

Ising model fog drip: the first two droplets

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Abstract. We present here a simple model describing coexistence of solid and vapour phases. The two phases are separated by an interface. We show that when the concentration of supersaturated vapour reaches the dew-point, the droplet of solid is created spontaneously on the interface, adding to it a monolayer of a “visible” size.

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1. Introduction: Condensation phenomenon in the Ising model

The phenomenon of droplet condensation in the framework of the Ising model was first described in the papers [DS1], [DS2]. It deals with the following situation. Suppose we are looking at the Ising spins $\sigma_t = \pm 1$ at low temperature β^{-1} , occupying a d -dimensional box T_N^d of the linear size $2N$ with periodic boundary conditions. If we impose the canonical ensemble restriction, fixing the total mean magnetization,

$$\frac{M_N}{|T_N^d|} \triangleq \frac{1}{|T_N^d|} \sum \sigma_t,$$

to be equal to the spontaneous magnetization, $m^*(\beta) > 0$, then the typical configuration that we see will look as a configuration of the (+)-phase. That means that the spins are taking mainly the values $+1$, while the values -1 are seen rarely, and the droplets of minuses in the box T_N^d are at most of the size of $K(d) \ln N$. We want now to put more -1 particles into the box T_N^d , and we want to see how the above droplet picture would evolve. That means, we want to look at the model with a different canonical constraint:

$$M_N = m^*(\beta) |T_N^d| - b_N,$$

$b_N > 0$. It turns out that if b_N -s are small, nothing is changed in the above picture; namely, if

$$\frac{b_N}{|T_N^d|^{\frac{d}{d+1}}} \rightarrow 0 \text{ as } N \rightarrow \infty,$$

then in the corresponding canonical ensemble all the droplets are still microscopic, not exceeding $K(d) \ln N$ in linear size. On the other hand, once

$$\liminf_{N \rightarrow \infty} \frac{b_N}{|T_N^d|^{\frac{d}{d+1}}} > 0,$$

the situation becomes very different: among many $(-)$ -droplets there is one of the linear size of the order of $(b_N)^{1/d} \geq N^{\frac{d}{d+1}}$, while all the rest of the droplets are still at most logarithmic. Therefore $b_N \sim |T_N^d|^{\frac{d}{d+1}}$ can be called the *condensation threshold*, or *dew-point*. The behavior of the system *at the threshold scale*, i.e. for $b_N = c |T_N^d|^{\frac{d}{d+1}} (1 + o_N(1))$, is considered in the 2D case in [BCK]. Sharp description of the transition *inside the threshold* is considered in [HIK].

The above condensation picture suffers from one (largely esthetic) defect: both below and immediately above the condensation threshold the droplets are “too small to be visible”, i.e. they are of the size sublinear with respect to the system size. This defect was to some degree bypassed in [BSS]. It is argued there on heuristic level, that in the low-temperature 3D Ising model in the regime when b_N is already of the volume order, i.e. $b_N \sim \nu N^3$, the sequence of condensations happens, with “visible” results. In such regime one expects to find in the box T_N^3 a droplet Γ of $(-)$ -phase, of linear size of the order of N , having the approximate shape of the Wulff crystal, which crystal at low temperatures has 6 flat facets. One expects furthermore that the surface Γ itself has 6 flat facets, at least for some values of b_N . However, when one further increases the “supersaturation parameter” b_N , by an increment of the order of N^2 , one expects to observe the condensation of extra $(-)$ -particles on one of the flat facets of Γ (randomly chosen), forming a monolayer \mathfrak{m} of thickness of one lattice spacing, and of linear size to be cN , with $c \geq c_{crit} = c_{crit}(\beta)$, with $c_{crit}N$ being smaller than the size of the facet. As b_N increases further, the monolayer \mathfrak{m} grows, until all the facet is covered by it. So one expects to see here the condensation of the supersaturated gas of $(-)$ -particles into a monolayer of linear size $\sim c_{crit}N$, which is “visible”. (Indeed, such monolayers were observed in the experiments of condensation of the Pb.) The rigorous results obtained in [BSS] are much more modest: the model studied there is the Solid-on-Solid model, and even in such simplified setting the evidence of appearance of the monolayer \mathfrak{m} of linear size is indirect.

The purpose of the present paper is to consider another 3D lattice model, where one can completely control the picture and prove the above behavior to happen. Namely, we consider a system of ideal particles in the phase transition regime, and we put these phases – the vapour phase and the solid phase – into coexistence by applying the canonical constraint, i.e. by fixing the total number of

particles. We study the interface Γ , separating them, and we show that when we increase the total number of particles, the surface Γ changes in the way described above. More precisely, we show that for some values of concentration the surface Γ is essentially flat, but when the concentration increases up to the dew-point, a monolayer \mathfrak{m} of a size at least $c_{crit}N$ appears on Γ , with N being the linear size of our system.

2. Informal description of the main result

In this section we describe our results informally. We will use the language of the Ising model, though below we treat rigorously a simpler model of the interface between two ideal particles phases. Ising model language makes the description easier; moreover, we believe that our picture holds for the Ising spins as well.

Suppose we are looking at the Ising spins $\sigma_t = \pm 1$ at low temperature β^{-1} in a 3D box B_N of the linear sizes $RN \times RN \times 2N$. The parameter R should be chosen sufficiently large in order to be compatible with the geometry of monolayer creation as described below. We impose (+)-boundary conditions in the upper half-space ($z > 0$), and (-)-boundary conditions in the lower half-space ($z < 0$). These (\pm)-boundary conditions force an interface Γ between the (+) and the (-) phases in V_N , and the main result of the paper [D1] is a claim that the interface Γ is rigid. It means that at any location, with probability going to 1 as the temperature $\beta^{-1} \rightarrow 0$, the interface Γ coincides with the plane $z = 0$. If we impose the canonical ensemble restriction, fixing the total mean magnetization M_N to be zero, then the properties of Γ stay the same.

We will now put more -1 particles into V_N ; that is, we fix M_N to be

$$M_N = -b_N = -\delta N^2,$$

and we will describe the evolution of the surface Γ as the parameter $\delta > 0$ grows. The macroscopic image of this evolution is depicted on Figure 1.

0. $0 \leq \delta < \delta^1$

Nothing is changed in the above picture – namely, the interface Γ stays rigid. It is essentially flat at $z = 0$; the local fluctuations of Γ are rare and do not exceed $K \ln N$ in linear size.

I. $\delta^1 < \delta < \delta^2$

The monolayer \mathfrak{m}_1 appears on Γ . This is a random outgrowth on Γ , of height one. Inside \mathfrak{m}_1 the height of Γ is typically $z = 1$, while outside it we have typically $z = 0$.

For δ close to δ^1 the shape of \mathfrak{m}_1 is *the Wulff shape*, given by the Wulff construction, with the surface tension function $\tilde{\tau}^{2D}(n)$, $n \in \mathbb{S}^1$, given by

$$\tilde{\tau}(n) = \left. \frac{d}{dn} \tau^{3D}(m) \right|_{m=(0,0,1)}. \quad (2.1)$$

Here $\tau^{3D}(m)$, $m \in \mathbb{S}^2$ is the surface tension function of the 3D Ising model, the derivatives in (2.1) are taken at the point $(0,0,1) \in \mathbb{S}^2$ along all the tangents

$n \in \mathbb{S}^1$ to the sphere \mathbb{S}^2 . The “radius” of \mathbf{m}_1 is of the order of N , i.e. it equals to $r_1(\delta)N$, and as $\delta \searrow \delta^1$ we have $r_1(\delta) \searrow r_{cr} > 0$. In particular, we never see a monolayer \mathbf{m} of radius smaller than $r_{cr}N$.

As we explain below r_{cr} should scale like $R^{2/3}$. In particular, it is possible to choose R in such a fashion that $R > 2r_{cr}$ or, in other words, for values of R sufficiently large the critical droplet fits into B_N .

As δ increases, the monolayer \mathbf{m}_1 grows in size, and at a certain moment $\delta = \delta^{1.5}$ it touches the faces of the box B_N . After that moment the shape of \mathbf{m}_1 is different from the Wulff shape. Namely, it is *the Wulff plaquette* (see [SchS]), made from four segments on the four sides of the $RN \times RN$ square, connected together by the four quarters of the Wulff shape of radius $\tilde{r}_1(\delta)N$. We have evidently $\tilde{r}_1(\delta^{1.5}) = R/2$. As $\delta \nearrow \delta^2$, the radius $\tilde{r}_1(\delta)$ decreases to some value $\tilde{r}_1(\delta^2)N$, with $\tilde{r}_1(\delta^2) > 0$.

II. $\delta^2 < \delta < \delta^{2.5}$

The second monolayer \mathbf{m}_2 is formed on the top of \mathbf{m}_1 . Asymptotically it is of Wulff shape with the radius $r_2(\delta)N$, with $r_2(\delta) \searrow r_2^+(\delta^2)$ as $\delta \searrow \delta^2$, with $r_2^+(\delta^2) > 0$. The first monolayer \mathbf{m}_1 has a shape of Wulff plaquette with radius $\tilde{r}_1(\delta)$, which satisfies

$$\tilde{r}_1(\delta) = r_2(\delta).$$

A somewhat curious relation is:

$$r_2^+(\delta^2) \text{ is strictly bigger than } \tilde{r}_1(\delta^2).$$

In other words, the Wulff-plaquette-shaped monolayer \mathbf{m}_1 undergoes a jump in its size and shape as the supersaturation parameter δ crosses the value δ^2 . In fact, the monolayer \mathbf{m}_1 shrinks in size: the radius $\tilde{r}_1(\delta)$ increases as δ grows past δ^2 .

II.5 $\delta^{2.5} < \delta < \delta^3$

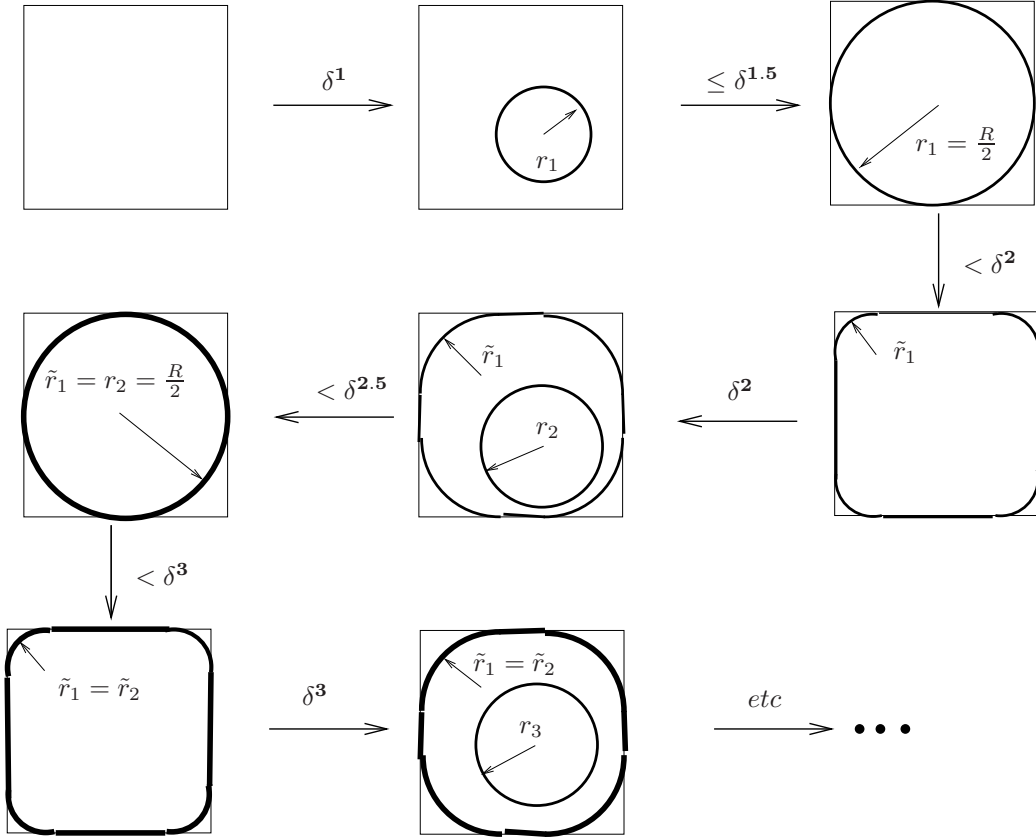
At the value $\delta = \delta^{2.5}$ the growing monolayer \mathbf{m}_2 meets the shrinking monolayer \mathbf{m}_1 , i.e. $r_2(\delta^{2.5}) = \tilde{r}_1(\delta^{2.5}) = R/2$. Past the value $\delta^{2.5}$ the two monolayers $\mathbf{m}_2 \subset \mathbf{m}_1$ are in fact asymptotically equal, both having the shape of the Wulff plaquette with the same radius $\tilde{r}_1(\delta) = \tilde{r}_2(\delta)$, decreasing to the value $\tilde{r}_1(\delta^3) = \tilde{r}_2(\delta^3)$ as δ increases up to δ^3 .

III. $\delta^3 < \delta < \delta^4$

The third monolayer \mathbf{m}_3 is formed, of the asymptotic radius $r_3(\delta)N$, with $r_3(\delta) \searrow r_3^+(\delta^3)$ as $\delta \searrow \delta^3$, with $r_3^+(\delta^3) > 0$. The radii of two bottom Wulff plaquettes $\tilde{r}_1(\delta) = \tilde{r}_2(\delta) = r_3(\delta)$ decrease to the value $r_3^+(\delta^3)$ as δ decreases down to δ^3 , with $r_3^+(\delta^3) > \tilde{r}_i(\delta^3)$, so the two Wulff plaquettes $\mathbf{m}_1, \mathbf{m}_2$ shrink, jumping to a smaller area, as δ passes the threshold value δ^3 .

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A complete investigation of the restricted Wulff variational problem (see (7.5) below) and, accordingly, a rigorous treatment of the interface repulsion phenomenon which shows up on the microscopic level in all the regimes from II.5 on is relegated to a forthcoming paper [IS]. For the rest of the paper we shall focus on


 FIGURE 1. Creation and evolution of macroscopic monolayers on Γ as δ grows

the regimes **0**, **I** and **II** in the context of a simplified model which we proceed to introduce.

3. Our model

We consider the following lattice model of two-phase coexistence. The 3D box

$$B_N = \Lambda_N \times \{-N - 1/2, -N + 1/2, \dots, N - 1/2, N + 1/2\}$$

is filled with two kinds of particles: v -particles (vapour phase) and s -particles (solid phase). Here Λ_N is a two-dimensional $RN \times RN$ box;

$$\Lambda_N = \{0, 1, \dots, RN - 1\}^2,$$

and R is a constant, which we shall set later on to be big enough, in order to make our picture clearer. We have $|B_N| = 2R^2N^3$. Vapour v -particles are occupying the

upper part of B_N , while solid s -particles – the lower part. Some sites of the box B_N can be empty. In our model the two phases are separated by an interface Γ , which is supposed to be an SOS-type surface; it is uniquely defined by a function

$$h_\Gamma : \Lambda_N^\circ \rightarrow \{-N, -N+1, \dots, N\},$$

where Λ_N° is the interior of Λ_N . We assume that the interface Γ is pinned at zero height on the boundary $\partial\Lambda_N$, that is $h_\Gamma \equiv 0$ on $\partial\Lambda_N$.

Such a surface Γ splits B_N into two parts; let us denote by $V_N(\Gamma)$ and $S_N(\Gamma)$ the upper and the lower halves. The set of configurations of our model consists thus from a surface Γ plus a choice of two subsets, $\sigma_v \subset V_N(\Gamma)$ and $\sigma_s \subset S_N(\Gamma)$; we have a vapour particle at a point $x \in B_N$ iff $x \in \sigma_v$, and similarly for solid particles.

The partition function $Z_N(\beta)$ of our model is now given by

$$Z_N(\beta) = \sum_{(\Gamma, \sigma_v, \sigma_s)} \exp\{-\beta|\Gamma| - (a|\sigma_v| + b|V_N(\Gamma) \setminus \sigma_v| + c|\sigma_s| + d|S_N(\Gamma) \setminus \sigma_s|)\}. \quad (3.1)$$

Here $|\Gamma|$ is the surface area of Γ , $|\sigma_v|$ is the number of vapour particles, ..., while a, b, c, d are four chemical potentials. We want the two phases to be in the equilibrium, so we suppose that

$$e^{-a} + e^{-b} = e^{-c} + e^{-d} \equiv e^{-f},$$

where the last equality is our definition of the free energy f . Accordingly, let us define microscopic occupation probabilities in vapour and solid states as

$$p^v = e^{f-a} \quad \text{and} \quad p^s = e^{f-c}.$$

To mimic the fact that the density of the solid state has to be higher, we impose the relation $p^v < p^s$.

We will study our model under the condition that the total number of particles is fixed, and in the leading order of N it is $2\rho R^2 N^3$, with ρ between the values p^v and p^s . Of course, flat interface at level zero should correspond to the choice

$$\rho_0 = \frac{p^s + p^v}{2}.$$

More generally, given $\rho = \rho_0 + \Delta$, one expects to find Γ to be located approximately at the height ℓN above zero level, where ℓ satisfies

$$\frac{\ell}{2} (p^s - p^v) = \Delta.$$

The above reasoning suggests that in our model the formation of macroscopic monolayers over flat interface should happen in canonical ensemble with total number of particles being fixed at

$$2\rho_0 R^2 N^3 + \delta N^2 \triangleq a_0 N^3 + \delta N^2 \quad (3.2)$$

with varying δ .

We will denote by \mathbb{P} the (“grand canonical”) probability distribution on triples $\{\Gamma, \sigma_v, \sigma_s\}$ corresponding to the above partition function. Our main interest in this paper is the study of the conditional distribution of the random surface Γ , under condition that the total *number of particles*

$$\Sigma \triangleq |\sigma_v| + |\sigma_s| \triangleq \Sigma_v + \Sigma_s,$$

is fixed, i.e. the distribution $\mathbb{P}\left(\Gamma \mid \Sigma = a_0 N^3 + \delta N^2\right)$.

To study this conditional distribution we rely on Bayes’ rule,

$$\mathbb{P}\left(\Gamma \mid \Sigma = a_0 N^3 + \delta N^2\right) = \frac{\mathbb{P}\left(\Sigma = a_0 N^3 + \delta N^2 \mid \Gamma\right) \mathbb{P}(\Gamma)}{\sum_{\Gamma'} \mathbb{P}\left(\Sigma = a_0 N^3 + \delta N^2 \mid \Gamma'\right) \mathbb{P}(\Gamma')}.$$

The control over the conditional probabilities $\mathbb{P}\left(\bullet \mid \Gamma\right)$ comes from volume order local limit theorems for independent Bernoulli variables, whereas a-priori probabilities $\mathbb{P}(\Gamma)$ are derived from representation of Γ in terms of a gas of non-interacting contours.

In the sequel c_1, c_2, \dots are positive constants which appear in various inequalities and whose values are fixed in such a way that the corresponding bounds hold true.

4. Volume order limit theorems

The study of probabilities $\Pr\left(\Sigma = a_0 N^3 + \delta N^2 \mid \Gamma\right)$ is easy, since we are dealing with independent variables. Indeed, let $B_N = S_N \cup V_N$ be the decomposition of B_N induced by Γ . Then, the $\mathbb{P}\left(\bullet \mid \Gamma\right)$ -conditional distribution of the overall number of particles is

$$\Sigma = \sum_{i \in S_N} \xi_i^s + \sum_{j \in V_N} \xi_j^v,$$

with iid Bernoulli(p^s) random variables ξ_i^s , and iid Bernoulli(p^v) random variables ξ_j^v .

Let $\alpha(\Gamma)$ be the signed volume under the interface Γ ,

$$\alpha(\Gamma) = \int \int h_\Gamma(x, y) dx dy, \quad (4.1)$$

where we set h_Γ to be equal to $h_\Gamma(i)$ in the unit box $i + [1/2, 1/2]^2$. Clearly, $|S_N| = R^2 N^3 + \alpha(\Gamma)$ and $|V_N| = R^2 N^3 - \alpha(\Gamma)$. Accordingly,

$$\mathbb{E}\left(\Sigma \mid \Gamma\right) = a_0 N^3 + \alpha(\Gamma) p^{sv},$$

where $p^{sv} \triangleq p^s - p^v$. Introducing the variances $D^s = p^s(1 - p^s)$, $D^v = p^v(1 - p^v)$ and $D = D^s + D^v$, we infer from the Local Limit Theorem (LLT) behavior: For

every K fixed there exist two positive constants c_1 and c_2 , such that

$$c_1 \leq \frac{\mathbb{P}\left(\Sigma = a_0 N^3 + \delta N^2 \mid \Gamma\right)}{\frac{1}{\sqrt{\pi D |B_N|}} \exp\left\{-\frac{(\alpha(\Gamma) p^{sv} - \delta N^2)^2}{D |B_N|}\right\}} \leq c_2, \quad (4.2)$$

uniformly in N , $|\delta| \leq K$ and Γ , provided $|\alpha(\Gamma)| \leq KN^2$.

5. Surface weights

We now want to describe the a-priori probability distribution $\mathbb{P}(\Gamma)$. It is convenient and natural to express it via the weights $\{w(\Gamma)\}$, so that

$$\mathbb{P}(\Gamma) \triangleq \text{Pr}(\Gamma) = \frac{w(\Gamma)}{\sum_{\Gamma} w(\Gamma)}, \quad (5.1)$$

where we shall use an additional symbol Pr in order to stress that the corresponding probabilities are computed in the contour model we are going to introduce now.

For our purposes it is necessary to introduce a contour parameterization of the set of all surfaces Γ . Contours will live on the bonds of the dual (two dimensional) box $\Lambda_N^* = \{1/2, 3/2, \dots, RN - 3/2\}^2$, and they are defined as follows: Given an interface Γ and, accordingly, the height function h_Γ which, by definition, is identically zero outside Λ_N° , define the following semi-infinite subset $\widehat{\Gamma}$ of \mathbb{R}^3 ,

$$\widehat{\Gamma} = \bigcup_{\substack{(x,y,k) \\ k < h_\Gamma(x,y)}} \left((x, y, k) + \widehat{C} \right),$$

where $\widehat{C} = [-1/2, 1/2]^3$ is the unit cube. The above union is over all $(x, y) \in \mathbb{Z}^2$ and $k \in 1/2 + \mathbb{Z}$.

Consider now the level sets of Γ , i.e. the sets

$$H_k = H_k(\widehat{\Gamma}) = \left\{ (x, y) \in \mathbb{R}^2 : (x, y, k) \in \widehat{\Gamma} \right\}, \quad k = -N, -N+1, \dots, N.$$

We define *contours* as the connected components of sets ∂H_k . The length $|\gamma|$ of a contour is defined in an obvious way. Since, by construction all contours are closed polygons composed of the nearest neighbour bonds of Λ_N^* , the notions of interior $\text{int}(\gamma)$ and exterior $\text{ext}(\gamma)$ of a contour γ are well defined. A contour γ is called a \oplus -contour (\ominus -contour), if the values of the function h_Γ at the immediate exterior of γ are smaller (bigger) than those at the immediate interior of γ .

Alternatively, let us orient the bonds of each contours $\gamma \subseteq \partial H_k$ in such a way that when we traverse γ the set H_k remains to the right. Then \oplus -contours are those which are clockwise oriented with respect to their interior, whereas \ominus -contours are counter-clockwise oriented with respect to their interior.

Let us say that two oriented contours γ and γ' are compatible, $\gamma \sim \gamma'$, if

1. Either $\text{int}(\gamma) \cap \text{int}(\gamma') = \emptyset$ or $\text{int}(\gamma) \subseteq \text{int}(\gamma')$ or $\text{int}(\gamma') \subseteq \text{int}(\gamma)$.

2. Whenever γ and γ' share a bond b , b has the same orientation in both γ and γ' .

A family $\Gamma = \{\gamma_i\}$ of oriented contours is called consistent, if contours of Γ are pair-wise compatible. It is clear that the interfaces Γ are in one-to-one correspondence with consistent families of oriented contours. The height function h_Γ could be reconstructed from a consistent family $\Gamma = \{\gamma\}$ in the following way: For every contour γ the sign of γ , which we denote as $\text{sign}(\gamma)$, could be read from its orientation. Then,

$$h_\gamma(x, y) = \text{sign}(\gamma)\chi_{\text{int}(\gamma)}(x, y) \quad \text{and} \quad h_\Gamma = \sum_{\gamma \in \Gamma} h_\gamma,$$

where χ_A is the indicator function of A .

We are finally ready to specify the weights $w(\Gamma)$ which appear in (5.1): Let $\Gamma = \{\gamma\}$ be a consistent family of oriented (signed) contours, Then,

$$w(\Gamma) = \exp \left\{ -\beta \sum_{\gamma \in \Gamma} |\gamma| \right\}. \tag{5.2}$$

By definition the weight of the flat interface $w(\Gamma_0) = 1$.

6. Estimates in the contour ensemble

In order to make the contour model (5.1) , (5.2) tractable one should, evidently, make certain assumptions on the largeness of β , e.g. e^β should be certainly larger than the connective constant of self-avoiding random walks on \mathbb{Z}^2 [MS]. In fact, it would be possible to push for optimal results in terms of the range of β along the lines of recent developments in the Ornstein-Zernike theory [I, CIV1, CIV2]. However, in order to facilitate the exposition and in order to focus on the phenomenon of monolayer creation per se, we shall just conveniently assume that β is so large that one or another form of cluster expansion goes through, see eg. [D2]. Due to the (\pm -contour) symmetry of the model the corresponding techniques would be quite similar to those developed in the context of the 2D low temperature Ising model in [DKS]. Consequently, instead of stating conditions on β explicitly we shall just assume that $\beta > \beta_0$, where β_0 is so large that all the claims formulated below are true.

In the sequel we shall employ the following notation: \mathcal{C} for clusters of non-compatible contours and $\Phi_\beta(\mathcal{C})$ for the corresponding cluster weights which shows up in the cluster expansion representation of partition functions.

Peierls estimate on appearance of γ . Given a contour γ and a consistent family of contours Γ , let us say that $\gamma \overset{k}{\in} \Gamma$, if γ appears in Γ exactly k times. Then,

$$\Pr \left(\gamma \overset{k}{\in} \Gamma \right) \leq e^{-k\beta|\gamma|}. \tag{6.1}$$

Indeed, every Γ satisfying $\gamma \stackrel{k}{\in} \Gamma$ can be decomposed as $\Gamma = \Gamma' \cup \gamma \cup \dots \cup \gamma$. Therefore,

$$\Pr\left(\gamma \stackrel{k}{\in} \Gamma\right) \leq \frac{\sum_{\Gamma'} w(\Gamma') e^{-k\beta|\gamma|}}{\sum_{\Gamma'} w(\Gamma')},$$

where the sums are over all consistent families which are compatible with γ , but do not contain it.

Fluctuations of $\alpha(\Gamma)$ and absence of intermediate contours. The following rough a-priori statement is a consequence of (6.1): There exist positive ν such that for every $b_0 > 0$ fixed,

$$\Pr(|\alpha(\Gamma)| > bN^2) \leq c_3 e^{-\nu N\sqrt{b}}, \quad (6.2)$$

uniformly in $b \geq b_0$ and in N large enough.

In view of (4.2) (computed with respect to the flat interface Γ_0 with $\alpha(\Gamma_0) = 0$) the bound (6.2) implies that the canonical distribution $\mathbb{P}\left(\bullet \mid \Sigma = a_0 N^3 + \delta N^2\right)$ is concentrated on Γ with

$$\alpha(\Gamma) \leq N^2 \max\left\{\frac{\delta^4}{\nu^2 D^2 R^4}, b_0\right\}. \quad (6.3)$$

Now let the interface Γ be given by a consistent collection of contours, and assume that $\gamma \sim \Gamma$. Of course $\alpha(\Gamma \cup \gamma) = \alpha(\Gamma) + \alpha(\gamma)$. Let us assume that the surface Γ satisfies the estimate (6.3). Then

$$\begin{aligned} & \mathbb{P}\left(\Gamma \cup \gamma \mid \Sigma = a_0 N^3 + \delta N^2\right) \\ & \leq \frac{\mathbb{P}\left(\Sigma = a_0 N^3 + \delta N^2 \mid \Gamma \cup \gamma\right)}{\mathbb{P}\left(\Sigma = a_0 N^3 + \delta N^2 \mid \Gamma\right)} \cdot \frac{\Pr(\Gamma \cup \gamma)}{\Pr(\Gamma)} \\ & \leq c_4 \exp\left\{c_5 \frac{|\alpha(\gamma)|}{N} - \beta|\gamma|\right\} \leq c_4 \exp\left\{c_6 \frac{|\gamma|^2}{N} - \beta|\gamma|\right\} \end{aligned}$$

where we have successively relied on Bayes' rule, (4.2) and on the isoperimetric inequality.

It follows that for every K there exists $\epsilon = \epsilon(\beta) > 0$ such that intermediate contours γ with

$$\frac{1}{\epsilon} \log N < |\gamma| < \epsilon N \quad (6.4)$$

are, uniformly in $|\delta| < K$, improbable under the conditional distribution

$$\mathbb{P}\left(\bullet \mid \Sigma = a_0 N^3 + \delta N^2\right).$$

In the sequel we shall frequently *ignore* intermediate contours, as if they do not contribute at all to the distribution (5.1). To avoid confusion, we shall use $\widehat{\Pr}$ for the restricted contour ensemble, which is defined exactly as in (5.1), except that the intermediate contours γ satisfying (6.4) are suppressed.

7. The surface tension and the Wulff shape

Since we are anticipating formation of a monolayer droplet on the interface, we are going to need the surface tension function in order to study such a droplet and to determine its shape. It is defined in the following way: Let λ be an oriented site self avoiding path on the dual lattice \mathbb{Z}_*^2 . An oriented contour γ is said to be compatible with λ ; $\gamma \sim \lambda$, if $\lambda \cap \text{int}(\gamma) = \emptyset$ and if whenever λ and γ share a bond b , the orientation of b is the same in both λ and γ . Accordingly, if \mathcal{C} is a cluster of (incompatible) contours, then $\mathcal{C} \sim \lambda$ if $\gamma \sim \lambda$ for every $\gamma \in \mathcal{C}$.

In the sequel $0^* = (1/2, 1/2)$ denotes the origin of \mathbb{Z}_*^2 . Let $x \in \mathbb{Z}_*^2$. Set,

$$T_\beta(x) = \sum_{\lambda: 0^* \rightarrow x} \exp \left\{ -\beta|\lambda| - \sum_{\mathcal{C} \neq \lambda} \Phi_\beta(\mathcal{C}) \right\},$$

where the sum is over all oriented self-avoiding paths from 0^* to x .

Let $n \in \mathbb{S}^1$ be a unit vector, and $n^\perp \in \mathbb{S}^1$ is orthogonal to it. The surface tension τ_β in direction n is defined as

$$\tau_\beta(n) = - \lim_{L \rightarrow \infty} \frac{1}{L} \log T_\beta(\lfloor Ln^\perp \rfloor).$$

Consider the Wulff variational problem, which is a question of finding the minimum $w_\beta(S)$ of the functional,

$$w_\beta(S) \equiv \min_{\{\lambda: \text{Area}(\lambda)=S\}} \mathcal{W}(\lambda).$$

Here

$$\mathcal{W}(\lambda) = \int_\lambda \tau_\beta(n_s) ds,$$

n_s being the unit normal to λ at the point $\lambda(s)$, and the minimum is taken over all closed self-avoiding loops λ , enclosing the area S . Of course, $w_\beta(S) = \sqrt{S}w_\beta(1)$. Let us denote by W_β the Wulff shape, which is the minimizing loop with area $S = 1$.

As in [DKS] it could be shown that if β is sufficiently large, then τ_β is well defined and strictly positive. Furthermore, the boundary of the optimal loop W_β is locally analytic and has uniformly positive and bounded curvature.

One can now apply to the present setting the machinery and the results of [DKS], [DS1], [DS2], [SchS] and [ISch]. They allow us to study the probabilities of the events

$$\Pr(A_b) \equiv \Pr \{ \Gamma : \alpha(\Gamma) = b \}, \quad (7.1)$$

where we consider here the probability distribution (5.1).

As it follows from local limit results in the restricted phase [DKS] without intermediate contours (6.4), for all values of b , the probability $\widehat{\Pr}(A_b)$ is bounded above by

$$\widehat{\Pr}(A_b) \leq c_7 \exp \left\{ -c_8 \frac{b^2}{N^2} \wedge N \right\}. \quad (7.2)$$

In particular, for the values of $b \ll N^{3/2}$ the main contribution to $\widehat{\text{Pr}}(A_b)$ comes from small contours; $|\gamma| < \epsilon^{-1} \log N$. In other words, for such values of b , conditional distribution $\widehat{\text{Pr}}(\cdot | A_b)$ is concentrated on the interfaces Γ which are essentially flat: all contours γ of a typical surface Γ are less than $\epsilon^{-1} \log N$ in length, while their density goes to zero as $\beta \rightarrow \infty$.

On the other hand, for values of $b \gg N^{3/2}$ long contours contribute, and the probabilities $\text{Pr}(A_b)$ satisfy

$$\log \text{Pr}(A_b) = -\sqrt{b} w_\beta(1) (1 + o_N(1)), \quad (7.3)$$

provided, of course, that the scaled Wulff shape $\sqrt{b/N^2} W_\beta$ fits into the square $[0, R]^2$. Under these two restrictions on b the analysis of [DKS] implies that the conditional distribution $\text{Pr}(\cdot | A_b)$ is concentrated on the interfaces Γ which are ‘‘occupying two consecutive levels’’. Namely, the set $\{\gamma_i\}$ of contours, comprising Γ , contains exactly one large contour, γ_0 , of diameter $\sim \sqrt{b}$, while the rest of them have their lengths not exceeding $\epsilon^{-1} \ln N$. The contour γ_0 is of \oplus -type, so for the majority of points inside γ_0 the value of the height function h_Γ is 1, while outside γ_0 it is mainly zero. Finally, the contour γ_0 has

- *Asymptotic shape*: The contour γ_0 is of size $\sim \sqrt{b}$, and it follows very close the curve $\sqrt{b} W_\beta$. Namely, the latter can be shifted in such a way that the Hausdorff distance

$$\rho_H(\gamma_0, \sqrt{b} W_\beta) \leq \sqrt[3]{b}. \quad (7.4)$$

Of course, all the claims above should be understood to hold only on the set of typical configurations, i.e. on the sets of (conditional) probabilities going to 1 as $N \rightarrow \infty$.

In the present paper we also we need to consider such values of $b \sim 2R^2 N^2$, when the scaled Wulff shape $\sqrt{b/N^2} W_\beta$ does not fit into the square $[0, R]^2$. This situation was partially treated in the paper [SchS], and the technique of that paper provides us with the following information about the typical behavior of Γ under the distribution $\widehat{\text{Pr}}(\cdot | A_b)$ for the remaining values of b .

Namely, instead of the Wulff variational problem we have to consider the following *restricted* Wulff variational problem, which is a problem of finding the minimum

$$w_\beta^{rst}(S) \equiv \min_{\{k; \lambda_1, \dots, \lambda_k\}} \mathcal{W}_S^{rst}(k; \lambda_1, \dots, \lambda_k) \equiv \mathcal{W}(\lambda_1) + \dots + \mathcal{W}(\lambda_k), \quad (7.5)$$

where

- the curves $\lambda_1, \dots, \lambda_k$ are closed piecewise smooth loops *inside* the unit square Q_1 ;
- the loops λ_i are nested: $\text{Int}(\lambda_k) \subseteq \text{Int}(\lambda_{k-1}) \subseteq \dots \subseteq \text{Int}(\lambda_1)$;
- $\text{Area}(\lambda_k) + \text{Area}(\lambda_{k-1}) + \dots + \text{Area}(\lambda_1) = S$.

The parameter k is not fixed; we have to minimize over k as well. For the area parameter S small enough, the minimum in (7.5) is attained at $k = 1$, while λ_1 is

the scaled Wulff shape, $\sqrt{S}W_\beta$. In other words, in this regime $w_\beta^{rst}(S) = w_\beta(S)$. Let S_1 be the maximal value, for which the inclusion $\sqrt{S}W_\beta \subset Q_1$ is possible. In the range $S_1 < S < 1$ the solution to (7.5) is given by $k = 1$, while the loop λ_1 is the corresponding Wulff plaquette, described above. In the range $1 < S < 2S_1$ the solution has the value $k = 2$, the curve λ_1 is the Wulff plaquette, while the curve $\lambda_2 \subset \lambda_1$ is the Wulff shape; they are uniquely defined by the two conditions:

1. $\text{Area}(\lambda_2) + \text{Area}(\lambda_1) = S$,
2. the curved parts of λ_1 are translations of the corresponding quarters of λ_2 .

In the range $2S_1 < S < 2$ we have $k = 2$, while the loops $\lambda_2 = \lambda_1$ are identical Wulff plaquettes.

The relation (7.3) is generalized to

$$\log \Pr(A_b) = -RNw_\beta^{rst} \left(\frac{b}{R^2N^2} \right) (1 + o_N(1)). \quad (7.6)$$

The function $w_\beta^{rst}(S)$ is evidently increasing in S . For S small it behaves as $c'\sqrt{S}$. In the vicinity of the point $S = 1$ it behaves as $c''\sqrt{S-1}$ for $S > 1$, and as $c'''\sqrt{1-S}$ for $S < 1$. Otherwise it is a smooth function of S , $0 \leq S < 2$. The two singularities we just pointed out, are responsible for the interesting geometric behavior of our model, which has been described informally in Section 2, and will be explicitly formulated in the next Section. Namely, each one is responsible for the appearance of the corresponding droplet.

Accordingly, once the Wulff shape $\sqrt{b/N^2} W_\beta$ does not fit into the square $[0, R]^2$, while $b \leq c(\beta) R^2 N^2$ (where the constant $c(\beta) \rightarrow 1$ as $\beta \rightarrow \infty$) the conditional distribution $\Pr(\cdot | A_b)$ is concentrated on the interfaces Γ which again are occupying two consecutive levels. The set $\{\gamma_i\}$ of contours, comprising Γ , contains one large contour, γ_0 , this time of diameter $\sim R$, which in some places is going very close to the boundary of our box. The rest of contours have their lengths not exceeding $\epsilon^{-1} \ln N$. The contour γ_0 is of \oplus -type, and for the majority of points inside γ_0 the value of the height function h_Γ is 1, while outside γ_0 it is mainly zero. Finally, the contour γ_0 has asymptotic shape of the Wulff plaquette, in the same sense as in (7.4).

In the remaining range $R^2N^2 \leq b \leq 2R^2N^2$ the set $\{\gamma_i\}$ of contours, comprising Γ , contains exactly two large contours, γ_0 and γ_1 , with $\gamma_1 \subset \text{Int}(\gamma_0)$, both of the \oplus -type. The interface Γ is, naturally, occupying three consecutive levels: it is (typically) at the height 2 inside γ_1 , at height 1 between γ_0 and γ_1 , and at height 0 outside γ_0 . Note that for b close to R^2N^2 the contour γ_1 is free to move inside γ_0 , so its location is random (as is also the case in the regime of the unique large contour, when the scaled Wulff shape $\sqrt{b/N^2} W_\beta$ fits into the square $[0, R]^2$). The contour γ_0 , on the other hand, is (nearly) touching all four sides of the boundary of our box, so it is relatively less free to fluctuate.

In the complementary regime, when b is close to $2R^2N^2$, the two contours γ_0 and γ_1 have the same size in the leading order (which is linear in N), while the

Hausdorff distance between them is only $\sim N^{1/2}$; it is created as a result of the entropic repulsion between them. In particular, in the limit as $N \rightarrow \infty$, and under the $\frac{1}{N}$ scaling, the two contours coincide, going in asymptotic shape to the same Wulff plaquette. The study of this case needs the technique, additional to that contained in [DKS], [DS1], [DS2], [SchS] and [ISch], since the case of two repelling large contours was not considered there. The case of the values b above $2R^2N^2$ is even more involved, since there we have to deal with several large mutually repelling contours. We will return to it in a separate publication, see [IS].

8. Main result

We are ready now to describe the monolayers creation in our model: Let us fix $p^s > p^v$ (and hence p^{sv} and D), and let β be sufficiently large. Let us also fix R large enough, so that the rescaled Wulff shape of area

$$\sqrt[3]{\frac{D^2 w_\beta^2(1)}{p^{sv}}} R^{4/3}$$

fits into the $R \times R$ square.

Theorem 8.1. *Let Γ be a typical interface drawn from the conditional distribution $\mathbb{P}(\bullet \mid \Sigma = a_0 N^3 + \delta N^2)$. Define*

$$\delta^1 = \frac{3}{2} \sqrt[3]{D^2 w_\beta^2 p^{sv}} R^{4/3}. \quad (8.1)$$

- *For values of δ satisfying $0 < \delta < \delta^1$, the interface Γ is essentially flat: all contours of Γ have lengths bounded above by $\epsilon^{-1} \log N$.*
- *There exists $\delta^2 > \delta^1$, such that for $\delta^1 < \delta < \delta^2$ the interface Γ has one monolayer. Precisely, Γ contains exactly one large contour γ_0 of approximately Wulff shape (or Wulff plaquette shape), such that*

$$\alpha(\gamma_0) > \frac{2\delta}{3p^{sv}} N^2. \quad (8.2)$$

The rest of contours of Γ are small; their lengths are bounded above by $\epsilon^{-1} \log N$.

- *Similarly, there exists a value δ_R , such that for $\delta^2 < \delta < \delta_R$ the interface Γ has two monolayers, and contains exactly two large contours, γ_0 and $\gamma_1 \subset \text{Int}(\gamma_0)$. The bigger one, γ_0 , has the shape of the Wulff plaquette, while the smaller one has the Wulff shape. Again, $\alpha(\gamma_1) > \frac{2\delta}{3p^{sv}} N^2$.*

9. Proof of the main result

Let us fix δ and consider the surface distribution $\mathbb{P}(\bullet \mid \Sigma = a_0 + \delta N^2)$. Since we can ignore intermediate contours (6.4) and since we already know how the typical surfaces looks like in the constraint ensembles $\widehat{\text{Pr}}(\bullet \mid A_b)$, it would be

enough to study conditional probabilities $\mathbb{P}(A_b | \Sigma = a_0 + \delta N^2)$. Namely, for every δ we need to know the range of the typical values of the “volume” observable b . To do this we will compare the probabilities $\mathbb{P}(A_b, \Sigma = a_0 + \delta N^2) \sim \mathbb{P}(\Sigma = a_0 + \delta N^2 | A_b) \widehat{\text{Pr}}(A_b)$ for various values of b , in order to find the dominant one.

There are three regimes to be worked out: Fix $\eta \in (0, 1/2)$ and c_9 small enough.

Case 1. $b \leq N^{1+\eta}$. By (4.2) and (7.2),

$$\begin{aligned} & c_{10} \exp \left\{ -\frac{\delta^2}{2DR^2} N - O\left(\frac{b^2}{N^2}\right) \right\} \\ & \leq N^{3/2} \mathbb{P}(\Sigma = a_0 + \delta N^2 | A_b) \widehat{\text{Pr}}(A_b) \\ & \leq c_{11} \exp \left\{ -\frac{\delta^2}{2DR^2} N \right\}. \end{aligned} \quad (9.1)$$

Case 2. $N^{1+\eta} < b \leq c_9 N^2$. By (4.2) and (7.2),

$$\mathbb{P}(\Sigma = a_0 + \delta N^2 | A_b) \widehat{\text{Pr}}(A_b) \leq c_{12} \exp \left\{ -\frac{\delta^2}{2DR^2} N + \frac{\delta p^{sv} b}{NR^2 D} - c_8 \frac{b^2}{N^2} \wedge N \right\}. \quad (9.2)$$

Obviously, once c_9 is chosen to be sufficiently small, the right hand side of (9.2) is negligible with respect to the lower bound on left-hand side of (9.1) (computed at $b \ll N^{1+\eta}$).

Case 3. $b = \rho N^2$ with $\rho > c_9$. By (7.6) and, once again, by volume order local limit result (4.2),

$$\begin{aligned} & \exp \left\{ -\frac{(\delta - p^{sv} \rho)^2}{DR^2} N - RN w_\beta^{rst} \left(\frac{\rho}{R^2} \right) - o(N) \right\} \\ & \leq \mathbb{P}(\Sigma = a_0 + \delta N^2 | A_b) \text{Pr}(A_b) \\ & \leq \exp \left\{ -\frac{(\delta - p^{sv} \rho)^2}{2DR^2} N - RN w_\beta^{rst} \left(\frac{\rho}{R^2} \right) + o(N) \right\}. \end{aligned} \quad (9.3)$$

Therefore, in order to figure out the dominant contribution between (9.1) and (9.3), we have to find the global minimum of the function

$$\frac{(\delta - p^{sv} \rho)^2}{2DR^2} + RN w_\beta^{rst} \left(\frac{\rho}{R^2} \right) \quad (9.4)$$

on the interval $\rho \in [0, 2R^2]$. This minimization problem needs just the elementary calculus, see e.g. [BCK]. For small values of ρ our function reduces to $\frac{(\delta - p^{sv} \rho)^2}{2DR^2} + w_\beta(1) \sqrt{\rho}$. After the following change of variables:

$$\lambda = \frac{p^{sv} \rho}{\delta} \quad \text{and} \quad \kappa = \kappa(\delta) = \frac{\delta^{3/2}}{2DR^2 w_\beta(1) \sqrt{p^{sv}}},$$

we have to look for global minimizers of

$$\phi_\kappa(\lambda) \triangleq \kappa(1-\lambda)^2 + \sqrt{\lambda}.$$

Set

$$\kappa_c = \kappa(\delta^1) = \frac{1}{2} \left(\frac{3}{2} \right)^{3/2}. \quad (9.5)$$

One easily sees that

- If $\kappa < \kappa_c$, then the global minimizer is 0.
- If $\kappa = \kappa_c$ then there are exactly two global minimizers; 0 and $\lambda_c = 2/3$.
- If $\kappa > \kappa_c$, then the global minimizer λ_m is the maximal solution of

$$4\kappa\sqrt{\lambda}(1-\lambda),$$

which, in particular, satisfies $\lambda_m > 2/3$.

A similar analysis applies in the vicinity of the singularity of the function $w_\beta^{rst}(\frac{\rho}{R^2})$ at $\frac{\rho}{R^2} \sim 1$. Since the function $w_\beta^{rst}(S)$ is monotone, and has the derivative equal to $+\infty$ at $S = 1$, the point of the global minimum of (9.4), which is a monotone function of δ , never belongs to some neighborhood of the point $\frac{\rho}{R^2} = 1$. Therefore at some $\delta = \delta^2$ it jumps from some value $\rho_- < R^2$ to $\rho_+ > R^2$.

The proof of Theorem 1 is, thereby, completed.

10. Conclusions

In this paper we have described a model of the interface between the vapour and liquid phases, evolving as the total number of particles increases. We have shown that the evolution of the interface goes via the spontaneous formation on it of one monolayer of the size of the system. We believe that the same result can be proven for the 3D Ising model with the same boundary conditions, i.e. periodic in two horizontal directions and \pm in the vertical one. It will be very interesting to establish the phenomenon of the monolayer formation in the 3D Ising model with (+)-boundary conditions, when the monolayer attaches itself to a facet of the Wulff-like (random) crystal. This problem, however, seems to be quite difficult, since one needs to control the rounded part of the crystal. This rounded part is probably behaving as a massless Gaussian random surface (compare with [K]), and this alone indicates enough the complexity of the problem.

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