very nearly the minimal value. This is the key to the estimation of the denominator in (1.9).

Though we have a good knowledge of the minimizers for certain values of the constraint, we do not have this knowledge for other values. In general, there is no rigorous *a-priori* argument to exclude the possibility that a minimizing profile takes values very close to ± 1 on sets of significant size. This would cause a difficulty since $|f'(m)|$, the absolute value of the derivative of f , tends to infinity as m tends to ± 1 . Nonetheless, the functional $\mathcal{F}(\sigma)$ is *nearly Lipschitz* continuous on its entire domain.

Theorem 3.1 (Near Lipschitz continuity of \mathcal{F}) *Let σ and σ_0 be two functions on \mathcal{T}_L with values in $[-1, +1]$, and suppose that*

$$\|\sigma - \sigma_0\|_\infty \leq h$$

with $2h \leq 1 - m_\beta$. Then there is a universal constant C so that

$$|\mathcal{F}(\sigma) - \mathcal{F}(\sigma_0)| \leq CL^d h |\log(h)|.$$

Proof Let $\varphi(r) := \sigma(r) - \sigma_0(r)$,

$$A_+ = \{r : \sigma_0(r) \geq 1 - 2h\} \quad \text{and} \quad A_- = \{r : \sigma_0(r) \leq -1 + 2h\}.$$

Finally, let B denote the complement of $(A_+ \cup A_-)$. We now seek an upper bound on $\mathcal{F}(\sigma) - \mathcal{F}(\sigma_0)$.

Since i is monotone increasing in the set $[m_\beta, 1]$, and due to our restriction on h , on the set A_+ ,

$$i(\sigma(r)) - i(\sigma_0(r)) \leq i(1) - i(1 - 2h).$$

Likewise, on the set A_- ,

$$i(\sigma(r)) - i(\sigma_0(r)) \leq i(-1) - i(-1 + 2h) = i(1) - i(1 - 2h).$$

Note that

$$i(1) - i(1 - 2h) \leq Ch |\log(h)|.$$

Next, on the set B ,

$$\begin{aligned} i(\sigma(r)) - i(\sigma_0(r)) &= i(\sigma_0(r) + \varphi(r)) - i(\sigma_0(r)) \\ &\leq \left(\sup_{-1+h \leq m \leq 1-h} |i'(m)| \right) h. \end{aligned} \tag{3.1}$$

Note that

$$\sup_{-1+h \leq m \leq 1-h} |i'(m)| = |i'(1 - h)| \leq C |\log(h)|.$$

Thus,

$$\int_{\mathcal{I}_L} [i(\sigma(r)) - i(\sigma_0(r))] dr \leq CL^d h |\log(h)|.$$

The interaction term poses no problem:

$$\begin{aligned} \sigma(r)J(|r - y|)\sigma(y) - \sigma_0(r)J(|r - y|)\sigma_0(y) \\ = \varphi(r)J(|r - y|)\sigma(y) + \sigma_0(r)J(|r - y|)\varphi(y), \end{aligned} \tag{3.2}$$

and so the interaction term is Lipschitz. Thus, we have the upper bound

$$\mathcal{F}(\sigma) - \mathcal{F}(\sigma_0) \leq CL^d h |\log(h)|.$$

By the symmetry of the hypotheses, we have the same upper bound for $\mathcal{F}(\sigma_0) - \mathcal{F}(\sigma)$, and this proves the Theorem. □

3.1 Proof of Theorem 2.1

For each given $\sigma_\delta \in \Omega_{L,\gamma}^{(\delta)}$ we consider the event

$$E(\sigma_\delta) = \{s \in \Omega_{L,\gamma} \mid \pi^{(\delta)}s = \sigma_\delta\}.$$

Given N , we have $n = N/|\Lambda_{L,\gamma}|$. We denote by $P(\sigma_\delta)$ the canonical probability $P_{\text{can},N}[E(\sigma_\delta)]$. We quote the following lemma from [1]:

Lemma 3.1 *Let $W_\ell(\sigma_\delta)$ be the cardinality of $E(\sigma_\delta)$. Then*

$$\left| \log W(\sigma_\delta) + \gamma^{-d} \int_{\mathcal{T}_L} i(\sigma_\delta(r)) \right| \leq cL^d k d 2^{d\ell} = cL^d \frac{\log(\gamma^{-1})}{\log 2} \gamma^{-d\delta}. \tag{3.3}$$

Proof Let C be any atom in the coarse-graining partition Q^{coarse} and $\bar{\sigma}$ be the average of σ on C . There are $N_C = 2^{d(k-\ell)} = \gamma^{-d(1-\delta)}$ atoms of the fine partition Q^{fine} in C and $\sigma(r) = -1$ on exactly $K(\bar{\sigma}) = \frac{1-\bar{\sigma}}{2} N_C$ cubes of Q^{fine} in C . Therefore, the number of compatible microscopic configurations in C is given by $\binom{N_C}{K(\bar{\sigma})}$. Using Stirling's formula in the form

$$\log n! = n \log n - n + \mathcal{O}(\log n),$$

and, by straightforward Stirling analysis, one can check that there is a constant c such that

$$\left| \log \binom{N_C}{K(\bar{\sigma})} + N_C i(\bar{\sigma}) \right| \leq c' \log N_C = cd(k - \ell).$$

Summing over the $L^d 2^{d\ell}$ C 's in Q^{coarse} gives the result. □

Lemma 3.2 *Let N_ℓ be the cardinality of $\Omega_{L,\gamma}^{(\delta)}$. Then there is a constant c such that*

$$\log N_\ell \leq cL^d 2^{d\ell} d(k - \ell) \leq c' L^d \gamma^{-d\delta} \log(\gamma^{-1}).$$

Proof The number of distinct values possible for $\bar{\sigma}$ is $2^{d(k-\ell)} = \gamma^{-d(1-\delta)}$ and there are $L^d 2^{d\ell} = L^d \gamma^{-d\delta}$ coarse-grained cells in the torus. □

Lemma 3.3 *There is a constant c such that for each $\sigma \in \Omega_{L,\gamma}$*

$$|H(\sigma) - H(\pi^{(\delta)}\sigma)| \leq cL^d 2^{-\ell} = cL^d \gamma^\delta$$

Proof By the definitions of H and $\pi^{(\delta)}$ we get:

$$H(\sigma) - H(\pi^{(\delta)}\sigma) = \int_{\mathcal{T}_L} dr \int_{\mathcal{T}_L} dr' \sigma(r)\sigma(r') [J(|r - r'|) - \pi^{(\delta)} \otimes \pi^{(\delta)} J(|r - r'|)].$$

But

$$|J(|r - r'|) - \pi^{(\delta)} \otimes \pi^{(\delta)} J(|r - r'|)| \leq \|\nabla J\|_\infty \sqrt{d} 2^{-\ell},$$

since $\sqrt{d} 2^{-\ell}$ is the diameter of the cube $C \in Q^{\text{coarse}}$. □

Lemma 3.4 *Let $\phi(r)$ be any continuously differentiable function on (\mathcal{T}_L) , taking values in $[-1, 1]$. Then there exists $\sigma_* \in \Omega_{L,\gamma}^{(\delta)}$ such that*

$$\|\sigma_* - \phi\|_\infty \leq c \|\nabla \phi\|_\infty [\gamma^\delta + \gamma^{d(1-\delta)}]$$

and

$$\int_{\mathcal{T}_L} \sigma_*(r) dr = \int_{\mathcal{T}_L} \phi(r) dr.$$

Proof The construction is based on three steps:

1. Replace ϕ by $\pi^{(\delta)}\phi$;
2. For each $C \in \mathcal{Q}^{\text{coarse}}$, replace the value of $\pi^{(\delta)}\phi$ in C by the closest value in the set of admissible values for the coarse-grained configurations, which are $-1 + \frac{2j}{2^{d(k-\ell)}}$, with j an integer between 0 and $2^{d(k-\ell)}$;
3. If the coarse-grained configuration produced in step 2 has too high an average to satisfy the constraint, we lower the values of σ_δ on the necessary fraction of C by an amount $2^{-d(k-\ell)-1}$ or rise it if it is too low.

The first step does not change the average and we have,

$$\|\pi^{(\delta)}\phi - \phi\|_\infty \leq \|\nabla\phi\|_\infty 2^{-\ell} \sqrt{d}.$$

In the second and third steps we shift the value by at most $2^{-d(k-\ell)-1}$. Putting these things together we get the proof of the lemma. □

Proof of Theorem 2.1 Let us pick a coarse-grained configuration $\sigma_\delta \in \Omega_{L,\gamma}^{(\delta)}$ such that

$$\frac{1}{L^d} \int_{\mathcal{T}_L} \sigma_\delta(x) dx = \frac{[mN]}{N}.$$

Then

$$Z_{\beta,\gamma,L,m} P(\sigma_\delta) = \sum_{\sigma \in E(\sigma_\delta)} e^{-\beta\gamma^{-d} H(\sigma)}.$$

We define

$$\psi(\delta) = cL^d \gamma^{-d} \{ \beta\gamma^\delta + \gamma^{d(1-\delta)} \log(\gamma^{-1}) \} \tag{3.4}$$

By Lemma 3.1 and Lemma 3.3, we get:

$$e^{-\beta\gamma^{-d} \mathcal{F}(\sigma_\delta) - \psi(\delta)} \leq \sum_{\sigma \in E(\sigma_\delta)} e^{-\beta\gamma^{-d} H(\sigma)} \leq e^{-\beta\gamma^{-d} \mathcal{F}(\sigma_\delta) + \psi(\delta)}.$$

We have to consider the partition function. In fact, the essential part of it comes from the microscopic configurations whose coarse-grained configuration corresponds to the minimizer of the free energy.

Let σ^* be the minimizer of the free energy under the mass constraint and note that it fulfills the conditions required for the application of Lemma 3.4. Indeed one gets immediately that the minimizer is of bounded variation, so that $\|\nabla\sigma^*\|_1$ is bounded. Moreover, by using the Euler Lagrange equation and a bootstrap argument, it can be easily proved that $\|\nabla\sigma^*\|_\infty$ is bounded.

Let σ_δ^* be the corresponding coarse-grained configuration provided by Lemma 3.4. Then

$$Z_{\beta,\gamma,L,m} \geq e^{-\beta\gamma^{-d} \mathcal{F}(\sigma_\delta^*) - \psi(\delta)}.$$

Similarly, we have

$$Z_{\beta,\gamma,L,m} \leq e^{-\beta\gamma^{-d} \mathcal{F}(\sigma_\delta^*) + \psi(\delta)} N_\ell.$$

By Lemma 3.2

$$Z_{\beta,\gamma,L,m} \leq e^{-\beta\gamma^{-d} \mathcal{F}(\sigma_\delta^*) + \phi(\delta)}$$

with

$$\phi(\delta) = cL^d \gamma^{-d} [\gamma^d + \gamma^{d(1-\delta)} \log \gamma^{-1}].$$

In conclusion,

$$-\gamma^{-d} \beta [\mathcal{F}(\sigma_\delta) - \mathcal{F}(\sigma_\delta^*)] - \phi(\delta) \leq \log P(\sigma_\delta) \leq -\gamma^{-d} \beta [\mathcal{F}(\sigma_\delta) - \mathcal{F}(\sigma_\delta^*)] + \psi(\delta).$$

We now replace $\mathcal{F}(\sigma_\delta^*)$ by $\mathcal{F}(\sigma^*)$ in the estimates. For the upper bound, it is enough to use

$$\mathcal{F}(\sigma_\delta^*) \geq \mathcal{F}(\sigma^*).$$

For the lower bound instead we use Theorem 3.1:

$$|\mathcal{F}(\sigma_\delta^*) - \mathcal{F}(\sigma^*)| \leq c\gamma^{-d} L^d |\sigma_\delta^* - \sigma^*|_\infty \log |\sigma_\delta^* - \sigma^*|_\infty.$$

By Lemma 3.4 then we obtain

$$|\mathcal{F}(\sigma_\delta^*) - \mathcal{F}(\sigma^*)| \leq c\gamma^{-d} L^d [\gamma^\delta + \gamma^{d(1-\delta)}] \log \gamma^{-1}$$

for a suitable constant c depending on $\|\nabla \sigma^*\|_\infty$.

The final estimate is

$$\begin{aligned} -\gamma^{-d} \beta [\mathcal{F}(\sigma_\delta) - \mathcal{F}(\sigma^*)] - c\gamma^{-d} L^d [\gamma^\delta + \gamma^{d(1-\delta)}] \log \gamma^{-1} \\ \leq \log P(\sigma_\delta) \leq -\gamma^{-d} \beta [\mathcal{F}(\sigma_\delta) - \mathcal{F}(\sigma^*)] + c\gamma^{-d} L^d [\gamma^\delta + \gamma^{2d(1-\delta)}] \log \gamma^{-1}. \quad \square \end{aligned}$$

4 Concluding Remarks

4.1 About the Shape Problem

In the analysis in [2] that leads to the crucial estimate (2.8), use was made of the Riesz Rearrangement Inequality for convolutions. For any measurable function σ on \mathbb{R}^d such that the Lebesgue measure $\{x : \sigma(x) > \lambda\}$ tends to 0 and λ tends to ∞ , let σ^* denote the radial function on \mathbb{R}^d such that for all $\lambda > 0$, the sets $\{x : \sigma(x) > \lambda\}$ and $\{x : \sigma^*(x) > \lambda\}$ have the same Lebesgue measure. (If the measure is infinite, the second set is all of \mathbb{R}^d .) Then the Riesz Rearrangement Inequality says that

$$\int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |\sigma(x) - \sigma(y)|^2 J(x - y) dx dy \geq \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |\sigma^*(x) - \sigma^*(y)|^2 J(x - y) dx dy. \quad (4.1)$$

In order to apply this to our profiles on the torus, we need to make some modifications of the profiles, “lifting” from \mathcal{T}_L to \mathbb{R}^d , without significantly affecting the value of \mathcal{F} , as explained in [2].

Once this is done, the rearrangement operation lowers the value of the free energy functional—because of the Riesz Rearrangement Inequality—and it makes the trial function σ radial. This facilitates the estimation of $\mathcal{F}(\sigma)$, and leads to (2.8), but in the process, all information about the shape of the set $C(\sigma)$ defined in (1.11), i.e., the droplet, is lost.

To solve the shape problem, we would like to know, quantitatively, *how much* the rearrangement operation lowers the free energy for profiles σ in which the droplet is not nearly

spherical. In purely mathematical terms, the question to be answered is this: Let A be a measurable set in \mathbb{R}^d with finite Lebesgue measure. Let B be the ball with the same Lebesgue measure as A . The *Fraenkel asymmetry* $F(A)$ is defined by

$$F(A) = \inf_{y \in \mathbb{R}^d} \left\{ \int_{\mathbb{R}^d} |1_A(x) - 1_B(x-y)| dx \right\}.$$

It measures “how out of round the shape of A is”.

As soon as one has an explicit lower bound on

$$\int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |1_A(x) - 1_A(y)|^2 J(x-y) dx dy - \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |1_B(x) - 1_B(y)|^2 J(x-y) dx dy \quad (4.2)$$

in terms of $F(A)$ and J , the methods of this paper translate such a bound into a solution of the shape problem. Such a lower bound in (4.2) may be seen as a quantitative “non-local isoperimetric inequality”. Indeed, if J is supported in a ball of radius $r > 0$, then $|1_A(x) - 1_A(y)| = 0$ unless both x and y are within a distance r of the boundary of A , so that as r tends to zero one would recover from this the usual isoperimetric inequality. Recent progress on the quantitative form of the classical isoperimetric inequality [3, 4] provides a basis for expecting such an inequality to be proved soon.

4.2 Local Interactions

We mention here that, as noted in [2], we expect the results derived there and here to apply to more general forms of $f(m)$ than that given in (1.14). More precisely, the $\beta^{-1}i(m)$ in (1.14) is the free energy of a lattice gas without any short range interaction. However the result should also be valid when, in addition to the Kac potential, also there are short range interactions, i.e. ones which do not scale with γ , as long as we are at values of β where these do not, by themselves, produce a phase transition. This corresponds to replace, in the free energy functional, $\beta^{-1}i(m)$ by a strictly convex function $f_0(\beta, m)$, the free energy of the “reference system”, as in references [5] and [6]. The technical problem in considering such system are the estimates as in Lemma 3.1. To obtain such estimates for systems with short range interactions requires an estimate of the finite size corrections to $f_0(\beta, m)$. We know that in the canonical ensemble they go to zero as $\gamma \rightarrow 0$. One expects that they behave like the ratio of surface area to volume, i.e. of $O(\gamma L^{-1})$. It is an open problem to prove that they go as a suitably small power of γL^{-1} . More is known in the grand-canonical ensemble for β small and we hope that the same is true for the canonical case, whenever $f_0(\beta, m)$ is strictly convex.

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