
Phase separation and sharp large deviations

Ostap Hryniv and Clare Wallace†*

Abstract. *Using a refined analysis of phase boundaries, we derive sharp asymptotics of the large deviation probabilities for the total magnetization of a low-temperature Ising model in two dimensions.*

1 Introduction

The phenomenon of “phase separation” has been at the heart of the theory of phase transitions in low-temperature lattice systems since its discovery by Minlos and Sinai [1, 2] in the late 1960s. Under suitable conditions, it makes possible to describe the canonical ensembles of such models in terms of (families of) large contours, or “phase boundaries”, and, as a result, to study the limiting behaviour of the corresponding probability distributions and their partition functions. This approach is especially successful in two dimensions, as the resulting phase boundaries are one-dimensional contours, whose statistical behaviour is well understood.

When combined with a careful analysis of the related variational problem, these results can provide a detailed description of the typical configurations in such ensembles.

Department of Mathematical Sciences, Durham University, Durham, UK; ostap.hryniv@durham.ac.uk

Department of Mathematical Sciences, Durham University, Durham, UK; clare.wallace@durham.ac.uk
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In the setting of the low-temperature Ising model on a two-dimensional torus, the famous Dobrushin-Kotecký-Shlosman theorem [3] rigorously justifies the so-called Wulff construction and approximates the rescaled phase boundary by that of the Wulff shape, a two-dimensional region enclosed by a curve with the smallest surface energy. In turn, this determines the asymptotics of the logarithm of large deviation probabilities for the total magnetization of the model.

To derive a sharp large deviation principle for the total spin, one needs to carefully analyse the shape dependence of the corresponding distribution. We illustrate the approach in the case of a low-temperature Ising model in two dimensions.

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2 Model

For integer $N, M \geq 1$ consider a finite box

$$V_{NM} := \{x = (x_1, x_2) \in (\mathbb{Z}^2)^* : |x_1| \leq N, |x_2| \leq M\}$$

of the (dual) two-dimensional integer lattice $(\mathbb{Z}^2)^* := \{x = (x_1, x_2) : x_1 + 1/2, x_2 + 1/2 \in \mathbb{Z}\}$. To each site $x \in V_{NM}$ associate a spin $\sigma_x \in \{-1, +1\}$ and write $\sigma = (\sigma_x, x \in V_{NM})$ for a configuration in $\Omega_{NM} := \{-1, +1\}^{V_{NM}}$. Write $x \sim y$ if sites x and y are neighbours in $(\mathbb{Z}^2)^*$, i.e., $|x - y| := |x_1 - y_1| + |x_2 - y_2| = 1$. For a subset $V \subset (\mathbb{Z}^2)^*$, use ∂V to denote the external boundary of V , namely, the set $\{y \in (\mathbb{Z}^2)^* \setminus V : \exists x \in V \text{ with } x \sim y\}$.

Given an angle $\varphi \in (-\pi/2, \pi/2)$, let $\bar{\sigma} = (\bar{\sigma}_x, x \in (\mathbb{Z}^2)^*)$ be the two-component boundary conditions, where $\bar{\sigma}_x = +1$ iff $x = (x_1, x_2)$ satisfies $x_2 \geq x_1 \tan \varphi$ for $x_1 > 0$ or $x_2 > x_1 \tan \varphi$ for $x_1 < 0$; otherwise, put $\bar{\sigma}_x = -1$. Notice that in $\bar{\sigma}$ the pairs of sites which are centrally symmetric with respect to the origin $(0, 0)$ have spins of the opposite sign, $\bar{\sigma}_{-x} \equiv -\bar{\sigma}_x$ for all x .

The Gibbs distribution in Ω_{NM} with boundary conditions $\bar{\sigma}$ is defined via

$$P_{V_{NM}}^{\bar{\sigma}}(\sigma) := (Z(V_{NM}, \bar{\sigma}))^{-1} \exp\{-\beta \mathcal{H}(\sigma | \bar{\sigma})\}, \quad \sigma \in \Omega_{NM}, \quad (1)$$

where the partition function is

$$Z(V_{NM}, \bar{\sigma}) = \sum_{\sigma \in \Omega_{NM}} \exp\{-\beta \mathcal{H}(\sigma | \bar{\sigma})\} \quad (2)$$

and the (joint) energy is given by

$$\mathcal{H}(\sigma|\bar{\sigma}) = -\frac{1}{2} \sum_{\{x\sim y\} \subset V_{NM}} \sigma_x \sigma_y - \sum_{x\sim y: x \in V_{NM}, y \in \partial V_{NM}} \sigma_x \bar{\sigma}_y, \quad (3)$$

where the first sum runs over all pairs of neighbouring sites in V_{NM} , while the second sum is restricted to boundary pairs (x, y) of neighbouring sites with $x \in V_{NM}$ and $y \in \partial V_{NM}$. In what follows we always assume that the temperature $1/\beta > 0$ is sufficiently low.

Of key interest is the distribution of the total magnetization $S_{V_{NM}} := \sum_{x \in V_{NM}} \sigma_x$ in large volumes, namely, the limiting behaviour of the probability

$$P_{V_{NM}}^{\bar{\sigma}}(b_N) := P_{V_{NM}}^{\bar{\sigma}}(\{\sigma \in \Omega_{NM} : S_{V_{NM}} = b_N\})$$

as $N \rightarrow \infty$, for a suitable sequence of integer values b_N ; of course, for the last probability to be positive b_N must be of the same parity as the number $|V_{NM}|$ of sites in V_{NM} , i.e., even, and satisfy the *a priori* bound $|b_N| \leq |V_{NM}|$. In what follows we assume that b_N satisfies these constraints.

For a given $\varphi \in (-\pi/2, \pi/2)$, assume additionally that $(2N)^{-2}b_N \rightarrow b$ as $N \rightarrow \infty$ with the limiting value satisfying $|b| < b(\varphi)$, for a suitably chosen constant $b(\varphi) > 0$, see below. Then the Dobrushin-Kotecký-Shlosman theory [3] implies that for some $\alpha \in (0, 1)$

$$\ln P_{V_{NM}}^{\bar{\sigma}}(b_N) = -2\beta N \mathcal{W}(\varphi, b) + O(N^\alpha) \quad \text{as } N \rightarrow \infty, \quad (4)$$

provided $\beta \geq \beta_0$ with suitably chosen $\beta_0 > 0$, and the aspect ratio M/N is uniformly bounded from below by a positive constant depending on φ . Here \ln denotes the natural logarithm, and the rate functional $\mathcal{W}(\varphi, b)$ can be expressed in terms of the surface energy of the Wulff profile, a unique solution to the related variational problem, see below.

Our aim here is to derive a sharp asymptotic of the probability $P_{V_{NM}}^{\bar{\sigma}}(b_N)$, equivalently, to improve the expansion in (4) up to the zero order term. To state our main result, we need to introduce some additional concepts.

Similarly to the Gibbs distribution (1)–(3) with two-component boundary conditions $\bar{\sigma}$, consider its analogue $P_{V_{NM}}^+(\sigma)$, $\sigma \in \Omega_{NM}$, where $\bar{\sigma}$ is replaced by the constant “plus” configuration $\sigma^+ = (\sigma_x^+, x \in (\mathbb{Z}^2)^*)$ with $\sigma_x^+ = 1$ for all x . The corresponding energy is

defined via

$$\mathcal{H}(\sigma|+) = -\frac{1}{2} \sum_{\{x \sim y\} \subset V_{NM}} \sigma_x \sigma_y - \sum_{x \sim y; x \in V_{NM}, y \in \partial V_{NM}} \sigma_x \sigma_y^+, \quad (5)$$

and the partition function is

$$Z(V_{NM}, +) = \sum_{\sigma \in \Omega_{NM}} \exp\{-\beta \mathcal{H}(\sigma|+)\}.$$

Then the *surface tension* in direction of the normal n_φ to the line $x_2 = x_1 \tan \varphi$ is

$$\tau(n_\varphi) := - \lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} \frac{\cos \varphi}{2\beta N} \ln \frac{Z(V_{NM}, \bar{\sigma})}{Z(V_{NM}, +)}. \quad (6)$$

Informally, $\tau(n_\varphi)$ is the price (per unit length) of the presence of the phase boundary induced by the two-component boundary conditions $\bar{\sigma}$, relative to the constant “plus” boundary conditions σ^+ . As shown in [3], $\tau(n_\varphi)$ also arises in the simultaneous limit $N \rightarrow \infty$ and $M \rightarrow \infty$ in (6) along a sequence of suitably shaped volumes; in particular, this holds for rectangular volumes V_{NM} with uniform condition $M \geq (1 + |\tan \varphi|)N$.

The related Wulff variational problem is to minimize the value of the Wulff functional,

$$\mathcal{W}(\gamma) := \int_\gamma \tau(n_s) ds, \quad (7)$$

in the class of all rectifiable curves γ enclosing area $|V(\gamma)| \geq 1$. Its solution $W = W_\beta$, known as the *Wulff shape*, is unique (up to translations), and can be constructed by a simple geometric procedure [3, 5]. The boundary of the Wulff shape W is strictly convex for all $\beta \geq \beta_0$ [3].

The rate functional $\mathcal{W}(\varphi, b)$ in (4) can be defined in terms of the surface energy of a suitable part of the Wulff shape boundary [4]. Without loss of generality, let $b < 0$. By strict convexity of the Wulff shape W_β there is a unique position of a straight line at angle φ to the horizontal intersecting W_β , such that the area a of the top part and the horizontal projection w of its straight boundary, see Fig. 1, satisfy the relation

$$a = w^2 |b| / (2m(\beta)), \quad (8)$$

where the spontaneous magnetization $m(\beta)$ is positive for all β large enough. Then,

rescaling the resulting shape (see the right part of Fig. 1) so that the horizontal projection of γ_0 equals one, we have

$$\mathcal{W}(\varphi, b) = \mathcal{W}(\gamma_1) - \mathcal{W}(\gamma_0),$$

recall (7). The strict convexity of the surface tension $\tau(n_\varphi)$ implies that $\mathcal{W}(\varphi, b) \geq 0$.

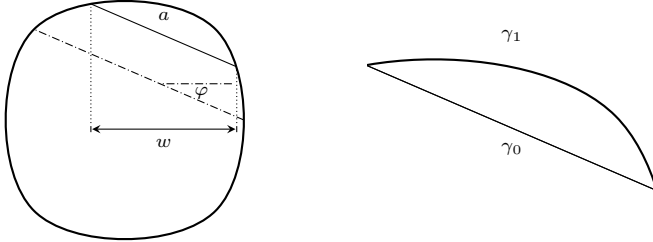


Figure 1: Construction of the Wulff profile corresponding to $\mathcal{W}(\varphi, b)$.

Let $a(\varphi)$ be the value of the area corresponding to the straight line at angle φ to the horizontal passing through the right-most point of W_β (the dashed line on the left of Fig. 1); write $w(\varphi)$ for the horizontal projection of the resulting shape. If $|a| < a(\varphi)$, the tangent at every point of the boundary γ_1 is non-vertical. As shown in [4], for such a the fluctuations of the phase boundary of the Ising model (1)–(3) around the suitably scaled curve γ_1 are asymptotically Gaussian.

The maximal value $b(\varphi)$, determining the validity of (4), is linked to $a(\varphi)$ via (8) with $w = w(\varphi)$. In what follows we assume that the sequence b_N of even numbers is φ -admissible in that there is $\varepsilon > 0$ such that for all N we have $(2N)^{-2}|b_N| < b(\varphi) - \varepsilon$.

Theorem 2.1 Let $|\varphi| < \pi/2$ and consider a φ -admissible sequence b_N with $b = \lim_{N \rightarrow \infty} (2N)^{-2}b_N$. Fix a sequence of volumes V_{NM} such that $M = M_N$ with $M/N \rightarrow c > 0$ as $N \rightarrow \infty$, for large enough $c = c(\varphi) > 0$. Then there exist $\beta_0 > 0$ and a positive constant $C = C(\varphi, b)$ such that for $\beta \geq \beta_0$,

$$P_{V_{NM}}^{\bar{\sigma}}(b_N) = \frac{C(\varphi, b)}{\sqrt{2\pi N^3}} \exp\{-2\beta N \mathcal{W}(\varphi, b)\} (1 + o(1)) \quad \text{as } N \rightarrow \infty. \quad (9)$$

Remark 2.2 The asymptotic (9) improves the error in (4) to $3/2 \ln N + \text{const}$. The constant $C(\varphi, b)$ can be expressed in terms of the covariances of the related tilted distributions.

proportional to $\exp\{-2\beta(|S| + \sum_{\Gamma \in \mathcal{G}(\sigma)} |\Gamma|)\}$, where $|\Gamma|$ denotes the length (number of edges) of polygon Γ .

To study the behaviour of the total magnetization one uses the tilted distribution

$$P_{V_{NM},h}^{\bar{\sigma}}(\sigma) = (Z(V_{NM}, h, \bar{\sigma}))^{-1} \exp\{-\beta(2|S| + 2 \sum_{\Gamma \in \mathcal{G}(\sigma)} |\Gamma| - hS_{V_{NM}}(\sigma))\}, \quad (11)$$

with suitably defined normalization $Z(V_{NM}, h, \bar{\sigma})$. This distribution, however, lacks the necessary analyticity properties, and, as in [3], one needs to restrict attention to configurations with cutoffs; subsequently, following the approach of [3, Chap. 3], one can relax the cutoff constraint for the events of interest.

As in [3], for $\omega_N > 0$ we let

$$\Omega_{NM}^{\omega_N} := \{\sigma \in \Omega_{NM} : \forall \Gamma \in \mathcal{G}(\sigma), \text{diam } \Gamma \leq \omega_N\}$$

be the configurations with cutoff ω_N , and for each $\sigma \in \Omega_{NM}^{\omega_N}$ put

$$P_{V_{NM},h,\omega_N}^{\bar{\sigma}}(\sigma) = (Z(V_{NM}, h, \bar{\sigma}, \omega_N))^{-1} \exp\{-\beta(2|S| + 2 \sum_{\Gamma \in \mathcal{G}(\sigma)} |\Gamma| - hS_{V_{NM}}(\sigma))\}, \quad (12)$$

with suitably defined normalization $Z(V_{NM}, h, \bar{\sigma}, \omega_N)$. As shown in [3, Chap. 3], if $\omega_N \geq K \ln |V_{NM}|$ with sufficiently large constant K , and if $|h|\omega_N < c < 1$, the limiting properties of the probability distributions (11) and (12) are similar. At the same time, for the partition function $Z(V_{NM}, h, \bar{\sigma}, \omega_N)$ the usual low-temperature cluster expansion holds, provided complex h satisfies $|h|\omega_N < c < 1$.

Step II. We then adapt the argument of [3, Chap. 3] to study the conditional distribution $P_{V_{NM},h,\omega_N}^{\bar{\sigma}}(\sigma|\{S\})$, generated by (12). Let

$$M(S) \equiv M_{V_{NM},h,\omega_N}^{\bar{\sigma}}(S) := E_{V_{NM},h,\omega_N}^{\bar{\sigma}}(S_{V_{NM}}|\{S\}) \quad (13)$$

be the expectation of the total spin $S_{V_{NM}}$ with respect to $P_{V_{NM},h,\omega_N}^{\bar{\sigma}}(\sigma|\{S\})$. For (even) integer b denote

$$q_{NM}^S(b) := \frac{2}{(2\pi|V_{NM}|d(\beta))^{1/2}} \exp\left\{-\frac{(b - M(S))^2}{2|V_{NM}|d(\beta)}\right\}, \quad (14)$$

where $d(\beta) > 0$ is the specific variance of a single spin in the pure plus phase, i.e., the

limit of the Gibbs distribution $P_{V_{NM}}^+(\sigma)$ with plus boundary conditions.

The following analogue of Theorem 3.18 in [3] holds.

Proposition 3.1 Fix a sequence of volumes V_{NM} as in Theorem 2.1. Let $h = h_N$ and $\omega_N \geq K \ln |V_{NM}|$, with $K = K(\beta) > 0$ large enough, be such that $|h|\omega_N < c < 1$. Then there exists $\beta_0 > 0$ such that for all $\beta \geq \beta_0$ we have

$$\lim_{N \rightarrow \infty} \frac{P_{V_{NM}, h_N, \omega_N}^{\bar{\sigma}}(S_{V_{NM}} = b | \{S\})}{q_{NM}^{\bar{S}}(b)} = 1 \quad (15)$$

for all even b satisfying $|b - M(S)| \leq K'(|V_{NM}|d(\beta))^{1/2}$ with some $K' < \infty$.

Remark 3.2 As shown in [3, Theorem 3.19], in the case $h_N \equiv 0$ the gaussian approximation (15) can be extended to all even b_N satisfying

$$\lim_{N \rightarrow \infty} \frac{|b_N - M(S)|}{|V_{NM}|^{2/3}} = 0,$$

where $M(S)$ is defined via (13) with $h = 0$.

The following analogue of Proposition 3.26 in [3] is also true.

Proposition 3.3 Let the cutoff levels ω_N satisfy $\lim_{N \rightarrow \infty} \omega_N / (\ln |V_{NM}|)^3 = 0$. For positive constants C and c , define

$$\alpha_{NM}(x) := \begin{cases} C \exp\{-cx^2/|V_{NM}|\}, & \text{if } |x| \leq |V_{NM}|/\omega_N, \\ C \exp\{-c|x|/\omega_N\}, & \text{if } |x| > |V_{NM}|/\omega_N. \end{cases}$$

Then there exist β_0 large enough, positive constants $C = C(\beta)$ and $c = c(\beta)$ such that

$$P_{V_{NM}, 0, \omega_N}^{\bar{\sigma}}(S_{V_{NM}} = b | \{S\}) \leq \alpha_{NM}(b - M(S)) \quad (16)$$

for all b , where $\beta > \beta_0$ and $M(S)$ is defined via (13) with $h = 0$.

As a result, the probability distribution $P_{V_{NM}, 0, \omega_N}^{\bar{\sigma}}(S_{V_{NM}} = b | \{S\})$ is well concentrated around the corresponding average $M(S)$.

Step III. We next describe dependence of the average $M(S)$ on the shape of the phase boundary S . Let $\Delta^+(S)$ (respectively, $\Delta^-(S)$) be the set of all $x \in V_{NM}$ such that $\sigma_x \equiv 1$ (respectively, $\sigma_x \equiv -1$) for all configurations $\sigma \in \Omega_{NM}$ compatible with S , i.e., $\sigma \sim S$.

Then the complement $V_{NM} \setminus (\Delta^+(\mathbb{S}) \cup \Delta^-(\mathbb{S}))$ decomposes into two regions, one of which is surrounded by only plus spins for all $\sigma \sim \mathbb{S}$ (denoted $V_+ = V_+(\mathbb{S})$) while the other is surrounded by only minus spins for all $\sigma \sim \mathbb{S}$ (and denoted $V_- = V_-(\mathbb{S})$), see Fig. 2. Then

$$M(\mathbb{S}) = |\Delta^+(\mathbb{S})| - |\Delta^-(\mathbb{S})| + E_{V_+,h,\omega_N}^+(S_{V_+}) + E_{V_-,h,\omega_N}^-(S_{V_-}),$$

with obvious interpretation of the last two averages. It is natural to expect that for typical \mathbb{S} and large V_{NM} we have

$$E_{V_+,h,\omega_N}^+(S_{V_+}) \approx m(\beta)|V_+|, \quad E_{V_-,h,\omega_N}^-(S_{V_-}) \approx -m(\beta)|V_-|,$$

where $m(\beta)$ is the spontaneous magnetization, so that

$$M(\mathbb{S}) \approx M_*(\mathbb{S}) := |\Delta^+(\mathbb{S})| - |\Delta^-(\mathbb{S})| + m(\beta)(|V_+| - |V_-|). \quad (17)$$

A naïve application of the shape dependence results from [3, Chap. 3] suggests that

$$|M(\mathbb{S}) - M_*(\mathbb{S})| \leq K(|\Delta^+(\mathbb{S})| + |\Delta^-(\mathbb{S})| + N + M),$$

with the right-hand side value of order N for typical \mathbb{S} . At the same time, for such \mathbb{S} the difference $\delta_-(\mathbb{S}) := |\Delta^+(\mathbb{S})| - |\Delta^-(\mathbb{S})|$ has symmetric distribution with zero mean, and it is intuitively “obvious” that the typical values of this difference are much smaller than

$$\delta_+(\mathbb{S}) := |\Delta^+(\mathbb{S})| + |\Delta^-(\mathbb{S})| \leq 4|\mathbb{S}|.$$

In fact, it is not difficult to show that for some $\alpha \in (1/2, 1)$ the rescaled difference $\delta_-(\mathbb{S})N^{-\alpha}$ has exponential tails. By applying a suitably adjusted version of the cluster expansions used in [4], one can verify that a similar property holds for $M(\mathbb{S}) - M_*(\mathbb{S})$, and therefore

$$M(\mathbb{S}) = m(\beta)(|V_+| - |V_-|) + O(N^\alpha) \quad (18)$$

for typical $\mathbb{S} \in \mathcal{G}_{NM}$.

Step IV. Let $q(\mathbb{S}) := (|V_+(\mathbb{S})| - |V_-(\mathbb{S})|)/2$ be the area defect created by the phase boundary \mathbb{S} , so that (18) becomes $M(\mathbb{S}) \approx 2m(\beta)q(\mathbb{S})$. Using this approximation in (14), it is easy to see that the simplified version of the local CLT asymptotics (15) is valid for

all b satisfying $|b - 2m(\beta)q(S)| \ll |V_{NM}|^{2/3}$. When combined with the uniform estimates (16) for the remaining values of b , one can see that the sum in (10) is essentially reduced to the phase boundaries S satisfying $q(S) = q$ with

$$\left| q - \frac{b_N}{2m(\beta)} \right| \ll N^{4/3}. \quad (19)$$

On the other hand, the area defect $q(S)$ has standard deviation of order $O(N^{3/2})$ and therefore the probability of the event $\{q(S) = q\}$ is almost constant for all q in (19). As a result, the sum in (10) is well approximated by the value

$$P_{V_{NM}}^{\sigma}(q(S) = b_N/2m(\beta)),$$

whose asymptotic can be derived from the results in [4]. The target relation (9) follows.

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