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Vortices and Magnetization in Kac's Model

H. El Bouanani[1] and M. Rouleux[1]

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We consider a 2-dimensional planar rotator on a large, but finite lattice with a ferromagnetic Kac potential $J_\gamma(i) = \gamma^2 J(\gamma i)$, J with compact support. The system is subject to boundary conditions with vorticity. Using a gradient-flow dynamics, we compute minimizers of the free energy functional at low temperature, i.e. in the regime of phase transition. We have the numerical evidence of a vortex structure for minimizers, which present many common features with those of the Ginzburg-Landau functional. We extend the results to spins valued in S^2 and compare with the celebrated Belavin and Polyakov model.

KEY WORDS: Kac's model, gradient-flow dynamics, vortex, Belavin and Polyakov model

INTRODUCTION

Vector spin model with an internal continuous symmetry group, such classical $O^+(q)$ models (XY or "planar rotator" for $q = 2$, and Heisenberg model for $q = 3$,) play an important rôle in Statistical Physics. In one or two dimensions, and for all inverse temperature β, if the range of the translation invariant interaction is finite, then a theorem of Dobrushin and Shlosman shows there is no breaking of the internal symmetry (that is, Gibbs states are invariant under $O^+(q)$) and furthermore, by a theorem of Bricmont, Fontaine and Landau, uniqueness of the Gibbs state holds (see e.g. Ref. 20, Chap. III).

Despite of this, a particular form for phase transition exists, which can be characterized by the change of behavior in the correlation functions. In the low temperature phase they have power law decay, showing that the system is in a long range order state (exhibiting in particular the so-called "spin waves,") but

[1] Centre de Physique Théorique and Université du Sud Toulon Var CPT, Campus de Luminy, Case 907 13288 Marseille cedex 9, France; e-mail: hicham.el-bouanani@cpt.univ-mrs.fr; rouleux@cpt.univ-mrs.fr.

they decay exponentially fast at high temperatures, breaking the long range order, even though thermodynamic quantities remain smooth across the transition. For the XY system, these transitions were described by Kosterlitz and Thouless in term of topological excitations called vortices: while these vortices are organized into dipoles at low temperature, a disordered state emerges at the transition. But the observation of the spatial distribution of defects shows that it is not uniform; rather, defects tend to cluster at temperatures slightly larger than the transition temperature, and there are still large ordered domains where the spins are almost parallel (see e.g. Refs. 7, 13, 14, and references therein).

Here we consider a Kac version of the classical XY or Heisenberg model on a "large" lattice $\Lambda \subset \mathbf{Z}^2$. It was studied in particular by Buttà and Picco.[7] The hamiltonian (except for the interaction with the boundary) is of the form

$$H_\gamma(\sigma_\Lambda) = -\frac{1}{2} \sum_{i,j\in\Lambda} \gamma^2 J(\gamma(i-j))\langle\sigma_\Lambda(i), \sigma_\Lambda(j)\rangle$$

where γ is a small coupling constant and J denotes a cutoff function. Kac potentials for fixed γ have finite interaction, but as we take an appropriate limit $\gamma \to 0$, they can be considered, to this respect, as long range. Thus, they share some features with the mean field model, though exhibiting better mechanisms of phase transitions, which depend in particular on the dimension, as for the short range case. For the mean field model with $O^+(q)$ symmetry, $q = 2, 3$, we know that there is no phase transition for inverse temperature $\beta \leq q$ (Gibbs measure is supported at the absolute minimum of the free energy functional,) while there is a phase transition for $\beta > q$, with internal symmetry group $O^+(q)$.

When the model possesses internal symmetry and common features with the mean field, it is hard to expect vortices at low temperature, unless the symmetry is somehow broken, for instance if the system is subject to boundary conditions. This situation is met in other domains of Condensed Matter Physics, as in supraconductivity, where vorticity is created by an exterior magnetic flux, or for superfluids. In that case, phase transitions of matter are well described by critical points of free energy (Ginzburg-Landau) functionals (Refs. 3, 15, etc. . .)

One of the main process consists in averaging the spins σ_Λ over some mesoscopic boxes, so to define the magnetization $m = m_{\Lambda^*}$ on another "coarser" or "mesoscopic" lattice Λ^*. The free energy (or excess free energy) functional $F_{\beta,\gamma}(m)$ at inverse temperature β in case of Kac models with internal symmetry, can be simply derived from a suitable renormalization of H_γ making use of the entropy $I(m)$ for the mean field that corresponds to Van der Waals free energy $f_\beta(m) = -\frac{1}{2}|m|^2 + \frac{1}{\beta}I(m)$ (see Sec. 1).

To understand the significance of $F_{\beta,\gamma}(m_{\Lambda^*})$, one should think also of the formal "stationary phase" argument, as $\Lambda \to \infty$, which suggests that an important rôle in the averaging with respect to Gibbs measure, is played by configurations close to those which produce the local critical points of $F_{\beta,\gamma}$. This occurs in computing correlations functions (see e.g. Ref. 21). These critical points consist in ground states, or metastable states.

They will be determined as the attractors of a certain dynamics, similar to this given by the "heat operator," but known in that context as the gradient-flow dynamics[8,9,18] .... Thus, we expect convergence of this dynamics toward a Gibbsian equilibrium, though this will not be rigorously established here.

Let us present our main results.

In Sec. 1, we describe in detail Kac's hamiltonian on the lattice, and recall briefly the renormalization scheme, that makes of the free energy functional a fairly good approximation for the density of Gibbs measure, i.e. $\mu_{\beta,\gamma,\Lambda} \approx \exp[-\beta\gamma^{-2}\mathcal{F}(m \mid m^c)]$. Here $\mathcal{F}(m \mid m^c)$ denotes the free energy functional subject to boundary conditions m^c on Λ^{*c}.

In Sec. 2, we present a simple, combinatorial averaging process, relating Kac's hamiltonian with the free energy functional. While exhibiting the main idea of renormalization, it is more suitable for effective computations on the lattice.

In Sec. 3, we study Euler-Lagrange equations for the free energy functional, and introduce the corresponding gradient-flow dynamics $m(x, t)$ (see Eq. (3.4)). Using that $\mathcal{F}(m \mid m^c)$ is a Lyapunov function, we show that $m(x, t)$ converges towards a critical point of $\mathcal{F}(m \mid m^c)$, generically, a local minimum. Unless $\beta \leq 2$, in which case $m = 0$ is the unique minimizer of $\mathcal{F}(m \mid m^c)$, as expected from the considerations above on the mean field, in general there cannot be uniqueness of the limiting orbits, at least for a finite lattice. Instead, local minimizers might depend on initial conditions $m(0, x)$ inside Λ^*.

Local minimizers however, have the property that their modulus be bounded by m_β, if this is true of the initial condition, and as expected from general results relative to the Gibbs states,[(7)] $|m|$ has to be close to m_β on large regions of Λ^*. Actually Proposition 3.4 indicates that if no vorticity is induced by the boundary, nor by the initial condition, then all magnetizations of the limiting configuration should point out in the same direction and have length about m_β.

In Sec. 4 we make numerical simulations, introducing a boundary condition with topological degree $d \in \mathbf{Z}$. Then, on the basis on conservation of vorticity, the limiting orbits for the gradient-flow dynamics show a vortex pattern. For $q = 2$, our main observation is the existence of vortices below the temperature of transition of phase for the mean field model, induced by the vorticity at the boundary of the lattice Λ, together with large ordered domains where the magnetizations m_{Λ^*} become parallel. We discuss in detail dependence on the shape of the lattice, and on initial conditions. In particular, the application of the "simulated annealing process" allows the limiting configurations to move away from local minima, and reach lower energies.

We also have some numerical evidence that, as in the case of Ginzburg-Landau functional, Kirchhoff-Onsager hamiltonian for the system of vortices gives a fairly good approximation of the minimizing free energy, despite of the non-local interactions.

Finally, for $q = 3$, we examine in Sec. 5 the situation of spin-waves in the spirit of Belavin and Polyakov.

1. MEAN FIELD APPROXIMATION AND RENORMALIZED KAC'S HAMILTONIAN

Consider the lattice $\mathbf{Z}^2$, consisting in a bounded, connected domain Λ (the interior region), and its complement (the exterior region) Λ^c. In practice, we think of Λ as a large rectangle with sides parallel to the axis of $\mathbf{Z}^2$, of length of the form $L = 2^n$, $n \in \mathbf{N}$. Physical objects make sense in the thermodynamical limit $\Lambda \to \mathbf{Z}^2$, but in this paper we work in large, but finite domains.

To each site $i \in \mathbf{Z}^2$ is attached a classical spin variable $\sigma_i \in \mathbf{S}^{q-1}$, $q = 2, 3$. The configuration space $\mathcal{X}(\mathbf{Z}^2) = (\mathbf{S}^{q-1})^{\mathbf{Z}^2}$ is the set of all such classical states of spin; it has the natural internal symmetry group $O^+(q)$ acting on $\mathbf{S}^{q-1}$. The state $\sigma \in \mathcal{X}(\mathbf{Z}^2)$ will denote the map $\sigma\colon \mathbf{Z}^2 \to \mathbf{S}^{q-1}$, $i \mapsto \sigma(i)$. Given the partition $\mathbf{Z}^2 = \Lambda \cup \Lambda^c$, we define by restriction the interior and exterior configuration spaces $\mathcal{X}(\Lambda)$ and $\mathcal{X}(\Lambda^c)$, and the restricted configurations by σ_Λ and σ_{Λ^c}. The Hamiltonian in $\mathbf{Z}^2$ describes the interaction between different sites through Kac's potential defined as follows.

Let $0 \le J \le 1$ be a function on $\mathbf{R}^2$ with compact support and normalized by $\int_{\mathbf{R}^2} J = 1$. We can think of J also as a function on the lattice. There is a lot of freedom concerning the choice of J, but for numerical purposes, we take J as 1/2 the indicator function $\widetilde{J}$ of the unit rhombus with center at the origin, in other words $J(x) = J(|x|_1)$ where $|\cdot|_1$ is the ℓ^1 norm in $\mathbf{R}^2$. Thus the support of $\widetilde{J}$ is thought of as a chip of area 2, and considered as a function on the lattice, $\widetilde{J}$ takes the value 1 at the center, and 1/4 at each vertex, so that $\sum_{i\in\Lambda} J(i) = 1$. For γ of the form 2^{-m}, we set $J_\gamma(x) = \gamma^2 J(\gamma x)$, and extend the definition above in the discrete case so that J_γ enjoys good scaling properties, namely the stratum of full dimension (i.e. the set of points interior to the chip) has weight 1, the strata of dimension 1 (the points on the sides on the chip) have weight 1/2, and those of dimension 0 (the vertices of the chip) have weight 1/4. Thus, again $\sum_{i\in\mathbf{Z}^2} J_\gamma(i) = 1$. The discrete convolution on Λ is defined as usual. For instance, $(J_\gamma * \sigma)(i) = \sum_{j\in\mathbf{Z}^2} J_\gamma(i-j)\sigma(j)$ represents, with conventions as above, the mean value of σ over the chip of size γ^{-1} and center i, with a weight that depends on the stratum containing j.

Note that we could replace the lattice $\mathbf{Z}^2$ by the torus $(\mathbf{Z}/L\mathbf{Z})^2$ or the cylinder $(\mathbf{Z}/L\mathbf{Z}) \times \mathbf{Z}$, which amounts to specify periodic boundary conditions in one or both directions. Thermodynamic limit is obtained as $L \to \infty$.

The coupling between spin at site i and spin at site j is given by $J_\gamma(i-j)$; this is known as Kac's potential. From Statistical Physics point of view, Kac's potential, for small γ, shares locally the main properties of the mean field, i.e. long range $\approx \gamma^{-1}$, large connectivity $\approx \gamma^{-2}$ of each site, small coupling constant $\approx \gamma^2$ of the bonds, and total strength of each site equal to 1.

Given the exterior configuration $\sigma_{\Lambda^c} \in \mathcal{X}(\Lambda^c)$, we define the Hamiltonian on $\mathbf{Z}^2$ as

$$H_\gamma(\sigma_\Lambda \mid \sigma_{\Lambda^c}) = -\frac{1}{2} \sum_{i,j \in \Lambda} J_\gamma(i-j)\langle \sigma(i), \sigma(j) \rangle - \sum_{(i,j) \in \Lambda \times \Lambda^c} J_\gamma(i-j)\langle \sigma(i), \sigma(j) \rangle \tag{1.1}$$

where $\sigma(i)$, for simplicity, stands for $\sigma_\Lambda(i)$ or $\sigma_{\Lambda^c}(i)$, and $\langle \cdot, \cdot \rangle$ is the standard scalar product in $\mathbf{R}^q$. We note that as $J \geq 0$, the interaction is ferromagnetic, i.e. energy decreases as spins align.

We give here some heuristic derivation of the model we will consider, starting from principles of Statistical Physics. A thermodynamical system at equilibrium is described by Gibbs measure at inverse temperature β. We assume an a priori probability distribution ν for the states of spin, and because of the internal continuous symmetry of $\mathcal{X}(\Lambda)$, we take ν as the normalized surface measure on $\mathbf{S}^{q-1}$, i.e. $\nu(d\sigma_i) = \omega_q^{-1} \delta(|\sigma_i| - 1) d\sigma_i$, where ω_q is the volume of $\mathbf{S}^{q-1}$. Then Gibbs measure on $\mathcal{X}(\Lambda)$ with prescribed boundary condition σ_{Λ^c} is given by

$$\mu_{\beta,\gamma}(d\sigma_\Lambda \mid \sigma_{\Lambda^c}) = \frac{1}{Z^\Lambda_{\beta,\gamma}(\sigma_{\Lambda^c})} \exp[-\beta H_\gamma(\sigma_\Lambda \mid \sigma_{\Lambda^c})] \prod_{i \in \Lambda} \nu(d\sigma_\Lambda(i)) \tag{1.2}$$

where $Z^\Lambda_{\beta,\gamma}(\sigma_{\Lambda^c})$, the partition function, is a normalization factor which makes of $\mu_{\beta,\gamma}$ a probability measure on $\mathcal{X}(\Lambda)$, conditioned by $\sigma_{\Lambda^c} \in \mathcal{X}(\Lambda^c)$. It is obtained by integration of $\mu_{\beta,\gamma}(d\sigma_\Lambda \mid \sigma_{\Lambda^c})$ over $\Omega_0 = (\mathbf{S}^{q-1})^\Lambda$.

Since we are working on $\mathbf{Z}^2$, there exists, for any $\beta > 0, \gamma > 0$, an infinite volume Gibbs state $\mu_{\beta,\gamma}$, i.e. a (unique) probability distribution $\mu_{\beta,\gamma}$ on the space $\mathcal{X}$ of all configurations obtained by taking the thermodynamic limit $\Lambda \to \mathbf{Z}^2$. This measure satisfies suitable coherence conditions, i.e. DLR equations.

Nevertheless, we are faced with various difficulties, indicating that $\mu_{\beta,\gamma}(d\sigma_\Lambda \mid \sigma_{\Lambda^c})$ should not be the object to be directly considered. It is known that (and this goes back to Van Hove for the Ising ferromagnet, i.e. $q = 1$, see [see Ref. 20, p. 31,]) in order to understand thermodynamical properties for spins models, one should instead average spins over mesoscopic regions and consider the image of Gibbs measure through this transformation, the so called "block-spin transformation." So we introduce the empirical magnetization in the finite box $\Delta \subset \mathbf{Z}^2$

$$m_\Delta(\sigma) = \frac{1}{|\Delta|} \sum_{i \in \Delta} \sigma(i) \tag{1.3}$$

and given any $m \in \mathbf{R}^q$, $|m| \leq 1$, we define the canonical partition function in Δ as

$$Z_{\beta,\gamma}^{\Delta,\sigma_{\Delta^c}}(m) = \int_{(\mathbf{S}^{q-1})^\Delta} \exp[-\beta H_\gamma(\sigma_\Delta|\sigma_{\Delta^c})] \prod_{i\in\Delta} \nu(d\sigma(i))\delta(m_\Delta(\sigma) - m) \quad (1.4)$$

see [see Ref. 20, p. 31]. Also for Kac's model, it can be shown, taking the thermodynamical limit $\Delta \to \mathbf{Z}^2$, that the quantity

$$F_\gamma(\beta, m) = -\lim_{\Delta\to\mathbf{Z}^2} \frac{1}{\beta|\Delta|} \log Z_{\beta,\gamma}^{\Delta,\sigma_{\Delta^c}}(m) \quad (1.5)$$

is well defined, and doesn't depend on the boundary condition on Δ^c; it will be interpreted as the thermodynamic free energy density of the system. It is defined for a system with finite interaction of range γ^{-1}, i.e. before taking the mean field limit $\gamma \to 0$.

So far, parameter γ was kept small but constant; the limit $\gamma \to 0$ is called Lebowitz-Penrose limit. Let

$$f_\beta(m) = -\frac{1}{2}|m|^2 + \frac{1}{\beta} I(m) \quad (1.6)$$

be the free energy for the mean field, $I(m)$ denotes the entropy, see (2.2) below.

Lebowitz-Penrose theorem (in this simplified context) states that

$$\lim_{\gamma\to 0} F_\gamma(\beta, m) = \mathrm{CE}(f_\beta(m)) \quad (1.7)$$

See Ref. 7 for the case of a 1-d lattice and continuous symmetry, the proof can be carried over to $\mathbf{Z}^2$. Here CE denotes the convex envelope, to account for Maxwell correction law.

From this we sketch the renormalization procedure that leads to Lebowitz-Penrose theorem, as stated e.g. in Ref. 18, Theorem 3.2.1 for $q = 1$, following earlier results by Ref. 2 (actually, this is the "pressure" version of Lebowitz-Penrose theorem, but the argument can easily be adapted to free energy.) The following result will not be used in the sequel, we just give it for completeness.

Since we will take (in this paragraph) a continuous limit, we do assume that J is a differentiable function, not necessarily of compact support, but with $\|\nabla J\|_1 < \infty$ (the L^1 norm.) The lattice dimension d can be arbitrary. We set, following (1.3), $\Delta = \tilde{\Lambda}(x)$ and $m_\sigma(x) = m_{\tilde{\Lambda}(x)}(\sigma)$. Here $\tilde{\Lambda}(x)$ will be a square "centered" at a variable $x \in \mathbf{Z}^2$, with sides of length $\frac{\delta}{\gamma}$, δ of the form 2^{-p}, $p \in \mathbf{N}$, $\frac{\delta}{\gamma}$ much smaller than the diameter of Λ, but still containing many sites, for instance diam $(\tilde{\Lambda}(x)) = \gamma^{-1/2}$. Actually, we need to replace (1.3) by an integral, which allows to extend $x \mapsto m_\sigma(x)$ on $\mathbf{R}^d$, but for simplicity, we present it as a discrete sum.

The averages $m_\sigma(x)$ are called (empirical) magnetizations. The set of all such magnetizations $m_\sigma \in \mathbf{R}^q$ is the image of $\mathcal{X}(\mathbf{Z}^2)$ by the block-spin transformation $\pi_\gamma : \sigma \to m_\sigma$, and will be denoted by $\tilde{\mathcal{X}}(\mathbf{Z}^2)$. This is the set of "coarsed-grained" configurations.

It has again the continuous symmetry group $O^+(q)$, and this is a subset of the convex set $\mathcal{M}$ of all functions $m : \mathbf{Z}^2 \to \mathbf{R}^q$ such that $|m(x)| \leq 1$ for all x. When considering microscopic interior and exterior regions as above, the partition $\mathbf{Z}^2 = \Lambda \cup \Lambda^c$ induces of course restricted configuration spaces $\tilde{\mathcal{X}}(\Lambda^*)$ and $\tilde{\mathcal{X}}(\Lambda^{*c})$, where $\Lambda^* = \{x \in \mathbf{Z}^2 : \tilde{\Lambda}(x) \subset \Lambda\}$ and $\Lambda^{*c} = \{x \in \mathbf{Z}^2 : \tilde{\Lambda}(x) \subset \Lambda^c\}$. So let $m \in \mathcal{M}$.

We introduce as in (1.4) the canonical Gibbs measure conditioned by the external configuration $\sigma_{\Lambda^c} = \sigma^c$:

$$\mu_{\beta,\gamma,\Lambda}(d\sigma; m \mid \sigma^c) = \frac{1}{Z_{\beta,\gamma,\Lambda}(\sigma^c)} \int_{\Omega_0} \prod_{i\in\Lambda} \nu(d\sigma(i)) \exp[-\beta H_\gamma(\sigma(i)|\sigma^c)]\delta(\pi_\gamma\sigma(i) - m) \tag{1.8}$$

where the partition function $Z_{\beta,\gamma,\tilde{\Lambda}}(\sigma_{\tilde{\Lambda}^c})$ was defined in (1.2). For simplicity, we have removed the index Λ from σ. By definition of the image of Gibbs measure through the block-spin transformation, we have

$$\int_{|m|<1} dm \mu_{\beta,\gamma,\Lambda}\big(d\sigma; m \mid \sigma_\gamma^c\big) = 1 \tag{1.9}$$

where dm is the normalized Lebesgue measure on the product space $\prod_{x\in\Lambda^*} B_q(0, 1)$. ($B_q(0, 1)$ denotes the unit ball of $\mathbf{R}^q$.) Let

$$\begin{aligned}\mathcal{F}(m \mid m^c) = &\frac{1}{4} \int_{\Lambda_0} dr \int_{\Lambda_0} dr' J(r - r')|m(r) - m(r')|^2 \\ &+ \frac{1}{2} \int_{\Lambda_0} dr \int_{\Lambda_0^c} dr' J(r - r')|m(r) - m(r')|^2 \\ &+ \int_{\Lambda_0} dr(f_\beta(m(r)) - f_\beta(m_\beta))\end{aligned} \tag{1.10}$$

be the continuous, free energy in a box $\Lambda_0 \subset \mathbf{R}^2$ of fixed size L_0, rescaled from Λ by a factor proportional to γ. Here m_β is the critical value for the mean field f_β, see Sec. 2. Assume, as before, that the diameter of all block spins $\tilde{\Lambda}(x)$ equals $\gamma^{-1/2}$. Then we can give a special meaning to the approximation $\mu_{\beta,\gamma,\Lambda} \approx \exp[-\beta\gamma^{-d}\mathcal{F}(m \mid m^c)]$ (in the logarithmic sense) stated in the Introduction, by establishing the analogue of Ref. 2, Lemma 3.2 in case of continuous symmetry, improving also Ref. 7, Lemma 3.1. Let $\hat{e}$ be any (fixed) unit vector in $\mathbf{R}^q$, and $\widehat{m}_\beta$ the constant function on Λ equal to $m_\beta\widehat{e}$, which we extend to be equal to m^c on Λ^c. We have the following:

Proposition 1.1. *Let $q = 2$. With the notations above, there are constants $C_1, C_2 > 0$ such that for any coarse-grained configuration m on Λ^*:*

$$\begin{aligned}-g(m) - (L_0\gamma^{-1})^d(C_2\beta\sqrt{\gamma}\|\nabla J\|_1 + C_1\gamma^{d/2}\log\gamma^{-1})\\ \leq \log[\mu_{\beta,\gamma,\Lambda}(d\sigma; m \mid \sigma^c)] + \beta\gamma^{-d}\mathcal{F}(m \mid m^c)\\ \leq g(m) + \beta\gamma^{-d}\inf_{\widehat{e}\in\mathbf{S}^1}\mathcal{F}(\widehat{m}_\beta|m^c)\\ + (L_0\gamma^{-1})^d(C_2\beta\sqrt{\gamma}\|\nabla J\|_1 + C_1\gamma^{d/2}\log\gamma^{-1})\end{aligned}$$

where $g(m) = \log\prod_{x\in\Lambda^*}(1 - |m(x)|)^{-1/2}$.

See Ref. 10 for details. The divergence of $g(m)$ as $|m|$ gets close to 1 reflects the fact that the entropy density $I(m)$ is singular at $|m| = 1$, precisely where the mean field approximation breaks down, see also Ref. 7, Theorem 2.2. So the approximation $\mu_{\beta,\gamma,\Lambda} \approx \exp[-\beta\gamma^{-d}\mathcal{F}(m \mid m^c)]$ holds true when the magnetization stays bounded away from 1, as is the case in most applications.

Having this construction in mind, we shall proceed the other way around, and make a simple renormalization of H_γ (see Proposition 2.1 below). Actually our sole purpose is to give a discrete analogue for the excess free energy functional as in (1.10), most adapted to numerical experiments on the lattice.

2. RENORMALIZED HAMILTONIAN ON THE LATTICE

We restrict here to $q = 2$, in Sec. 5 we show how these considerations easily extend to $q = 3$. Recall from (1.6) the free energy for the mean field, $I(m)$ is the entropy function of the a priori measure ν, which can be computed following.[7] Namely, introduce the moment generating function

$$\phi(h) = \int_{S^{q-1}} e^{\langle h,\sigma\rangle}d\nu(\sigma) \tag{2.1}$$

and define $I(m)$ as Legendre transformation

$$I(m) = \hat{I}(|m|) = \sup_{h\in\mathbf{R}^q}(\langle h, m\rangle - \log\phi(h)) \tag{2.2}$$

We denote by I_n the modified Bessel function of order n. For $q = 2$, we have $\phi(h) = \hat{\phi}(|h|) = I_0(|h|)$. Function $\rho \mapsto \hat{I}(\rho)$ is convex, strictly increasing on [0, 1], $\hat{I}(\rho) \sim \rho^2$ as $\rho \to 0$, $\hat{I}(\rho) \sim -\frac{1}{2}\log(1 - \rho)$, as $\rho \to 1$, and these relations can be differentiated. We have also $\hat{I}' = ((\log\hat{\phi})')^{-1}$ and $(\log\hat{\phi})'(t) = I_1(t)/I_0(t)$, this is of course a real valued function. The phase transition of mean field type is given by the critical point of the free energy f_β, i.e. the positive root of equation $\beta m_\beta = \hat{I}'(m_\beta)$, which exists iff $\beta > \hat{I}''(0) = 2$. So the critical manifold has again $O^+(2)$ invariance.

Now we specify the choice of mesoscopic boxes $\tilde{\Lambda}(x)$ and construct the excess free energy functional by the procedure sketched above. When $q = 2$, it is convenient to use the underlying complex structure of $\mathcal{X}(\mathbf{Z}^2)$, so we shall write (1.1), with obvious notations, as

$$H_\gamma(\sigma_\Lambda \mid \sigma_{\Lambda^c}) = -\frac{1}{2} \sum_{i,j\in\Lambda} J_\gamma(i-j)\sigma(i)\overline{\sigma(j)} - \mathrm{Re} \sum_{(i,j)\in\Lambda\times\Lambda^c} J_\gamma(i-j)\sigma(i)\overline{\sigma(j)} \tag{2.3}$$

We introduce in detail the mesoscopic ensemble averages, or coarse graining approximation to renormalize H_γ. Let $\delta > 0$ be small, but still much larger than γ, we take again $\delta = 2^{-m}$, for some $m \in \mathbf{N}$. We take for $\tilde{\Lambda}(x)$, $x \in \mathbf{Z}^2$, a square "centered" at x, of diameter $\frac{\delta}{\gamma}$, and of the form $\tilde{\Lambda}_\delta(x) = \{i = (i_1, i_2) \in \mathbf{Z}^2 : i_k \in \frac{\delta}{\gamma}[x_k, x_k + 1[\}$ where we define as in (1.2), $m_\delta(x) = (\frac{\gamma}{\delta})^2 \sum_{i\in\tilde{\Lambda}(x)} \sigma(i)$. Thus we magnify by a factor δ/γ the "coarse graining" (or mesoscopic ensemble) labelled by $x \in \mathbf{Z}^2$, to the "smooth graining" (or microscopic ensemble) labelled by $i \in \mathbf{Z}^2$. We have:

Proposition 2.1. *There is* $0 < \alpha < \frac{1}{4}$ *such that*

$$\left(\frac{\gamma}{\delta}\right)^2 H_\gamma(\sigma_\Lambda \mid \sigma_{\Lambda^c}) + U_{\mathrm{ext}}(m_\delta) + U_{\mathrm{int}}(m_\delta) - |\Lambda| f_\beta(m_\beta) = \mathcal{F}\big(m_\delta \,\big|\, m_\delta^c\big) + |\Lambda| \mathcal{O}(\delta^{2\alpha}) \tag{2.4}$$

where

$$\begin{aligned}
\mathcal{F}\big(m_\delta \,\big|\, m_\delta^c\big) &= \frac{1}{4} \sum_{x,y\in\Lambda^*} J_\delta(x-y)|m_\delta(x) - m_\delta(y)|^2 \\
&\quad + \frac{1}{2} \sum_{(x,y)\in\Lambda^*\times\Lambda^{*c}} J_\delta(x-y)|m_\delta(x) - m_\delta(y)|^2 + \sum_{x\in\Lambda^*} f_\beta(m_\delta(x)) - f_\beta(m_\beta) \\
U_{\mathrm{ext}}(m_\delta) &= \frac{1}{2} \sum_{(x,y)\in\Lambda^*\times\Lambda^{*c}} J_\delta(x-y)|m_\delta(y)|^2 \\
U_{\mathrm{int}}(m_\delta) &= \frac{1}{\beta} \sum_{x\in\Lambda^*} I(m_\delta(x))
\end{aligned} \tag{2.5}$$

Proof: To start with, consider the first term in (1.1)

$$\begin{aligned}
\left(\frac{\gamma}{\delta}\right)^2 \sum_{i,j\in\Lambda} J_\gamma(i-j)\sigma(i)\overline{\sigma(j)} &= \sum_{x,y\in\Lambda^*} J_\delta(x-y) m_\delta(x)\overline{m_\delta(y)} \\
&\quad + \gamma^2 \sum_{x,y\in\Lambda^*} \sum_{(i,j)\in\tilde{\Lambda}_\delta(x)\times\tilde{\Lambda}_\delta(y)} (J(\gamma(i-j)) - J(\delta(x-y)))\sigma(i)\overline{\sigma(j)}
\end{aligned} \tag{2.6}$$

and denote by $R(\Lambda^*)$ the second sum in the RHS of (2.6). Let $C_0 = B_1(0, \frac{1}{\delta})$ be the rhombus (or ℓ^1-ball in $\mathbf{R}^2$) of center 0 and radius $\frac{1}{\delta}$, corresponding to the shape of the interaction J, and for $x' \in \mathbf{Z}^2$, its translate $C_{x'} = \frac{1}{\delta}x' + C_0$, we denote also by $C^*_{x'} \subset \Lambda^*$ the corresponding lattice obtained from $C_{x'}$ by deleting 2 of its sides, so that $\Lambda^* = \bigcup_{x'\in\mathbf{Z}^2} C^*_{x'}$ (disjoint union), and Λ^* is covered by those $C^*_{x'}$ with $x' = (x'_1, x'_2), x'_j \in \{\pm 1, \dots, \pm\gamma L\}$. Let also $E(x, y) = \{(i, j) \in \tilde\Lambda_\delta(x) \times \tilde\Lambda_\delta(y) : J(\gamma(i - j)) - J(\delta(x - y)) \neq 0\}$. We can consider $E(x, y)$ as a symmetric relation $E : \Lambda^* \to \Lambda^*$, $E(x) = \{y \in \Lambda^* : E(x, y) \neq \emptyset\}$. By translation invariance of J, for any $x' \in \mathbf{Z}^2$, we have $|E(x, y)| = |E(x - \frac{1}{\delta}x', y - \frac{1}{\delta}x')|$, so that

$$\sum_{x,y\in\Lambda^*} |E(x, y)| \leq 4\left(\frac{\gamma L}{\delta}\right)^2 \sum_{x,y\in C^*_0} |E(x, y)| \tag{2.7}$$

With the choice of ℓ^1 norm, we have $E(x, y) \neq \emptyset$ for all $x, y \in C^*_0$, and $\max_{x\in C^*_0} |E(x)| = (1 + \frac{1}{2\delta})^2$, while $\min_{x\in C^*_0} |E(x)|$ is of order unity. In any case, $|E(x)|$ depends on x and δ, but not on γ, and it is easy to see that for some $0 < \alpha < \frac{1}{4}$, $\sum_{x\in C^*_0} |E(x)| = \mathcal{O}(\delta^{-2(1-\alpha)})$, $\delta \to 0$. [Actually, this kind of estimate is well-known, see e.g. Ref. 6 and references therein for related results, and applies whenever the support of J is a convex set.]

On the other hand, we have the rough estimate $|E(x, y)| \leq |\tilde\Lambda_\delta(x) \times \tilde\Lambda_\delta(y)| = (\frac{\delta}{\gamma})^4$, and since $|\sigma(i)| = 1$,

$$\left| \sum_{x,y\in C^*_0} \sum_{(i,j)\in\tilde\Lambda_\delta(x)\times\tilde\Lambda_\delta(y)} (J(\gamma(i - j)) - J(\delta(x - y)))\sigma(i)\overline{\sigma(j)} \right|$$

$$\leq \left(\frac{\delta}{\gamma}\right)^4 \sum_{x\in C^*_0} |E(x)| = \left(\frac{\delta}{\gamma}\right)^4 \mathcal{O}\big(\delta^{-2(1-\alpha)}\big)$$

This, together with (2.7), shows that $R(\Lambda^*) \leq \text{Const.}\, \delta^{2\alpha} L^2$. A similar argument gives an estimate on the remainder $R(\Lambda^* \mid \Lambda^{*c})$ for the second term in (1.1). Once we have replaced $(\frac{\gamma}{\delta})^2 \sum_{i,j} J_\gamma(i - j)\sigma(i)\overline{\sigma(j)}$ by $\sum_{x,y} J_\delta(x - y)m_\delta(x)\overline{m_\delta(y)}$ modulo $R(\Lambda^*)$ and $R(\Lambda^* \mid \Lambda^{*c})$, which verify the estimate given in (2.4), we use the identity

$$-2\,\mathrm{Re}\, m_\delta(x)\overline{m_\delta(y)} = |m_\delta(x) - m_\delta(y)|^2 - |m_\delta(x)|^2 - |m_\delta(y)|^2$$

and express the "density" term $\frac{1}{2}|m|^2$ in term of the mean field free energy $f_\beta(m)$ as in (2.1). Summing over (x, y) and making use of the fact that J_δ is normalized in $\ell^1(\mathbf{Z}^2)$ eventually gives the Proposition. □

Remark. (1) In homogenization problems, one usually associates the discrete configuration $\sigma \in \mathcal{X}(\Lambda)$ with the function σ_γ on $\mathbf{R}^2$ taking the constant value

$\sigma(i)$ on the square "centered" at γi, $i = (i_1, i_2)$, i.e. on $[\gamma i_1, \gamma(i_1+1)[\times[\gamma i_2, \gamma(i_2+1)[$. Furthermore the size of the domain Λ is normalized, so that taking the thermodynamic limit $\Lambda \to \infty$ is a problem of convergence for piecewise constant functions (or discrete measures) in some suitable functional space. As we have seen in Sec. 1, it is convenient to take a smooth interaction J. Thus a version of Proposition 2.1 was obtained in Ref. 7 by replacing the discrete average $m_\delta(x)$ around $x \in \Lambda$ by an integral, or in Refs. 8, 9, 18, ... by averaging J_γ over boxes of type $C_{x'}$ as above. (For short we refer henceforth to the review article Ref. 18). Since our ultimate purpose here consists in numerical simulations on a lattice, we chose instead to give a discrete renormalization for H_γ.

(2) Our renormalized Hamiltonian is now given by $\mathcal{F}(m_\delta \mid m_\delta^c)$, the quantities we have subtracted are $-U_{\mathrm{ext}}(m_\delta)$, attached to the configuration space $\mathcal{X}(\Lambda^c)$, and $-U_{\mathrm{int}}(m_\delta)$ that can be interpreted as β^{-1} times the entropy of the system in Λ. Note we have also included self-energy terms $i = j$ in the original Hamiltonian. Of course, relevance of this free energy to Gibbs measure (or rather its image through the block-spin transformation) after taking the thermodynamic limit, is a rather subtle question which will not be discussed here, since we content to finite lattices.

3. EULER-LAGRANGE EQUATIONS AND NON LOCAL DYNAMICS

We are interested in the critical points of $\mathcal{F}(m_\delta \mid m_\delta^c)$. Denote as usual resp. by ∂_m and $\overline{\partial}_m$ the holomorphic and anti-holomorphic derivatives, we have for $m = m_\delta$ (for short), and any tangent vector of type (1,0) in the holomorphic sense, $\delta m \in T_m^{(1,0)}\tilde{\mathcal{X}}(\mathbf{Z}^2)$:

$$\begin{aligned}\langle \partial_m \mathcal{F}(m \mid m^c), \delta m\rangle = \frac{1}{2} &\sum_{(x,y)\in\Lambda^*\times\Lambda^{*c}} J_\delta(x-y)(\bar{m}(x) - \bar{m}(y))\delta m(x)\\ &+ \frac{1}{2}\sum_{x,y\in\Lambda^*} J_\delta(x-y)(\bar{m}(x)-\bar{m}(y))\delta m(x)\\ &+ \sum_{x\in\Lambda^*}\left(-\frac{1}{2}\bar{m}(x) + \frac{1}{\beta}\frac{\partial I(m)}{\partial m}(x)\right)\delta m(x)\end{aligned}$$

Using again the normalization of J_δ in $\ell^1(\mathbf{Z}^2)$, the relation $I(m) = \hat{I}(|m|)$, and setting as before $J_\delta * m(x) = \sum_{y\in\mathbf{Z}^2} J_\delta(x-y)m(y)$, we obtain

$$\langle \partial_m \mathcal{F}(m \mid m^c), \delta m\rangle = \frac{1}{2}\sum_{x\in\Lambda^*}\left(-J_\delta * \overline{m}(x) + \frac{1}{\beta}\frac{\hat{I}'(|m|)}{|m|}\overline{m}(x)\right)\delta m(x) \quad (3.1)$$

Since $\mathcal{F}$ is real, this gives Euler-Lagrange equation:

$$-J_\delta * m(x) + \frac{1}{\beta}\frac{\hat{I}'(|m|)}{|m|}m(x) = 0 \tag{3.2}$$

Let $f = (\hat{I}')^{-1} = \frac{\hat{\phi}'}{\hat{\phi}}$ denote the inverse of the function $\hat{I}'$. Thus $f : [0, +\infty[\to [0, 1[$ is strictly concave, $f(0) = 0$, $f'(0) = 1/2$, and $f(\rho) \to 1$ as $\rho \to +\infty$. Since the inverse of $m \mapsto \hat{I}'(|m|)\frac{m}{|m|}$ defined on the unit disk is given by $n \mapsto f(|n|)\frac{n}{|n|}$, $n \in \mathbf{C}$, (3.2) takes the form

$$-m + f(\beta|J_\delta * m|)\frac{J_\delta * m}{|J_\delta * m|} = 0 \tag{3.3}$$

Following, Ref. 18 to find the critical points minimizing the excess free energy functional $\mathcal{F}$ we solve the "heat equation"

$$\frac{dm}{dt} = -m + f(\beta|J_\delta * m|)\frac{J_\delta * m}{|J_\delta * m|} \text{ in } \Lambda^* \tag{3.4}$$

with prescribed (time independent) boundary condition on Λ^{*c}, and initial condition $m_{|\Lambda^*} = m_0$. By Cauchy-Lipschitz theorem, Eq. (3.4) has a unique solution, defined for all $t > 0$, valued in $\tilde{\mathcal{X}}(\Lambda^*)$. Monotonicity of $\mathcal{F}$ is given in the following:

Proposition 3.1. *$\mathcal{F}$ is a Lyapunov function for Eq.* (3.4)*, i.e. there exists a free energy dissipation rate function $\mathcal{I} : \tilde{\mathcal{X}}(\Lambda^*) \to \mathbf{R}^+$, $\mathcal{I}(m) = 0$ iff m solves* (3.3)*, and*

$$\frac{d}{dt}\mathcal{F}(m(\cdot, t)|m^c) = -\mathcal{I}(m(\cdot, t))$$

along the integral curves of (3.4).

Proof: We have, using (3.1) and (3.4)

$$\begin{aligned}\mathcal{I}(m(\cdot, t)) &= -\frac{d\mathcal{F}}{dt} = -\left\langle \partial_m \mathcal{F}, \frac{\partial m}{\partial t}\right\rangle - \left\langle \bar{\partial}_m \mathcal{F}, \frac{\partial \bar{m}}{\partial t}\right\rangle \\ &= \frac{1}{\beta}\operatorname{Re}\sum_{x\in\Lambda^*}\left(-\beta J_\delta * \bar{m}(x) + \frac{\hat{I}'(|m|)}{|m|}\bar{m}(x)\right) \\ &\quad \times \left(m(x) - f(\beta|J_\delta * m|)\frac{\beta J_\delta * m}{|\beta J_\delta * m|}(x)\right)\end{aligned} \tag{3.5}$$

Let $m = \rho e^{i\theta}$, $\beta J_\delta * m = \rho' e^{i\theta'}$, $\mathcal{I}(m(\cdot, t))$ equals a sum of terms of the form

$$R = \frac{2}{\beta}(\rho' f(\rho') + \rho \hat{I}'(\rho) - (\rho\rho' + f(\rho')\hat{I}'(\rho))\cos(\theta - \theta'))$$

then using $(\rho - f(\rho'))(\hat{I}'(\rho) - \rho') \geq 0$ for any ρ, ρ' since $\hat{I}'$ is increasing, we obtain the lower bound $R \geq \frac{2}{\beta}(1 - \cos(\theta - \theta'))(\rho\rho' + f(\rho')\hat{I}'(\rho)) \geq 0$. And because $\rho\rho' + f(\rho')\hat{I}'(\rho) = 0$ iff $\rho = 0$ or $\rho' = 0$, this estimate easily implies the Proposition. □

From Proposition 3.1 and a compactness argument as in Ref. 18, follow that in the closure of each orbit of Eq. (3.4) there is a solution of (3.3), or equivalently, of Euler-Lagrange Eq. (3.2), i.e. a critical point for $\mathcal{F}$. As suggested by numerical simulations, this critical point is not unique, and depends on initial conditions (except of course when $\beta \leq 2$.) We expect however some uniqueness in the thermodynamical limit $\Lambda^* \to \infty$, modulo the symmetry group.

Now we give estimates on solutions of (3.4) or (3.3), borrowing some ideas to Ref. 18. Equation (3.4) can be rewritten in the integrated form:

$$m(x,t) = e^{-t}m(x,0) + \int_0^t dt_1 e^{t_1-t} f(\beta|J_\delta * m|)\frac{J_\delta * m}{|J_\delta * m|}(x,t_1) \tag{3.6}$$

An effective construction of the solution is given by the "time-delayed" approximations. It will also be used, discretizing time, in the numerical simulations below. We define inductively $m_h(x,t)$, $h > 0$, on the intervals $[hk, h(k+1)[$, $k \in \mathbf{N}$, by $m_h(x,t) = e^{-t}m_0(x)$ for $0 \leq t < h$, and for $hk \leq t < h(k+1)$, $k \geq 1$:

$$m_h(x,t) = e^{kh-t}m_h(x,kh) + \int_{hk}^t dt_1 e^{t_1-t} f(\beta e^{-h}|J_\delta * m_h|)\frac{J_\delta * m_h}{|J_\delta * m_h|}(x,t_1-h) \tag{3.7}$$

Using Lipschitz properties of the coefficients, it is easy to see that, as $h \to 0$, $m_h(x,t)$ tends to the solution $m(x,t)$ of (3.4) uniformly for $x \in \Lambda^*$ and t in compact sets of $\mathbf{R}_+$. We prove estimates on $m(x,t)$ using sub- and supersolutions of (3.4). We start with:

Lemma 3.2. *Assume $\beta > 2$, and let $\lambda(t)$, $t > 0$ be the solution of*

$$\frac{d\lambda}{dt}(t) + \lambda(t) - f(\beta\lambda(t)) = 0, \quad \lambda(0) = \lambda \in [0,1[\tag{3.8}$$

If $\lambda \geq m_\beta$, then $\lambda(t) \leq \lambda$ for all $t > 0$.

Proof: Write (3.8) in the integrated form as in (3.6) and consider the approximating sequence $\lambda_h(t)$. Since $\lambda_h(t)$ tends to $\lambda(t)$ uniformly on compact sets of $\mathbf{R}_+$, it suffices to show the property stated in the Lemma for λ_h, and $h > 0$ small enough. For $0 \leq t < h$, $\lambda_h(t) = \lambda e^{-t}$, so the property holds, while for $h \leq t < 2h$, performing the integration in (3.7), we get $\lambda_h(t) = e^{-t}\lambda + \int_h^t dt_1 e^{t_1-t} f(\beta e^{-t_1}\lambda)$. Since $x > f(\beta x)$ iff $\beta x < \hat{I}'(x)$ (whence iff $x > m_\beta$), if $\lambda > m_\beta$, and $h > 0$ small enough, then $f(\beta e^{-t_1}\lambda) \leq e^{-t_1}\lambda$, and $\lambda_h(t) \leq \lambda$. By induction, using also that f is increasing, but without changing $h > 0$ anymore, it is easy to see that this property carries over for all $t > 0$. By a continuity argument, this holds true for all $\lambda \geq m_\beta$. □

Then we claim that the modulus of the magnetization doesn't increase beyond m_β. More precisely we have:

Proposition 3.3. *Assume $\beta > 2$, and let $m(x,t)$ be the solution of* (3.4) *such that $m_0(x) = m(x,0)$ satisfies $|m_0(x)| \leq \lambda < 1$, for some $\lambda \geq m_\beta$, and all $x \in \mathbf{Z}^2$ (so including the boundary condition on the exterior region.) Then $|m(x,t)| \leq \lambda$ for all $x \in \mathbf{Z}^2$, and all $t > 0$.*

Proof: Equation (3.6) shows that

$$|m(x,t)| \leq e^{-t}|m_0(x)| + \int_0^t dt_1 e^{t_1 - t} f(\beta|J_\delta * m|)(x,t_1) \tag{3.9}$$

Now by the monotony properties of the convolution and the function f, we have $f(\beta|J_\delta * m|)(x,t_1) \leq f(\beta J_\delta * |m|)(x,t_1)$, so the solution $\lambda(t)$ of (3.8) with $\lambda(0) = \lambda$ is a supersolution for (3.9), and Lemma 3.2 easily implies the Proposition. □

We now look for lower bounds on $m(x,t)$. Since there are in general vortices, one cannot expect a global, positive lower bound on $|m(x,t)|$, unless there is no vorticity on initial and boundary values. On the other hand, we know (at least for a 1-d lattice, see Ref. 7), that the Gibbs measure of the configurations at equilibrium $m_\delta \in \tilde{\mathcal{X}}(\Lambda^* \mid \Lambda^{*c})$ with $|m_\delta(x)|$ arbitrarily close to m_β, has to be large. We have:

Proposition 3.4. *Assume $\beta > 2$, and let $m(x,t)$ be the solution of (3.4) such that $m_0(x) = m(x,0)$ as in Proposition* 3.3 *satisfies* $\mathrm{Re}(\nu m_0(x)) > \mu$*, for some fixed $\nu \in \mathbf{S}^1 \approx \{z \in \mathbf{C}, |z| = 1\}$ and $\mu > 0$ and all $x \in \mathbf{Z}^2$. Assume furthermore that μ satisfies $(\mu^2 + \lambda^2)^{1/2} < \beta f(\beta\lambda)$, where λ is as in Proposition* 3.3. *Then* $\mathrm{Re}(\nu m(x,t)) \geq \mu$ *for all $x \in \Lambda^*$, and all $t > 0$.*

Proof: As in the proof of Proposition 3.3 we make use of a comparison function. So let $\mu(t)$ verify the differential equation

$$\frac{d\mu}{dt}(t) + \mu(t) - \beta f(\beta\lambda)\frac{\mu(t)}{(\mu(t)^2 + \lambda^2)^{1/2}} = 0, \quad \mu(0) > \mu \tag{3.10}$$

Write (3.10) in the integrated form as in (3.6) and consider the approximating sequence $\mu_h(t)$ as in (3.7). We shall show that $\mu_h(t) \geq \mu$ for all $t > 0$ provided $\mu(0) > \mu$ verifies the inequality given in the Proposition. Namely, this holds for $0 \le t < h$, because then $\mu_h(t) = \mu(0)e^{-t} \ge \mu$ for $h > 0$ small enough, while for $h \le t < 2h$, performing the integration as in (3.7), we get $\mu_h(t) = e^{h-t}\mu(0) + \beta f(\beta\lambda) \int_h^t dt_1 e^{t_1 - t} \mu e^{-t_1}((\mu e^{-t_1})^2 + \lambda^2)^{-1/2}$. By hypothesis, $\mu e^{-t_1} \beta f(\beta\lambda)((\mu e^{-t_1})^2 + \lambda^2)^{-1/2} \ge \mu$ for h small enough. So again $\mu_h(t) \ge \mu$. By induction, using that the function $\rho \mapsto \rho(\rho^2 + \lambda^2)^{-1/2}$ is increasing on $\mathbf{R}_+$, it is easy to see that $\mu_h(t) \ge \mu$ holds for all $t > 0$. Because the coefficients of (3.10) are uniformly Lipschitz, $\mu_h(t)$ tends to $\mu(t)$ uniformly on compact sets in $\mathbf{R}_+$, and this property holds again for $\mu(t)$.

Now we turn to the equation for $m(x, t)$. Possibly after rotating the coordinates, we may assume $\nu = 1$, i.e. $\mathrm{Re}\, m_0(x) \ge \mu$ and all $x \in \Lambda^*$ (again, we have included the boundary condition in the initial configuration.) Write $m(x, t) = u(x, t) + iv(x, t)$, u, v real and take real part of (3.4). The integrating form of the resulting equation writes:

$$u(x, t) = e^{-t}u(x, 0) + \int_0^t dt_1 e^{t_1 - t} f(\beta|J_\delta * m|) \frac{\beta J_\delta * u}{\beta|J_\delta * m|}(x, t_1) \qquad (3.11)$$

As $\rho' \mapsto \frac{f(\rho')}{\rho'}$ is decreasing on $\mathbf{R}_+$, and by Proposition 3.2, $|J_\delta * m| \le (|J_\delta * u|^2 + \lambda^2)^{1/2}$, we have

$$\frac{f(\beta|J_\delta * m|)}{\beta|J_\delta * m|} \ge \frac{f(\beta(|J_\delta * u|^2 + \lambda^2)^{1/2})}{\beta(|J_\delta * u|^2 + \lambda^2)^{1/2}} \ge \frac{f(\beta\lambda)}{\beta(|J_\delta * u|^2 + \lambda^2)^{1/2}}$$

the last inequality because f is increasing. Since $u(x, 0) \ge \mu$, by continuity we have $u(x, t) > 0$ at least for small $t > 0$, and (3.11) gives

$$u(x, t) \ge e^{-t}u(x, 0) + \beta f(\beta\lambda) \int_0^t dt_1 e^{t_1 - t} (J_\delta * u)((J_\delta * u)^2 + \lambda^2)^{-1/2}(x, t_1) \qquad (3.12)$$

Now, using the monotony of the convolution, and again the fact that the function $\rho \mapsto \rho(\rho^2 + \lambda^2)^{-1/2}$ is increasing on $\mathbf{R}_+$, we can easily show that the solution $\mu(t)$ of (3.10) with $\mu(0) = \mu$ is actually a subsolution for (3.12), for all $t > 0$; the properties proved already for $\mu(t)$ then imply the Proposition. $\square$

Of course, by continuity, Propositions 3.3 and 3.4 imply the corresponding estimates for the solutions of (3.3), or equivalently for the solutions of Euler-Lagrange Eq. (3.2). Our last result states that if $\beta \le 2$, then $m(x, t)$ tends to 0 $t \to \infty$, which is consistent with the absence of phase transition (or spontaneous magnetization) at high temperature.

Proposition 3.5. *Assume $\beta \le 2$, and let $m(x, t)$ be the solution of* (3.4). *Then $m(x, t) \to 0$ on Λ^* as $t \to +\infty$.*

Proof: Using that $f(\rho') \le \frac{1}{2}\rho'$, all $\rho' > 0$, (3.9) shows that

$$|m(x,t)| \le e^{-t}|m_0(x)| + \frac{\beta}{2}\int_0^t dt_1 e^{t_1-t} J_\delta * |m|(x,t_1)$$

So by taking convolution

$$J_\delta * |m|(x,t_1) \le e^{-t_1} J_\delta * |m_0|(x) + \frac{\beta}{2}\int_0^{t_2} dt_2 e^{t_2-t_1} J_\delta^{*2} * |m|(x,t_2)$$

and integrating the resulting inequality:

$$|m(x,t)| \le e^{-t}\left[|m_0(x)| + \frac{\beta t}{2} J_\delta * |m_0|(x) + \left(\frac{\beta}{2}\right)^2 T^{(2)}\big(e^{(\cdot)} J_\delta^{*2} * |m|(x,\cdot)\big)(t)\right]$$

where $T^{(k)}u(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{k-1}} dt_k u(t_k)$ denotes the k-fold integral of u, and J_δ^{*k} the k-fold convolution product of J_δ with itself. By induction, we get:

$$\begin{aligned}|m(x,t)| \le e^{-t}\bigg[&|m_0(x)| + \frac{\beta}{2} t J_\delta * |m_0|(x) + \cdots + \left(\frac{\beta}{2}\right)^k \frac{t^k}{k!} J_\delta^{*k} * |m_0|(x) \\ &+ T^{(k+1)}\big(e^{(\cdot)} J_\delta^{*(k+1)} * |m|(x,\cdot)\big)(t)\bigg]\end{aligned}$$

The series is uniformly convergent for t in compact sets so we can write

$$|m(x,t)| \le e^{-t} \sum_{k=0}^{+\infty} \left(\frac{\beta}{2}\right)^k \frac{t^k}{k!} J_\delta^{*k} * |m_0|(x)$$

When $\beta < 2$, using $J_\delta^{*k} * |m|(x,0) \le |m_0(x)| \le 1$, it follows that $m(x,t) \to 0$ for all $x \in \Lambda^*$ as $t \to \infty$. This holds again for $\beta = 2$ since we may assume that m_0 has compact support, and we know (see Ref. 11, Lemma 1.3.6) that $J_\delta^{*k} \to 0$ uniformly on $\mathbf{R}^2$ (or on $\mathbf{Z}^2$ in the discrete case), as $k \to \infty$. □

4. VORTICES

We consider here the problem of finding numerically the critical points of Euler-Lagrange Eq. (3.3) by solving (3.4) subject to a boundary condition on Λ^{*c} presenting vorticity.

4.1. Generalities

First we recall some facts about the degree of a map. Let $m : \mathbf{R}^2 \to \mathbf{C}$ be a differentiable function, considered as a vector field on $\mathbf{R}^2$, and subject to the condition $|m(x)| \to \ell > 0$ as $|x| \to \infty$ uniformly in $\hat{x} = x/|x|$. Then the integer

$$\deg_R m = \frac{1}{2\pi} \int_{|x|=R} d(\arg m) = \frac{1}{2i\pi} \int_{|x|=R} \frac{dm}{m} \tag{4.1}$$

is independent of R when $R > 0$ is large enough, is called the (topological) degree of m at infinity, and denoted by $\deg_\infty m$.

We define in the same way the local degree (or topological defect) $\deg_{x_0} m$ of m near x_0, provided $m(x) \neq 0$, $x \neq x_0$, by integrating on a small loop around x_0. The local degree takes values $d_j \in \mathbf{Z}$. When m has finitely many zeros x_j inside the disc of radius R, its total degree (or vorticity) is defined again as the sum of all local degrees near the x_j's. In many boundary value problems (or generalized boundary value problems, in the sense that the boundary is at infinity,) such as Ginzburg-Landau equations, total vorticity is conserved, i.e. $\deg_\infty m = \sum_j \deg_{x_j} m$. Generically $d_j = \pm 1$ ("simple poles.") Our aim is to check this conservation principle in the present situation.

We can define analogously the degree of a discrete map, which makes sense at least in the thermodynamical limit. If $m(x) = \rho(x)e^{i\theta(x)}$, the degree of m at infinity is the degree restricted to the lattice Λ^{*c}, e.g. by

$$d = \deg_{\Lambda^{*c}} m = \frac{1}{2\pi} \sum_j (\theta_{j+1} - \theta_j) \tag{4.2}$$

along some closed loop $\Gamma_\iota \subset \Lambda^{*c}$ encircling Λ^*, the sites along Γ_ι being labelled by j, assuming that this integer takes the same value on each Γ_ι.

The local degree near x_0, where $m(x_0) = 0$, is identified again by computing the angle circulation on a loop encircling x_0. Local degrees are also expected to take, generically, values ± 1.

We chose our parameters as follows. We start with prescribing the degree of the spin variable σ on Λ^c, and take on Γ_ι, the ι:th loop away from Λ, containing N_ι sites, ($N_\iota = 4\iota + P$, where P is the perimeter of Λ, we take enough ι's to cover the range of interaction), with a uniform distribution:

$$\sigma_j = \exp i(2\pi dj/N_\iota + \phi_0), \quad 1 \leq j \leq N_\iota \tag{4.3}$$

here ϕ_0 is a constant (e.g. $\phi_0 = 1$) that "breaks" the symmetry of the rectangle Λ. We shall also randomize these boundary conditions.

To this spin distribution on Λ^c, we apply the block spin transformation (1.3), so to have a distribution of magnetization on Λ^{*c}, then we prescribe initial conditions inside Λ^*. The simplest way is to take zero initial values, which gives a particular symmetry to the solution. Otherwise, we can choose them as random numbers, either small, or with absolute value less than m_β. All these cases will be discussed.

We usually fix the inverse temperature $\beta = 5$, so $m_\beta = 0.72$; the results do not depend on β in an essential way, we just observe that magnetization tends to 0 as $\beta \to 2^+$. The diameter L of the lattice Λ ranges from 2^6 to 2^{10}, the size δ/γ of the diameter of the block-spin $\Delta(x)$ is set to 4 (most of the time) so the diameter L^* of the lattice Λ^* ranges from 2^4 to 2^8. The lattice is either a square, or a rectangle.

The size $1/\delta$ of the length of interaction in Λ^* ranges from 2 to 32, thus the corresponding interaction in Λ has length $1/\gamma = 4/\delta$ between 8 to 128.

Equation (3.4) is solved by "time-delayed" approximations as in (3.7), implemented by the second order trapezoidal method to compute the integrals.

These experiments lead to the following observations, vortices display in a different way, according to the initial configuration on Λ^*, but always obey the conservation of total vorticity.

4.2. Some Typical Configurations

We consider here the case of a uniform distribution of spins on the boundary.

The particular case of zero initial values and a square lattice, gives raise to interesting symmetries (or degeneracies) in the picture: namely, vortices tend to occupy most of Λ^* so to cope with the symmetry of the square. So for $d = 1$ there is a single vortex in the center, for $d = 2$ (cf Fig. 1(a)) a vortex of multiplicity 2, (unless the degeneracy is lifted and turns into 2 nearby vortices,) for $d = 4 - 1$, (cf Fig. 2(a)) one vortex of degree -1 surrounded by 4 vortices of degree $+1$ near the corners, for $d = 4$, 4 vortices of degree $+1$ near the corners, for $d = 4 + 1$, same configuration as for $d = 3$, for $d = 4 + 2$ the picture looks alike, with a double vortex at the center, for $d = 2 \times 4 - 1$, 4 new vortices appear near the center (cf Fig. 3(a)), etc... So the configuration depends essentially of the residue of d modulo 4: new vortices show up from the middle towards the corners along the diagonals of Λ^*.

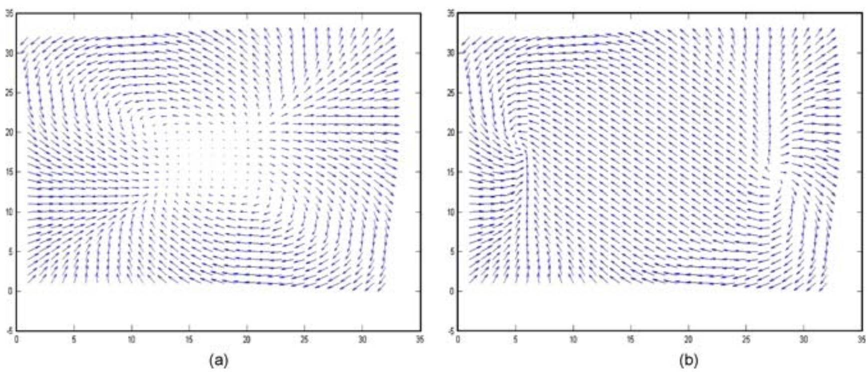

Fig. 1. (a) $L^* = 128$, $d = 2$, zero initial condition. (b) $L^* = 128$, $d = 2$, random initial condition.

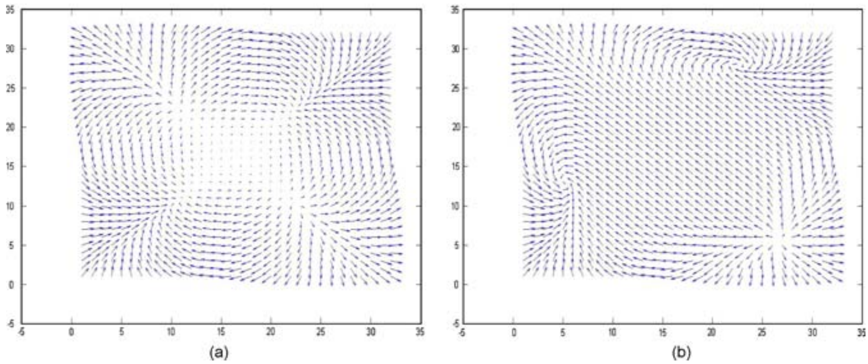

Fig. 2. (a) $L^* = 128$, $d = 3$, zero initial condition. (b) $L^* = 128$, $d = 3$, random initial condition.

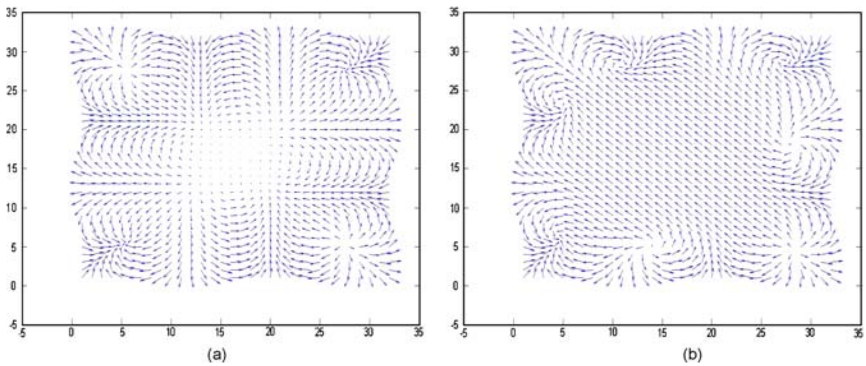

Fig. 3. (a) $L^* = 128$, $d = 7$, zero initial condition. (b) $L^* = 128$, $d = 7$, random initial condition.

Next we consider the case of a square lattice, but with random initial conditions, that is, we pick initial magnetizations with random direction and random length, provided the length is much smaller than m_β, typically $|m_0(x)| \leq 0.05$. Then vortices are simple (i.e. have local degree ± 1, total vorticity is of course conserved,) and tend to display at the periphery of Λ^*, in a pretty regular way, leaving some large ordered domain near the center.

Thus, these configurations maximize the area of the lattice where the magnetizations are aligned , with an absolute value close to m_β, (in accordance with the fact that energy H_γ decreases as the spins align.) Their direction, in general, points out along one of the diagonals of Λ^*. This is illustrated in Fig. 1, 2, 3(b) above, for a vorticity $d = 2, 3, 7$ respectively. In particular, Fig. 2 shows the topological bifurcation from $d = 4 - 1$ to $d = 3$. These simulations also suggest that the equilibrium configurations depend on the initial conditions, but exceptional configurations due to symmetry, for zero initial conditions, are essentially removed as soon as a small disorder is introduced.

Now we vary the shape of the lattice, changing the square into a rectangle, keeping in mind that thermodynamic limit, most of the time, should be taken in the sense of Fisher, i.e. the length of the rectangle Λ^* doesn't exceed a constant times $|\Lambda^*|^{1/2}$. As expected, vortices tend to align along the largest dimension, but again, limiting configurations depend on whether the initial condition inside Λ^* is set to zero or not.

Thus, for zero initial condition, vortices display along the largest median of Λ^*, with possible extra vortices near the corners (inheriting the features of the square lattice.) Namely, they tend to repel each other so the energy cost in clustering is minimized by occupying the corners. Typically, such configurations occur if $d \geq 4$ and the length of Λ^* is only twice its width. But for sufficiently long lattices, or small degree, they just stand the median line. See Fig. 4(a) and 4(c).

For small random initial conditions as above (Fig. 4(b)), we recover the general picture of square lattices, i.e. vortices set along the boarder of Λ^*, leaving a large space in the middle with parallel magnetizations. In any case, degeneracies are lifted, and all vortices have degree $+1$.

4.3. The Simulated Annealing

If we increase the initial conditions, still keeping $|m_0(x)| \leq m_\beta$, we obtain similar pictures, but with a non uniform distribution of defects: conservation of total degree holds, but at the same time, many vortices spread over the lattice, and the corresponding long range order region shrinks correspondingly. This suggest that the gradient-flow dynamics converges only to a local minimum of the free energy.

For reaching lower energies, we let the system explore other regions of the configuration space. This can be achieved through simulated annealing, see e.g. Ref. 12. Replace the dynamics (3.4) by

$$\frac{dm}{dt} = -m + f(\beta(t)|J_\delta * m|)\frac{J_\delta * m}{|J_\delta * m|} \text{ in } \Lambda^* \tag{4.4}$$

where $\beta(t)$ depends continuously on $t \in [0, t_1]$, starting with $\beta_0 < \beta_1 = \beta$, with negative slope at $t = 0$, so that the system is heated initially up to a peak $\beta_2^{-1} \approx 1/2$ (the critical temperature) around $t = t_2$, and then gradually cooled down to β at $t = t_1$. Function $\beta(t)$ is oscillating between successive warm and cool periods, so to "shake" sufficiently the system. Then we keep the temperature constant till we reach equilibrium.

It is not difficult to optimize, empirically, the annealing function $\beta(t)$, and our choice was the following.

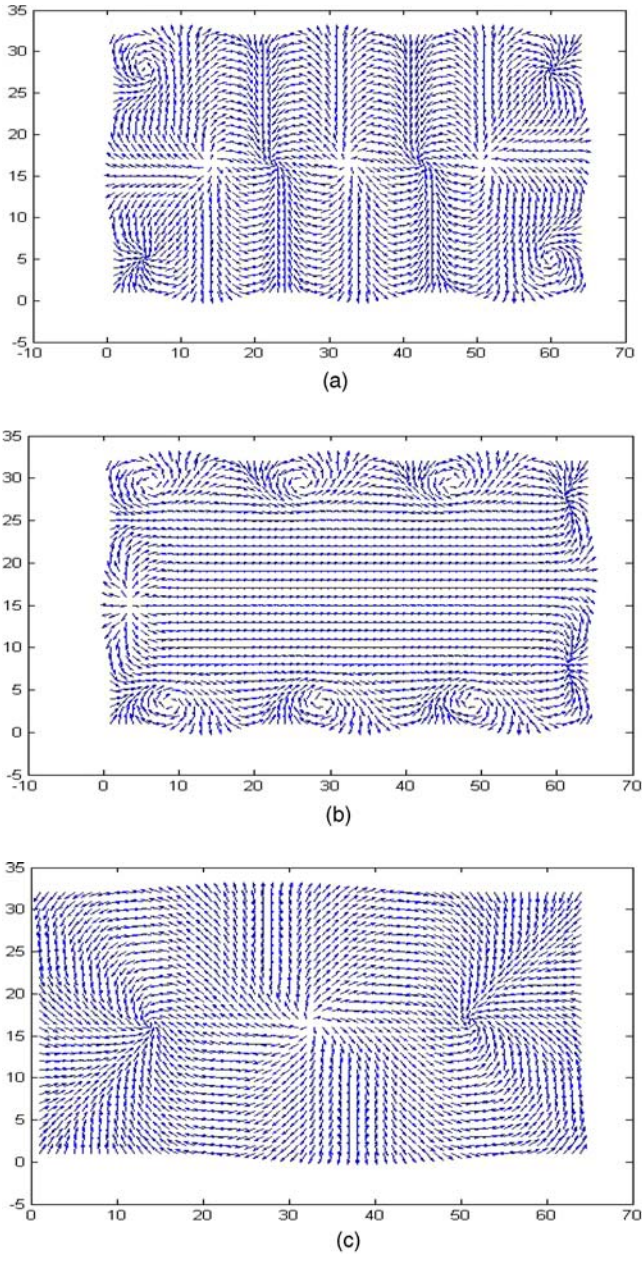

Fig. 4. (a) $L^* = 256$, $\ell^* = 128$, $d = 9$, zero initial condition. (b) $L^* = 256$, $\ell^* = 128$, $d = 9$, random initial condition. (c) $L^* = 256$, $\ell^* = 128$, $d = 3$, zero initial condition.

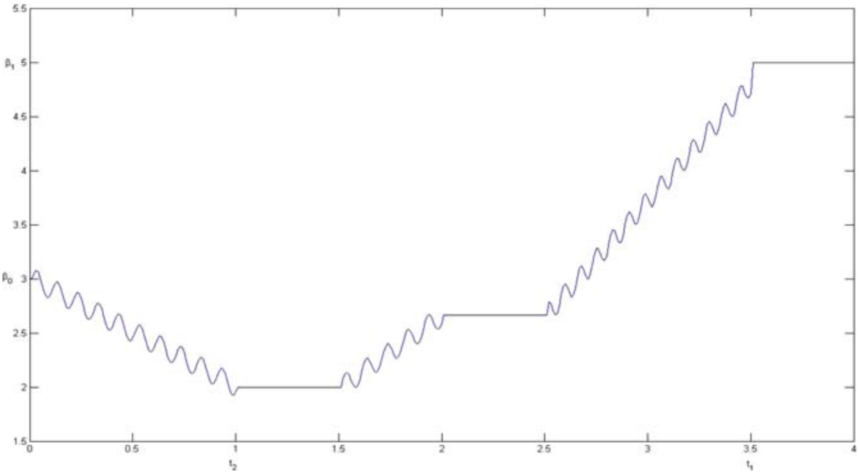

Fig. 5. The annealing function $\beta(t)$.

We applied this method first to the case of a square lattice, when the equilibrium configuration corresponding to some total degree d_0 is used as an initial condition for a dynamics with degree d_1. We fix $\beta_1 = 5$, $L^* = 128$.

Consider first the case $d_1 = 3$, the equilibrium configuration, with 0 initial condition, is given in Fig. 2(a), and the corresponding free energy is $E = 99$. We use simulated annealing to compute the equilibrium, starting from $d_0 = 4, -3, 5$, and find respectively $E = 23, 53, 51$, see Fig. 6. So the energies obtained this way are less than with zero initial conditions, though the initial magnetizations are rather large. At the same time, symmetries get lost. Thus the cost for the 3 vortices to be aligned along one of the diagonals of the square as in Fig. 6(b) is less than to form a domino near the center as in Fig. 2(a).

In Fig. 7 we show how to pass from $d_0 = 3$ to $d_1 = 5$. The configuration with zero initial condition and $d_1 = 5$ is given in Fig. 5(a), and energy is $E = 113$. Taking instead the equilibrium configuration for $d_0 = 3$ as an initial condition yields, without simulated annealing, to Fig. 7(b), with $d_1 = 6 - 1$, and $E = 216$. Using simulated annealing gives instead Fig. 7(c), which looks like Fig. 7(a), and corresponding energy $E = 115$. Actually, the 3 vortices on the anti-diagonal of the square in Fig. 7(b) collapse into a single one at the center.

Note also that the degeneracy in case of $d_1 = 2$ (a vortex of multiplicity 2 at the center for zero initial condition, $E = 24$,) is lifted through annealing from $d_0 = 4$: the 2 vortices move far apart, and $E = -19$. Other applications of simulated annealing will be given in the next subsection.

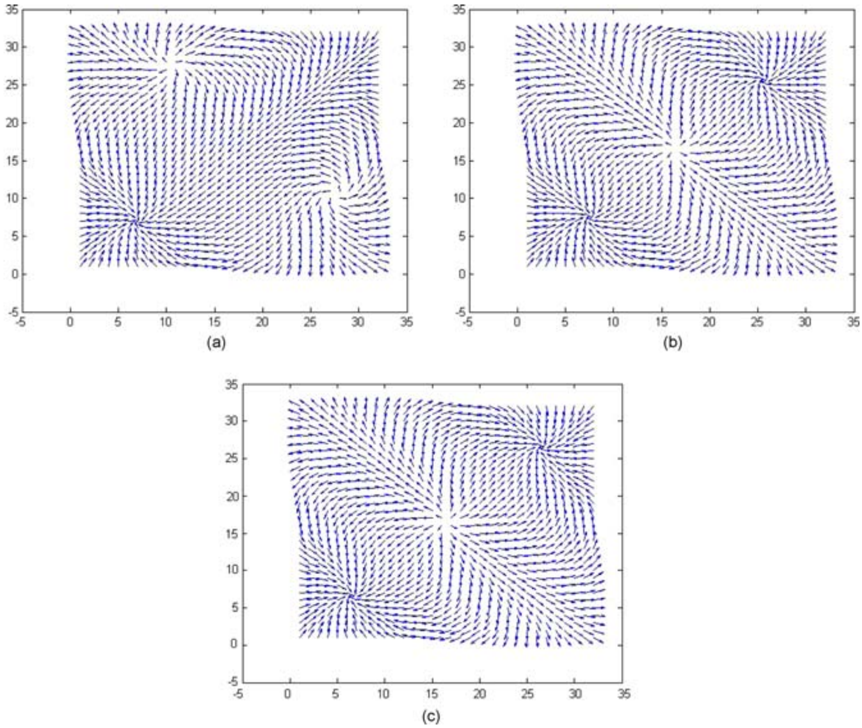

Fig. 6. (a) $d_0 = 4, d_1 = 3, E = 23$. (b) $d_0 = -3, d_1 = 3, E = 53$. (c) $d_0 = 5, d_1 = 3, E = 51$.

4.4. More General Configurations

We examine here the rôle of random fluctuations in the distribution of spins on the boundary Λ^{*c}, so to account for possible defects in the structure. With notations of Sec. 4.1, we take $\sigma_j = \exp(2i\pi d(j/N_\iota + \varepsilon_{\iota,j}))$, where $\varepsilon_{\iota,j}$ are uniform i.i.d. random variables with $\sum_{j=1}^{N_\iota} \varepsilon_{\iota,j} = 0$, and $(\varepsilon_{\iota,j})_{\iota,1\leq j\leq N_\iota-1}$, and variance small enough. The total degree is still equal to d, but the variation of the direction of spins at the boundary is not uniform. As expected, the picture does not depart drastically from the previous cases. Vortices change their place according to the initial value, and tend again to gather inside Λ^*, but take always the value $+1$ (assuming $d > 0$.) The sole effect of randomness in the boundary condition is to change the place of the vortices: namely they tend to get even closer to the boundary, so to leave larger ordered regions in the middle.

In Fig. 8(a,b), we have shown equilibrium configurations, obtained for $d = 7$, from the same initial and boundary conditions, but with (resp. without) simulated annealing. Initial magnetization has been chosen at random, but a priori larger

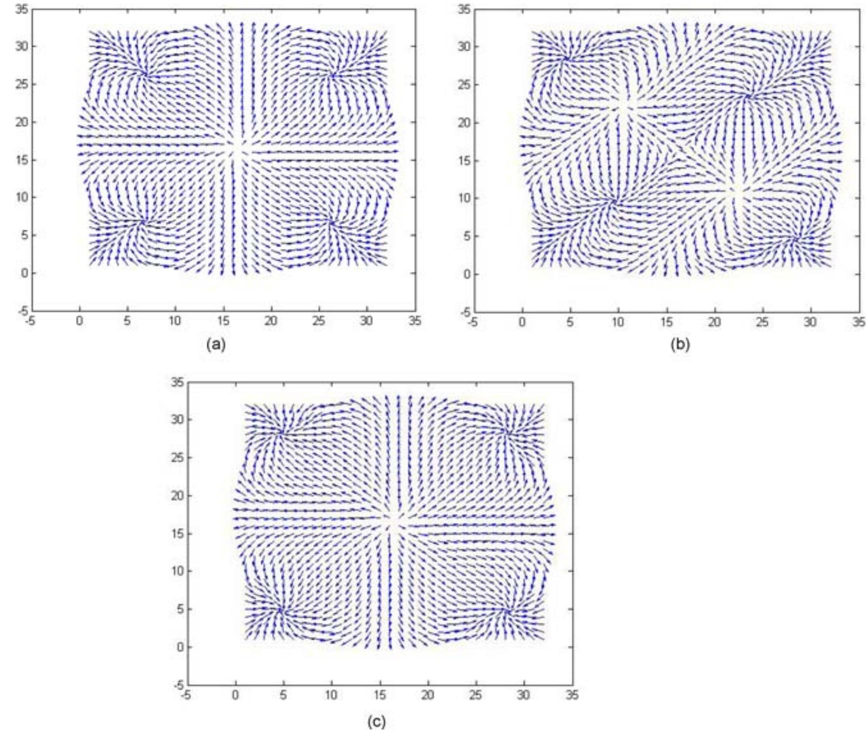

Fig. 7. (a) $d_1 = 5, d = 7$, zero initial condition. (b) $d_0 = 3, d_1 = 5$, without annealing. (c) $d_0 = 3, d_1 = 5$, with annealing.

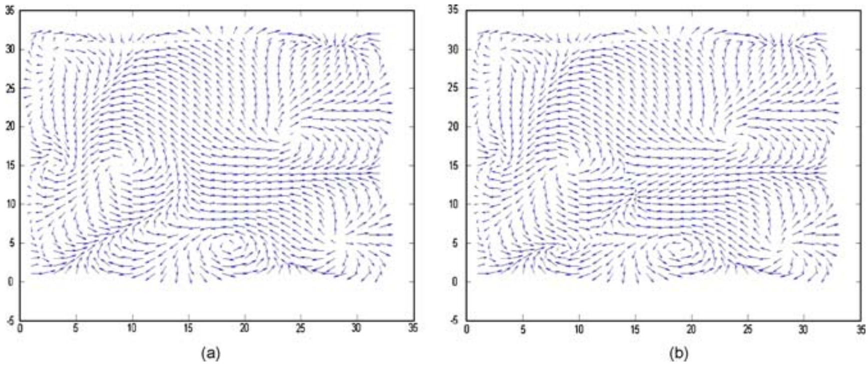

Fig. 8. (a) $d = 8 - 1$, $E = 277$, without annealing. (b) $d = 7$, $E = 240$, with annealing.

than before, the sole requirement being that $|m_0(x)| \leq m_\beta$. Random fluctuations on the boundary have been prescribed as above.

4.5. The Kirchoff-Onsager Correction

Another interesting result concerns the value of energy for the minimizing configurations. In case of Ginzburg-Landau equation, $-\Delta\psi + (|\psi|^2 - 1)\psi = 0$, where ψ is subject to a boundary condition with vorticity, it is known that energy of the minimizer vs. vorticity, has an asymptotic, as the n vortices x_j become distant from each other, the leading order term is given by a"proper energy," proportional to $\sum_{i=1}^n d_i^2$, and the next correction is the inter-vortex energy given by so-called Kirchhoff-Onsager hamiltonian, of the form

$$W_0 = -\pi \sum_{i \neq j} d_i d_j \log |x_i - x_j| \tag{4.5}$$

(see e.g. Ref. 3, 16 for precise statements.) It can be interpreted as the electrostatic energy for a system of charges d_j interacting through Coulomb forces. It turns out that, despite forces in action have no electrostatic character, Kirchhoff-Onsager correction holds with a good accuracy in our case, even for long range interactions (i.e. for small γ,) but provided the inter-vortex distance is bounded below by the range of the interaction. We have listed below some graphs of $K = \mathcal{F}(\cdot|m^c) - W_0$, obtained with uniform boundary conditions, which show that K roughly grows linearly with d (cf. Fig. 9).

Figure 9(b) shows that several random trials for initial conditions give approximately the same renormalized energy K.

5. THE HEISENBERG MODEL

We consider here "stationary spin waves" for $q = 3$, in a setting similar to this of Belavin and Polyakov, Ref. 4, 17, Chap. 6.

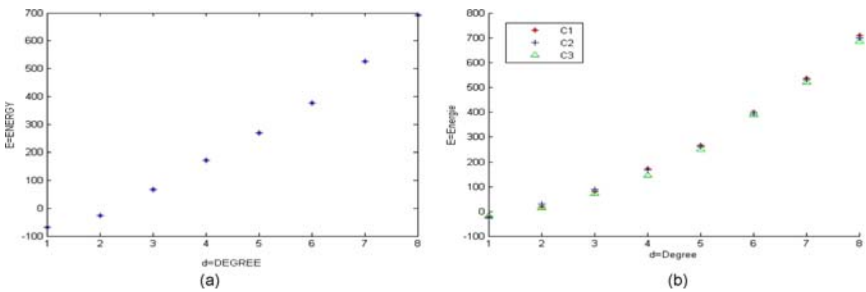

Fig. 9. (a) $L^* = 128$, zero initial condition. (b) $L^* = 128$, 3 random initial conditions.

Let us first recall the model. We look for minimizers of $H(\sigma) = \int_{\mathbf{R}^2} |\nabla\sigma(x)|^2 dx$, among all configurations $\sigma : \mathbf{R}^2 \to \mathbf{S}^2$ subject to the condition $\sigma(x) \to (0, 0, 1)$ as $|x| \to \infty$. This boundary condition not only ensures a finite energy on the whole plane, but also allows to extend σ as a map on the one point compactification $\mathbf{S}^2$ of $\mathbf{R}^2$, so we may consider its degree $D(\sigma) \in \mathbf{Z}$, or winding number, on the sphere. Differentiable maps $\mathbf{S}^2 \to \mathbf{S}^2$ are classified by their degree, in the sense that $\sigma, \tilde{\sigma} : \mathbf{S}^2 \to \mathbf{S}^2$ are homotopic iff they have the same degree. The main result of Belavin and Polyakov asserts that there exist solutions of that minimization problem, with given degree; they are called instantons, and expressed (in suitable coordinates associated with the stereographic projection $\mathbf{C} \to \mathbf{S}^2$) by arbitrary meromorphic functions of the form $\prod_{j=1}^{d} \frac{z-a_j}{z-b_j}$. Here $(a_j, b_j) \in \mathbf{C}^2$ play the role of vortices in the case $q = 2$; they have a natural structure of dipoles, with poles placed at a_j and b_j. So the minimization problem (for a given homotopy class) has a continuous degeneracy, parametrized by the family (a_j, b_j) which we interprete as moduli. The energy of all such instantons is a constant proportional to D.

It is then natural to consider the contribution of all instantons of same energy D. Somewhat heuristically,[17] obtains, after summing over $D \in \mathbf{N}$, a grand partition function of the form

$$\Xi(\lambda) = \sum_{D\geq 0} \frac{\lambda^{2D}}{(D!)^2} \int \prod_j da_j db_j \exp\left[\sum_{i<j} (\log|a_i - a_j|^2 + \log|b_i - b_j|^2) - \sum_{i,j} \log|a_i - b_j|^2\right] \tag{5.1}$$

and each instanton behaves as if it consisted of a pair of opposite Coulomb charges, placed at a_j and b_j. Since the 2 dimensional Coulomb energy is given by $(1/4\pi)\log|a_j - b_j|^2$, the exponent in (5.1) reminds us of the Kirchoff-Onsager hamiltonian (4.5), and formally, $\Xi(\lambda)$ is the grand partition function of a plasma at inverse temperature $\beta = 4\pi$.

It is not known to which extend these instantons are stable relatively to perturbations of $H(\sigma)$, e.g. due to the influence of temperature.

We start with some considerations on the degree of a map on $\mathbf{Z}^2$. Let $m : \mathbf{S}^2 \to \mathbf{S}^2$ be a discrete map, defined through the stereographic projection $\mathbf{Z}^2 \to \mathbf{S}^2$, the one point compactification of $\mathbf{Z}^2$ given by $\bar{\mathbf{Z}}^2 \approx \mathbf{Z}^2 \cup \{\omega\}$. The coordinates on the source and target space are given by the polar and azimuthal angles (θ, φ), and $(\tilde{\theta}, \tilde{\varphi})$ respectively.

Consider the complex $\mathcal{C} = (\mathbf{Z}^2, L_{\mathbf{Z}^2}, P_{\mathbf{Z}^2})$ and its homology group. Here $L_{\mathbf{Z}^2}$ is the set of bonds of unit length indexed by closest neighbors $x, x' \in \mathbf{Z}^2$, and $P_{\mathbf{Z}^2}$ the set of chips of unit area (plaquettes) around $x \in \mathbf{Z}^2$. See e.g.[1] for concepts of polyedral topology.

We define as usual the discrete jacobian $\operatorname{Jac} m(x) = \frac{\partial(\tilde{\theta},\tilde{\varphi})}{\partial(\theta,\varphi)}$ computed on the plaquette around x. Let $y_0 = m(x_0), x_0 \in \mathbf{Z}^2$ be a regular value of m, i.e. $\operatorname{Jac} m(x_0) \neq 0$. The integer

$$D_{x_0}(m) = |\{x \in m^{-1}(\{y_0\}) : \det \operatorname{Jac} m(x) > 0\}| \\ - |\{x \in m^{-1}(\{y_0\}) : \det \operatorname{Jac} m(x) < 0\}|$$

is called local degree of m at x_0. In case where $D_{x_0}(m)$ takes the same value for all $x_0 \in \mathbf{Z}^2$, we call it the degree of m and denote by $D(m)$. This is the general case, and $D(m)$ counts the number of coverings of the sphere. Then $D(m)$ will be given by the discrete analogue of the integral

$$D(m) = \frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \frac{\partial(\tilde{\theta},\tilde{\varphi}),}{\partial(\theta,\varphi)}$$

computed on the complex $\mathcal{C}$ defined above. When the values of m avoid a neighborhood of ω, we put $D(m) = 0$. If $D_{x_0}(m) = d$ for all x_0 in a neighborhood of $\omega \in \mathbf{Z}^2$, we call d the degree of m at infinity and denote $d = D_\omega(m)$. See e.g. Ref. 5 and references therein for a more complete study of topological properties of discrete maps.

We conjecture that for Kac-Heisenberg model, if m is a minimizer for the free energy $\mathcal{F}(\cdot, |m^c)$, i.e. m solves (3.2) or (3.3) with $D_\omega(m_0) = d$, after we take the thermodynamical limit $\Lambda \to \mathbf{Z}^2$, then either m vanishes at some point $x \in \mathbf{Z}^2$, or $\frac{m}{|m|} : \mathbf{Z}^2 \to \mathbf{S}^2$ has degree D. In practice however, we have only observed configurations with $0 \leq D \leq d$. So m shares some features with Belavin and Polyakov instantons, though with less symmetries or degeneracies, and a possible "degree loss" from infinity, since we are not really working in the thermodynamical limit.

It is straightforward to extend the constructions of Secs. 2 and 3 to the case $q = 3$. Let us sketch the main steps. The moment generating function is now $\phi(h) = \hat{\phi}(|h|) = \frac{\sinh|h|}{|h|}$, see Ref. 7, and for the entropy function $I(m) = \hat{I}(|m|)$ defined in (2.2), we have $\hat{I}' = ((\log\hat{\phi})')^{-1}$, and $(\log\hat{\phi})'(t) = L(t) = \frac{\cosh t}{\sinh t} - \frac{1}{t}$ (the function f before) is known as Langevin function. This is a concave, increasing function on $\mathbf{R}^+$, $L(t) \sim t/3$ as $t \to 0$, and $L(t) \to 1$ as $t \to \infty$. There is a phase transition of mean field type i.e. a positive root for equation $\beta m_\beta = \hat{I}'(m_\beta)$, iff $\beta > \hat{I}''(0) = 3$. We derive Euler-Lagrange equations for $\mathcal{F}(m_\delta \mid m_\delta^c)$, as in Sec. 3 (here we simply see m as a vector in the unit ball of $\mathbf{R}^3$, the complex representation of m was not essential,) and find

$$-m + L(\beta|J_\delta * m|)\frac{J_\delta * m}{|J_\delta * m|} = 0 \qquad (5.2)$$

For the corresponding gradient-flow dynamics (3.4), there is again a free energy dissipation rate function, which we compute exactly as in Proposition 3.1.

Furthermore, we have estimates on $m(x,t)$ as in Propositions 3.3 and 3.4; more precisely.

Proposition 5.1. *Assume $\beta > 3$, and let $m(x,t)$ be the solution of* (5.2) *such that $m_0(x) = m(x,0)$ satisfies $|m_0(x)| \leq \lambda < 1$, for some $\lambda \geq m_\beta$, and all $x \in \mathbf{Z}^2$. Then $|m(x,t)| \leq \lambda$ for all $x \in \Lambda^*$, and all $t > 0$. Assume moreover the z-component $m_0^z(x)$ of $m_0(x)$ satisfies $m_0^z(x)) \geq \mu > 0$, for all $x \in \mathbf{Z}^2$, and some $\mu > 0$ with $(\mu^2 + \lambda^2)^{1/2} < \beta L(\beta\lambda)$. Then $m^z(x,t)) \geq \mu$ for all $x \in \Lambda^*$, and $t > 0$.*

So choosing $\sigma^z(i) > 0$ on Λ^c (i.e. spins pointing to the z direction at the boundary) and also initial condition $m_0^z(x) > 0$ on Λ^*, Proposition 5.1 shows that $m^z(t,x) > 0$ stays bounded away from zero uniformly in time, so is the case for the limiting orbit $m(x)$ on $\mathbf{Z}^2$, thus $D(m) = 0$. Our conjecture is again comforted by the following numerical experiments, which also show that $m(x)$ depends in a more essential way on the initial conditions than for the planar rotator.

We start with prescribing the spins variables on Λ^c as in (4.3), taking a family of loops $\Gamma_i \subset \Lambda^c$, $i = 0, 1, 2 \dots$ along which $\sigma_j = (\cos\Phi_{ij}\sin\theta_i, \sin\Phi_{ij}\sin\theta_i, \cos\theta_i)$, $\Phi_{ij} = 2\pi dj/N_i + \phi_0$, and $0 \leq \theta_i \leq \theta_0$, decreasing with i, $\theta_{i_0} = 0$ on the last loop Γ_{i_0} interacting with Λ, and θ_0 small enough to fit with Belavin-Polyakov conditions. So fixing the precession number $d = D_\omega(m)$, we get a "stationary spin wave pattern" on the boundary. Inside Λ^* we choose random initial values, $|m_0(x)| \leq m_\beta$.

We represent here a few sample of (x,y) and (y,z) projections of the field m, which yield the following observations. In general, the solution is very sensitive to the choice of initial conditions, and many patterns show up, which reflects the moduli in Belavin-Polyakov model. For relatively small β (e.g. $\beta = 5$ with $L^* = 128$) spin waves fluctuate, and m^z can take negative values, but the domain where spins point downwards is not sufficiently large to start revolving around the sphere. So the degree is $D = 0$. We still get 2 dimensional "vortices" in the (x,y) plane, there are typically 1, 2 or 3 such "vortices"when $d = 1$, and up to 4 when $d = 2$. Exceptionally, we can also get a 3 dimensional vortex, i.e. x_0 such that $m(x_0)$ becomes quite small. Such a m is no longer homotopic to a function on the sphere.

Increasing β generally prevents getting too small values for m, and allows larger negative m^z. For $\beta = 10$ and $L^* = 128$, there are random trials where the winding number D is non zero. Thus Fig. 10 is obtained for $d = 1$ and suggests also $D = 1$. In Fig. 11 we still have $d = 1$, but $D = 0$, although 2 large symmetric regions contain negative values of m^z. Figure 12 gives an example where $D = 1$ for $d = 2$. Nevertheless, we have not observed winding numbers $D = 2$ for $d = 2$.

Further increasing β for a given L^* doesn't reveal anything new; namely, if small temperature seems to favors long range order and existence of non trivial instantons, it also creates stiffness and a need for space. In any case, one should

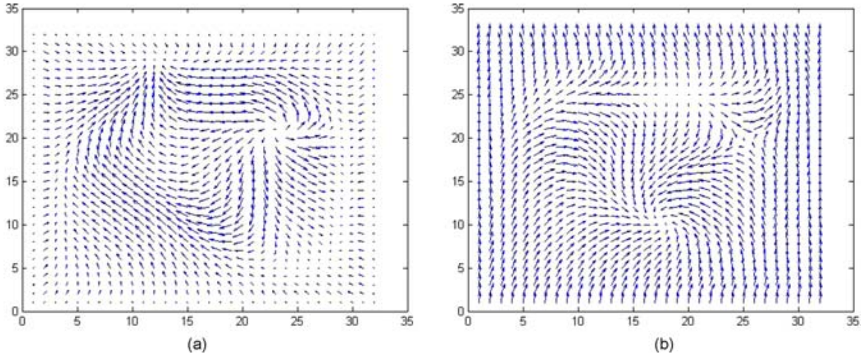

Fig. 10. (a) $L^* = 128$, $d = 1$, XY plane. (b) $L^* = 128$, $d = 1$, YZ plane.

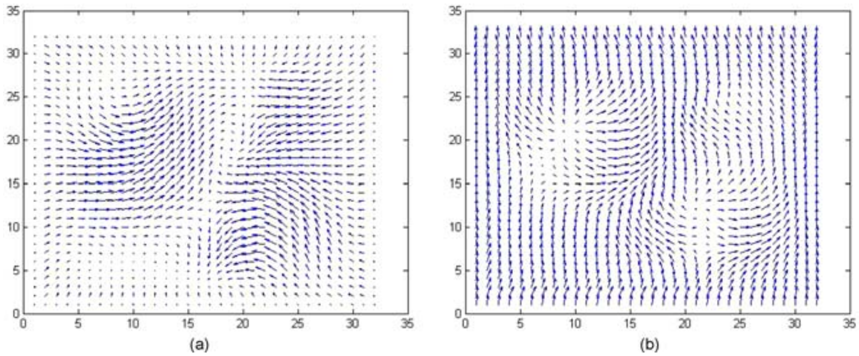

Fig. 11. (a) $L^* = 128$, $d = 1$, XY plane. (b) $L^* = 128$, $d = 1$, YZ plane.

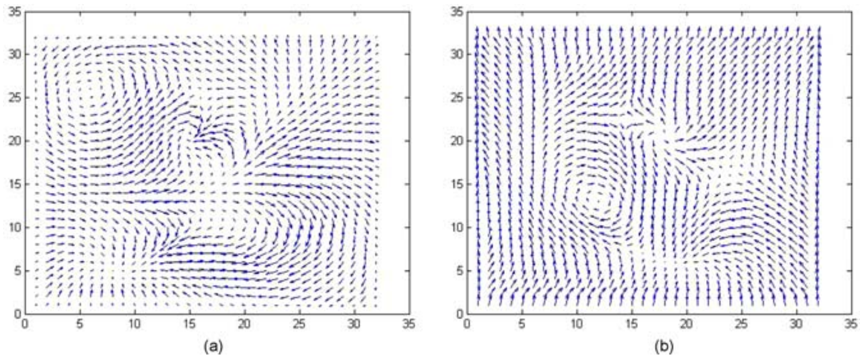

Fig. 12. (a) $L^* = 128$, $d = 2$, XY plane. (b) $L^* = 128$, $d = 2$, YZ plane.

keep in mind that Belavin-Polyakov instantons can be reproduced only as $\beta \to \infty$, and in the thermodynamic limit $|\Lambda| \to \infty$. Of course, everything can be again improved through simulated annealing.

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