

# Quantization of probability distributions and gradient flows in space dimension 2

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## Abstract

In this paper we study a perturbative approach to the problem of quantization of probability distributions in the plane. Motivated by the fact that, as the number of points tends to infinity, hexagonal lattices are asymptotically optimal from an energetic point of view [10,12,15], we consider configurations that are small perturbations of the hexagonal lattice and we show that: (1) in the limit as the number of points tends to infinity, the hexagonal lattice is a strict minimizer of the energy; (2) the gradient flow of the limiting functional allows us to evolve any perturbed configuration to the optimal one exponentially fast. In particular, our analysis provides a new mathematical justification of the asymptotic optimality of the hexagonal lattice among its nearby configurations.

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## 1. Introduction

The term *quantization* refers to the process of finding an *optimal* approximation of a  $d$ -dimensional probability density by a convex combination of a finite number  $N$  of Dirac masses. The quality of such an approximation is measured in terms of the Monge–Kantorovich or Wasserstein metric.

The need for such approximations first arose in the context of information theory in the early 1950s. The idea was to see the quantized measure as the digitalization of an analog signal which should be stored on a data storage medium or transmitted via a channel [5,11]. Another classical application of the quantization problem concerns numerical integration, where integrals with respect to certain probability measures needs to be replaced by integrals with respect to a good discrete approximation of the original measure [16]. For instance, quasi-Monte Carlo methods

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use low discrepancy sequences, and the notion of discrepancy can be regarded as one approach to the quantization problem. See [7] for an introduction to this subject, especially section 5 for a presentation of the notion of discrepancy of a sequence, and section 7 for applications in the context of rarefied gas dynamics. Moreover, this problem has applications in cluster analysis, pattern recognition, speech recognition, stochastic processes (sampling design) and mathematical models in economics (optimal location of service centers). For a detailed exposition and a complete list of references see the monograph [13].

We now introduce the theoretical setup of the problem. Given  $r \geq 1$ , consider  $\rho$  a probability density on an open set  $\Omega \subset \mathbf{R}^d$  with finite  $r$ -th order moment,

$$\int_{\Omega} |y|^r \rho(y) dy < \infty.$$

Given  $N$  points  $x^1, \dots, x^N \in \Omega$ , we seek the best approximation of  $\rho$ , in the sense of Monge–Kantorovich, by a convex combination of Dirac masses centered at  $x^1, \dots, x^N$ . Hence one minimizes

$$\inf \left\{ MK_r \left( \sum_i m_i \delta_{x^i}, \rho(y) dy \right) : m_1, \dots, m_N \geq 0, \sum_{i=1}^N m_i = 1 \right\},$$

with

$$MK_r(\mu, \nu) := \inf \left\{ \int_{\Omega \times \Omega} |x - y|^r d\gamma(x, y) : \pi \in \Pi(\mu, \nu) \right\},$$

where  $\Pi(\mu, \nu)$  is the set of all Borel probability measures on  $\Omega \times \Omega$  whose marginals onto the first and second component are given by  $\mu$  and  $\nu$  respectively. In other words, a Borel probability  $\pi$  measure on  $\Omega \times \Omega$  belongs to  $\Pi(\mu, \nu)$  if

$$\iint_{\Omega \times \Omega} (\phi(x) + \psi(y)) \pi(dx dy) = \int_{\Omega} \phi(x) \mu(dx) + \int_{\Omega} \psi(y) \nu(dy)$$

for each  $\phi, \psi \in C_c(\Omega)$  (see [2,17] for more details on the Monge–Kantorovich distance between probability measures).

As shown in [13], the following facts hold:

- (1) The best choice of the masses  $m_i$  is given by

$$m_i := \int_{V(x^i|\{x^1, \dots, x^N\})} \rho(y) dy,$$

where

$$V(x^i|\{x^1, \dots, x^N\}) := \{y \in \Omega : |y - x^i| \leq |y - x^j|, j \in 1, \dots, N\}$$

is the so-called *Voronoi cell* of  $x^i$  in the set  $x^1, \dots, x^N$ .

- (2) The following identity holds:

$$\inf \left\{ MK_r \left( \sum_i m_i \delta_{x^i}, \rho(y) dy \right) : m_1, \dots, m_N \geq 0, \sum_{i=1}^N m_i = 1 \right\} = \mathcal{Q}_{N,r}(x^1, \dots, x^N),$$

where

$$\mathcal{Q}_{N,r}(x^1, \dots, x^N) := \int_{\Omega} \min_{1 \leq i \leq N} |x^i - y|^r \rho(y) dy.$$

Assume that the points  $x^1, \dots, x^N$  are chosen in an optimal way so as to minimize the quantization functional  $\mathcal{Q}_{N,r} : (\mathbf{R}^d)^N \rightarrow \mathbf{R}^+$ ; then in the limit as  $N$  tends to infinity these points distribute themselves accordingly to a probability density proportional to  $\rho^{d/d+r}$ . In other words, by [13, Chapter 2, Theorem 7.5] one has

$$\frac{1}{N} \sum_{i=1}^N \delta_{x^i} \rightharpoonup \frac{\rho^{d/d+r}(x)dx}{\int_{\Omega} \rho^{d/d+r}(y)dy} \tag{1.1}$$

weakly in the sense of Borel probability measures on  $\Omega$  as  $N \rightarrow \infty$ .

These issues are relatively well understood from the point of view of the calculus of variations [13, Chapter 1, Chapter 2], and [14]. Moreover, in [6] we considered a gradient flow approach to this problem in dimension 1. Now we will explain the heuristic of the dynamical approach and the main difficulties in extending our result to higher dimensions.

### 1.1. A dynamical approach to the quantization problem

Given  $N$  points  $x_0^1, \dots, x_0^N$ , we consider their evolution under the gradient flow generated by  $\mathcal{Q}_{N,r}$ , that is, we solve the system of ODEs in  $(\mathbf{R}^d)^N$

$$\begin{cases} (\dot{x}^1(t), \dots, \dot{x}^N(t)) = -\nabla \mathcal{Q}_{N,r}(x^1(t), \dots, x^N(t)), \\ (x^1(0), \dots, x^N(0)) = (x_0^1, \dots, x_0^N). \end{cases} \tag{1.2}$$

As usual in gradient flow theory, as  $t$  tends to infinity one expects that the points  $(x^1(t), \dots, x^N(t))$  converge to a minimizer  $(\bar{x}^1, \dots, \bar{x}^N)$  of  $\mathcal{Q}_{N,r}$ . Hence, in view of (1.1), the empirical measure

$$\frac{1}{N} \sum_{i=1}^N \delta_{\bar{x}^i}$$

is expected to converge weakly in the sense of probability measures to

$$\frac{\rho^{d/d+r}}{\int_{\Omega} \rho^{d/d+r}(y)dy} dx$$

as  $N \rightarrow \infty$ .

Our approach of this problem involves exchanging the limits as  $t \rightarrow +\infty$  and  $N \rightarrow \infty$ . More precisely, we first pass to the limit in the ODE above as  $N \rightarrow \infty$ , and take the limit in the resulting PDE as  $t \rightarrow +\infty$ . For this, we take a set of reference points  $(\hat{x}^1, \dots, \hat{x}^N)$  and we parameterize a general family of  $N$  points  $x^i$  as the image of  $\hat{x}^i$  via a slowly varying smooth map  $X : \mathbf{R}^d \rightarrow \mathbf{R}^d$ , that is

$$x^i = X(\hat{x}^i).$$

In this way, the functional  $\mathcal{Q}_{N,r}(x^1, \dots, x^N)$  can be rewritten in terms of the map  $X$  and (a suitable renormalization of it) should converge to a functional  $\mathcal{F}[X]$ . Hence, we can expect that the evolution of  $x^i(t)$  for  $N$  large is well-approximated by the  $L^2$ -gradient flow of  $\mathcal{F}$ .

Although this formal argument may sound convincing, already the 1-dimensional case is rather delicate. We briefly review the results of [6] below.

### 1.2. The 1D case

Without loss of generality let  $\Omega$  be the open interval  $(0, 1)$ , and consider  $\rho$  a smooth probability density on  $\Omega$ . In order to obtain a continuous version of the functional

$$\mathcal{Q}_{N,r}(x^1, \dots, x^N) = \int_0^1 \min_{1 \leq i \leq N} |x^i - y|^r \rho(y) dy,$$

with  $0 \leq x^1 \leq \dots \leq x^N \leq 1$ , assume that

$$x^i = X\left(\frac{i - 1/2}{N}\right), \quad i = 1, \dots, N$$

with  $X : [0, 1] \rightarrow [0, 1]$  a smooth non-decreasing map such that  $X(0) = 0$  and  $X(1) = 1$ . Then,

$$N^r \mathcal{Q}_{N,r}(x^1, \dots, x^N) \longrightarrow C_r \int_0^1 \rho(X(\theta)) |\partial_\theta X(\theta)|^{r+1} d\theta := \mathcal{F}[X]$$

as  $N \rightarrow \infty$ , where  $C_r := \frac{1}{2^{r(r+1)}}$ .

By a standard computation, we obtain the gradient flow PDE for  $\mathcal{F}$  for the  $L^2$ -metric,

$$\partial_t X(t, \theta) = C_r \left( (r + 1) \partial_\theta (\rho(X(t, \theta)) |\partial_\theta X(t, \theta)|^{r-1} \partial_\theta X(t, \theta)) - \rho'(X(t, \theta)) |\partial_\theta X(t, \theta)|^{r+1} \right), \tag{1.3}$$

coupled with the Dirichlet boundary condition

$$X(t, 0) = 0, \quad X(t, 1) = 1. \tag{1.4}$$

Our main result in [6] shows that, provided that  $r = 2$ , one has  $\|\rho - 1\|_{W^{2,\infty}(0,1)} \ll 1$ , and that the initial datum is smooth and increasing, the discrete and the continuous gradient flows remain *uniformly* close in  $L^2$  for *all* times. In addition, by entropy-dissipation inequalities for the PDE, we show that the continuous gradient flow converges exponentially fast to the stationary state for the PDE, which is seen in Eulerian variables to correspond to the measure

$$\frac{\rho^{1/3}(x) dx}{\int_0^1 \rho^{1/3}(y) dy}$$

as predicted by (1.1).

### 1.3. The 2D case: setting and main result

Our goal is to extend the result above to higher dimensions. As a first step, it is natural to consider the quantization problem for the uniform measure in space dimension 2. The main advantage in this situation is that optimal configurations are known to be asymptotically hexagonal lattices [10,12,15]. (Notice however that the reference [15] considers the 2-dimensional quantization problem in the Monge–Kantorovich distance of exponent 1, i.e. with  $r = 1$ , at variance with our approach in the present paper which assumes  $r = 2$ .) Hence, it will be natural to use the vertices of the optimal, hexagonal lattice as reference points  $\hat{x}^i$ , and to assume that the time-dependent configuration of points are obtained as slowly varying deformations of the optimal configuration.

More precisely, we shall consider the following setting. Let us consider a regular hexagonal tessellation of the Euclidean plane  $\mathbf{R}^2$ . Up to some inessential displacement, one can choose the centers of the hexagons to be the vertices of the regular lattice

$$\mathcal{L} := \mathbf{Z}e_1 \oplus \mathbf{Z}e_2 \quad \text{where } e_1 = (1, 0) \text{ and } e_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right).$$

Let  $\Pi$  be the fundamental domain of  $\mathbf{R}^2/\mathcal{L}$  centered at the origin defined as follows:

$$\Pi := \{x_1 e_1 + x_2 e_2 : |x_1|, |x_2| \leq \frac{1}{2}\}.$$

Henceforth, we consider the sequence of scaled lattices homothetic to  $\mathcal{L}$ , of the form  $\epsilon \mathcal{L}$  with  $\epsilon = 1/n$  and  $n \in \mathbf{N}^*$ .

The slowly varying deformations of  $\mathcal{L}$  used in this work are discrete sets of the form  $\mathcal{X}_\epsilon := X(\epsilon\mathcal{L})$  with  $\epsilon = 1/n$  and  $n \in \mathbf{N}^*$ , where  $X \in \text{Diff}^1(\mathbf{R}^2)$ , i.e.  $X$  is a  $C^1$ -diffeomorphism of  $\mathbf{R}^2$  onto itself. We shall assume that  $X$  satisfies the following properties:

(a)  $X$  is a periodic perturbation of the identity map, i.e.

$$X(x+l) = X(x) + l \quad \text{for all } x \in \mathbf{R}^2 \text{ and } l \in \mathcal{L};$$

(b)  $X$  is  $C^1$ -close to the identity map, i.e.,

$$\|X - \text{id}\|_{W^{1,\infty}} < \eta \quad \text{where } \eta \ll 1;$$

(c)  $X$  is centered at the origin, i.e.

$$\int_{\Pi} X(x) dx = 0.$$

(This last condition does not restrict the generality of our approach: if  $X$  fails to satisfy property (c), set

$$\langle X \rangle := \int_{\Pi} X(x) dx = \int_{\Pi} (X(x) - x) dx;$$

then  $\langle X \rangle < \eta$  and  $\hat{X}(x) = X(x) - \langle X \rangle$  satisfies properties (a) and (c), and property (b) where  $\eta$  is replaced by  $2\eta$ .)

If  $\eta$  is sufficiently small, then for every  $x \in \mathcal{X}_\epsilon$  the Voronoi cell  $V(x|\mathcal{X}_\epsilon)$  centered in  $x$  with respect to the set of points  $\mathcal{X}_\epsilon$  is an hexagon. Indeed, the angle between two adjacent edges starting from any vertex in the deformed configuration  $\mathcal{X}_\epsilon$  is  $\pi/3 + O(\eta)$  by the mean value theorem. Hence the center of the circumscribed circle to any triangle with nearest neighbor vertices in the deformed configuration lies in the interior of this triangle, and the perpendicular bisectors of the edges of the triangle intersect at the center of the circumscribed circle with an angle  $2\pi/3 + O(\eta)$ . Hence the family of all such centers are the vertices of an (irregular) hexagonal tessellation of the plane, which is the Voronoi tessellation of the deformed configuration.

To avoid all difficulties pertaining to boundary conditions, we formulate our quantization problem in the ergodic setting. In other words, we consider the discrete quantization functional averaged over disks with radius  $L \gg 1$ :

$$\mathcal{G}_{\epsilon,L}(\mathcal{X}_\epsilon) := \int_{B(0,L)} \text{dist}(y, \mathcal{X}_\epsilon)^2 dy.$$

Our first main result describes the asymptotic behavior of  $\mathcal{G}_{\epsilon,L}$  as follows.

**Theorem 1.1.** *Assume that  $X \in \text{Diff}^1(\mathbf{R}^2)$  satisfies the properties (a–c) above, and that  $\eta$  is small enough. For each  $\epsilon = 1/n$  with  $n \in \mathbf{N}^*$*

$$\frac{1}{\pi L^2} \mathcal{G}_{\epsilon,L}(\mathcal{X}_\epsilon) \rightarrow \int_{X(\Pi)} \text{dist}(y, \mathcal{X}_\epsilon)^2 dy \quad \text{as } L \rightarrow \infty.$$

Moreover

$$\int_{X(\Pi)} \text{dist}(y, \mathcal{X}_\epsilon)^2 dy \sim \epsilon^2 \mathcal{F}(X) \quad \text{as } \epsilon \rightarrow 0,$$

where  $\mathcal{F}$  is given by

$$\mathcal{F}(X) := \int_{\Pi} F(\nabla X(x)) dx.$$

In this expression, the function  $F$  is defined by the formula

$$F(M) := \frac{1}{48} \sum_{\omega \in \{e_1, e_2, e_1 - e_2\}} |M\omega|^4 \Phi(\omega, M) (3 + \Phi(\omega, M)^2),$$

where

$$\Phi(e, M) := \sqrt{\frac{|MRe|^2 |MR^T e|^2}{\frac{3}{4} |\det(M)|^2} - 1}$$

for each invertible  $2 \times 2$ -matrix  $M$  with real entries and each unit vector  $e$ , and where  $R$  designates the rotation of an angle  $\frac{\pi}{3}$  centered at the origin.

The proof of [Theorem 1.1](#) occupies sections 2 and 3 below.

Observe that the integrand in the definition of  $\mathcal{F}$  depends exclusively on the gradient of the map  $\nabla X$ . In particular, the integrand in  $\mathcal{F}$  involves the Jacobian determinant  $\det(\nabla X)$  of the deformation map. However the dependence of  $\mathcal{F}$  on  $\det(\nabla X)$  becomes singular as  $\det(\nabla X) \rightarrow 0$ . Therefore, our analysis is restricted to small perturbations of the uniform, hexagonal tessellation of the plane. This is obviously consistent with the fact that we postulated that our configuration of points remains close to the uniform hexagonal tessellation in order to arrive at the explicit expression of  $\mathcal{F}$  given in [Theorem 1.1](#).

On the other hand, at variance with the 1D case, the limiting function  $\mathcal{F}$  does not depend on  $X$  only through its Jacobian determinant. This seriously complicates the Eulerian formulation of the 2D case, which was relatively simple in the 1D case, and which we used in a significant manner in our earlier work [\[6\]](#).

Our second result is a simplified expression for  $F$  near the identity matrix.

**Theorem 1.2.** *Let*

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

There exists  $0 < \eta_0 \ll 1$  such that, for all  $M \in GL_2(\mathbf{R})$  satisfying  $|M - I| \leq \eta_0$ , one has

$$\begin{aligned} F(M) &= \frac{1}{16\sqrt{3}} \det(M) \operatorname{trace}(M^T M (2S - I)) \\ &\quad + \frac{1}{64\sqrt{3}} \frac{\operatorname{trace}(M^T M)^2 \operatorname{trace}(M^T M S)}{\det(M)} \\ &\quad - \frac{1}{192\sqrt{3}} \frac{\operatorname{trace}(M^T M)^3}{\det(M)} - \frac{1}{48\sqrt{3}} \frac{\operatorname{trace}(M^T M S)^3}{\det(M)}. \end{aligned}$$

Moreover, for each  $2 \times 2$ -matrix  $N$  with real entries, one has

$$\begin{aligned} 48F(I + \epsilon N) &= \frac{10}{\sqrt{3}} + \frac{20}{\sqrt{3}} \epsilon \operatorname{trace}(N) \\ &\quad + \frac{1}{\sqrt{3}} \epsilon^2 \left( 14 \det(N) + 10 \operatorname{trace}(N)^2 + 3 \operatorname{trace}(N^T N) \right) + O(\epsilon^3). \end{aligned}$$

The proof of [Theorem 1.2](#) is given in section 5 below.

Our third main result bears on the basic properties of the  $L^2$ -gradient flow of the asymptotic quantization functional  $\mathcal{F}$  obtained in [Theorem 1.1](#).

**Theorem 1.3.** *Let  $X^{in} \in \operatorname{Diff}(\mathbf{R}^2)$  satisfy the properties (a–c) above, together with the condition*

$$\|X^{in} - \operatorname{id}\|_{W^{\sigma,p}(\Pi)} \leq \epsilon_0, \tag{1.5}$$

with  $p > 2$  and  $1 + 2/p < \sigma$ . Consider the PDE defining the  $L^2$ -gradient flow of  $\mathcal{F}$ :

$$\begin{cases} \partial_t X_j(t, x) = -\frac{\delta \mathcal{F}}{\delta X_j(t, x)}, & j = 1, 2, \\ X(0, x) = X^{in}(x). \end{cases} \tag{1.6}$$

The  $L^2$ -gradient flow of  $\mathcal{F}$  starting from any initial diffeomorphism  $X^{in}$  satisfying the conditions above exists and is unique. In other words, the Cauchy problem (1.6) has a unique solution  $X$  defined for all  $t > 0$ , and  $X(t, \cdot)$  satisfies

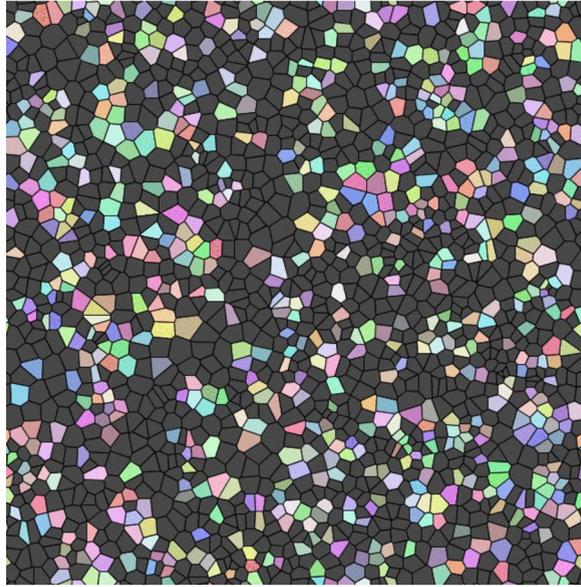


Fig. 1.1. 720 points at time 0.

properties (a–c) for all  $t > 0$ . Besides, the solution  $t \mapsto X(t, \cdot)$  of (1.6) converges exponentially fast to the identity map as  $t \rightarrow +\infty$ : for each  $X^{in}$  satisfying (a–c) and (1.5), there exist  $C, \mu > 0$  (depending on  $\epsilon_0$ ) such that

$$\|X(t, \cdot) - \text{id}\|_{L^\infty(\Pi)} \leq C e^{-\mu t}$$

for all  $t > 0$ .

Since  $\mathcal{F}$  depends on  $\det(\nabla X)$ , one cannot hope that  $\mathcal{F}$  has any convexity property. Moreover, since the dependence of  $\mathcal{F}$  in  $\det(\nabla X)$  is singular, one cannot hope that some compensations would offset the lack of convexity coming from the determinant. For this reason, we consider initial configurations that are small perturbations of the hexagonal lattices, and we study in detail the linearization at the equilibrium configuration of the system of equations defining the gradient flow of  $\mathcal{F}$ . Combining this with some general  $\epsilon$ -regularity theorems for parabolic systems, we prove that the nonlinear evolution is governed by the linear dynamics, and in this way we can prove exponential convergence to the hexagonal (equilibrium) configuration. As we shall see, our proof of [Theorem 1.3](#), which occupies [section 6](#) below, is based on tools coming from the regularity theory for parabolic systems, and this is why we need assumptions on the initial data in appropriate Sobolev spaces.

Moreover, our numerical simulations confirm the asymptotic optimality of the hexagonal lattice as the number of points tends to infinity — see [Figs. 1.1, 1.2, and 1.3](#). The colored polygons in [Figs. 1.1, 1.2, and 1.3](#) are the hexagons. [Fig. 1.3](#) suggests that the minimizers may have some small 1-dimensional defects with respect to the hexagonal lattice. This may be caused by the boundary conditions used in the numerical simulation which are not periodic, at variance with the setting used in [Theorems 1.1 and 1.3](#). Another possible explanation is that the particle system may remain frozen in some local minimum state. Also, the hexagonal tessellation is not the global minimizer for a finite number  $N$  of points, and this is another difference between the discrete and the continuous problems.

## 2. The contribution of a single Voronoi cell of the deformed lattice

From now on, we adopt the setting defined in the previous section, and we begin with some elementary geometrical observations used in computing the continuous functional  $\mathcal{F}$ . This is the first step in the proof of [Theorem 1.1](#).

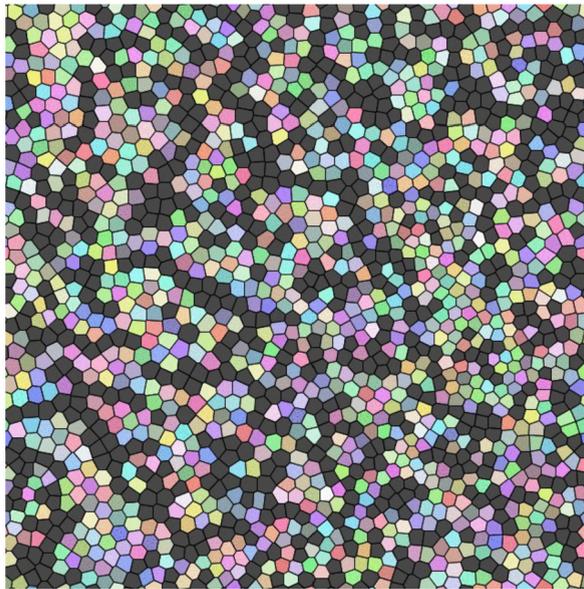


Fig. 1.2. 720 points after 19 iterations.

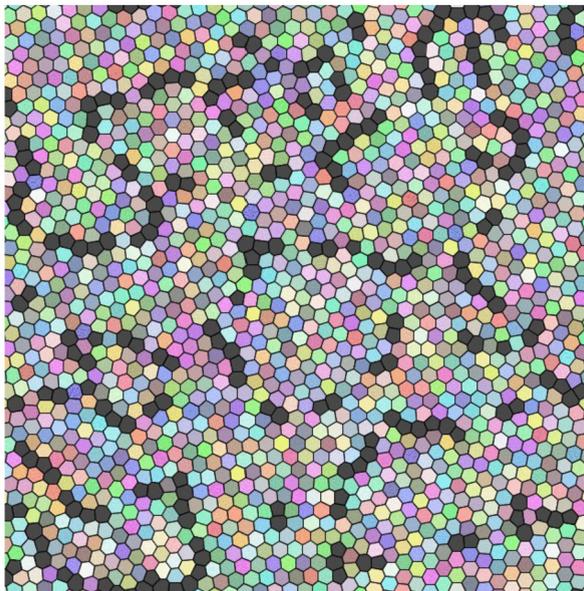


Fig. 1.3. 720 points after 157 iterations.

Under the assumptions of [Theorem 1.1](#), our goal is to compute

$$\int_{V(X(\epsilon(k_1 e_1 + k_2 e_2)) | \mathcal{X}_\epsilon)} |y - X(\epsilon(k_1 e_1 + k_2 e_2))|^2 dy$$

in terms of the displacement  $X(\epsilon(k_1 e_1 + k_2 e_2))$  and of the centers of the adjacent cells  $V(X(\epsilon(k_1 e_1 + k_2 e_2)) | \mathcal{X}_\epsilon)$ , i.e.:

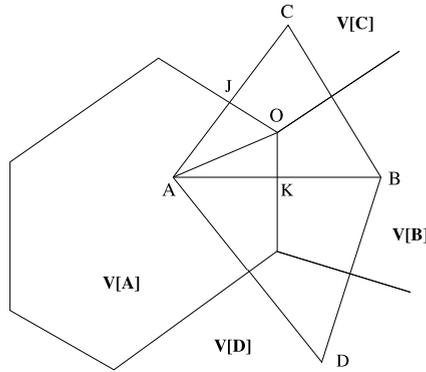


Fig. 2.1. Voronoi cell.

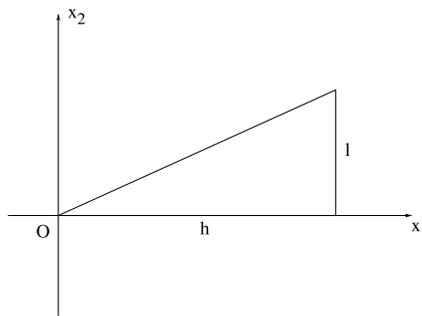


Fig. 2.2. Right triangle.

$$\begin{aligned} X(\epsilon((k_1 + 1)e_1 + k_2e_2)), & \quad X(\epsilon((k_1 - 1)e_1 + k_2e_2)), \\ X(\epsilon((k_1 - 1)e_1 + (k_2 + 1)e_2)), & \quad X(\epsilon((k_1 + 1)e_1 + (k_2 - 1)e_2)), \\ X(\epsilon(k_1e_1 + (k_2 - 1)e_2)), & \quad X(\epsilon(k_1e_1 + (k_2 + 1)e_2)). \end{aligned}$$

To do that, up to sets of measure zero, we can partition each hexagon into 12 right triangles, each of them similar either to  $AOK$  or to  $AOJ$  in Fig. 2.1. We start integrating the function  $|y - X(\epsilon(k_1e_1 + k_2e_2))|^2$  on one of these right triangles. Let  $T$  be a right triangle with adjacent sides to the right angle of length  $h$  and  $l$  (see Fig. 2.2).

With the notation of Fig. 2.2,

$$\begin{aligned} \int_T (x_1^2 + x_2^2) dx_1 dx_2 &= \int_0^h \int_0^{lx_1/h} (x_1^2 + x_2^2) dx_2 dx_1 = \int_0^h \left( \frac{lx_1}{h} x_1^2 + \frac{l^3 x_1^3}{3h^3} \right) dx_1 \\ &= \int_0^h x_1^3 \left( \frac{l}{h} + \frac{l^3}{3h^3} \right) dx_1 = \frac{1}{4}lh(h^2 + \frac{1}{3}l^2). \end{aligned}$$

Coming back to the notation of Fig. 2.1, we obtain

$$\int_{V[A]} |\vec{A}y|^2 dy = \int_{AOK} |\vec{A}y|^2 dy + \int_{AOJ} |\vec{A}y|^2 dy + 10 \text{ similar terms.}$$

Let us focus on the first term on the right hand side. We compute it in the triangle  $ABC$ .

Recalling the notation in Fig. 2.3

$$\int_{AOK} |\vec{A}y|^2 dy = \frac{1}{8}c|OK| \left( \frac{1}{4}c^2 + \frac{1}{3}|OK|^2 \right).$$

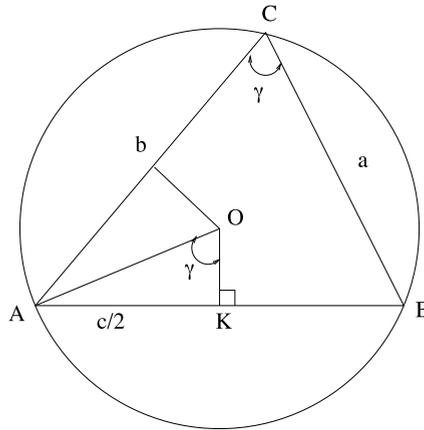


Fig. 2.3. Triangle ABC.

In the triangle  $ABC$ , we have

$$\widehat{AOK} = \widehat{ACB} = \gamma,$$

and

$$|OK|^2 = |OA|^2 - \frac{1}{4}c^2 = \frac{1}{4}c^2 \left( \frac{1}{\sin^2 \gamma} - 1 \right).$$

Moreover, denoting by  $S$  the surface of the triangle  $ABC$ ,

$$2S = |\vec{CA} \wedge \vec{CB}| = ab \sin \gamma.$$

Thus,

$$|OK|^2 = \frac{1}{4}c^2 \left( \frac{a^2b^2}{4S^2} - 1 \right),$$

so that

$$\begin{aligned} \int_{AOK} |\vec{Ay}|^2 dy &= \frac{1}{16}c^2 \sqrt{\frac{a^2b^2}{4S^2} - 1} \left( \frac{1}{4}c^2 + \frac{1}{12}c^2 \left( \frac{a^2b^2}{4S^2} - 1 \right) \right) \\ &= \frac{1}{192}c^4 \sqrt{\frac{a^2b^2}{4S^2} - 1} \left( \frac{a^2b^2}{4S^2} + 2 \right). \end{aligned}$$

In other words,

$$\int_{AOK} |\vec{Ay}|^2 dy = \frac{1}{192}|\vec{AB}|^4 \sqrt{\frac{|\vec{CB}|^2|\vec{CA}|^2}{|\vec{CA} \wedge \vec{CB}|^2} - 1} \left( \frac{|\vec{CB}|^2|\vec{CA}|^2}{|\vec{CA} \wedge \vec{CB}|^2} + 2 \right).$$

Exchanging  $B$  and  $C$ , we find by symmetry that

$$\int_{AOJ} |\vec{Ay}|^2 dy = \frac{1}{192}|\vec{AC}|^4 \sqrt{\frac{|\vec{BC}|^2|\vec{BA}|^2}{|\vec{BA} \wedge \vec{BC}|^2} - 1} \left( \frac{|\vec{BC}|^2|\vec{BA}|^2}{|\vec{BA} \wedge \vec{BC}|^2} + 2 \right).$$

Let us now write the latter expression for  $A = X(\epsilon(k_1e_1 + k_2e_2))$ , where the points  $B$  and  $C$  are the centers of the Voronoi cells adjacent to the Voronoi cell centered in  $A$ . For simplicity of notation, we define

$$X(\epsilon(k_1e_1 + k_2e_2)) =: X_{k_1, k_2}.$$

Thus, the contribution to

$$\int_{V(X(\epsilon(k_1 e_1 + k_2 e_2))), \mathcal{X}_\epsilon} |y - X(\epsilon(k_1 e_1 + k_2 e_2))|^2 dy$$

of the terms related to the triangle  $ABC$  with  $A = X_{k_1, k_2}$ ,  $B = X_{k_1+1, k_2}$  and  $C = X_{k_1, k_2+1}$  is:

$$\begin{aligned} & \int_{AOK} |\vec{A}y|^2 dy + \int_{AOJ} |\vec{A}y|^2 dy \\ &= \frac{1}{192} |X_{k_1+1, k_2} - X_{k_1, k_2}|^4 \sqrt{\frac{|X_{k_1+1, k_2} - X_{k_1, k_2+1}|^2 |X_{k_1, k_2} - X_{k_1, k_2+1}|^2}{|(X_{k_1, k_2} - X_{k_1, k_2+1}) \wedge (X_{k_1+1, k_2} - X_{k_1, k_2+1})|^2}} - 1 \\ & \quad \times \left( \frac{|X_{k_1+1, k_2} - X_{k_1, k_2+1}|^2 |X_{k_1, k_2} - X_{k_1, k_2+1}|^2}{|(X_{k_1, k_2} - X_{k_1, k_2+1}) \wedge (X_{k_1+1, k_2} - X_{k_1, k_2+1})|^2} + 2 \right) \\ &+ \frac{1}{192} |X_{k_1, k_2+1} - X_{k_1, k_2}|^4 \sqrt{\frac{|X_{k_1, k_2+1} - X_{k_1+1, k_2}|^2 |X_{k_1, k_2} - X_{k_1+1, k_2}|^2}{|(X_{k_1, k_2} - X_{k_1+1, k_2}) \wedge (X_{k_1, k_2+1} - X_{k_1+1, k_2})|^2}} - 1 \\ & \quad \times \left( \frac{|X_{k_1, k_2+1} - X_{k_1+1, k_2}|^2 |X_{k_1, k_2} - X_{k_1+1, k_2}|^2}{|(X_{k_1, k_2} - X_{k_1+1, k_2}) \wedge (X_{k_1, k_2+1} - X_{k_1+1, k_2})|^2} + 2 \right). \end{aligned} \tag{2.1}$$

The total contribution of the integral on the Voronoi cell

$$\int_{V(X(\epsilon(k_1 e_1 + k_2 e_2))), \mathcal{X}_\epsilon} |y - X(\epsilon(k_1 e_1 + k_2 e_2))|^2 dy$$

is therefore the sum of 6 terms analogous to the right hand side of (2.1).

### 3. The continuous functional $\mathcal{F}$

In order to derive the formula for the continuous function  $\mathcal{F}$ , we need to replace the finite differences appearing on the right hand side of (2.1) with (partial) derivatives of the deformation, i.e. of the map  $X$ . This is done by using Taylor’s formula, and we arrive at the leading order term in the form:

$$\begin{aligned} & \int_{AOK} |\vec{A}y|^2 dy + \int_{AOJ} |\vec{A}y|^2 dy \\ & \sim \frac{1}{192} \epsilon^4 |e_1 \cdot \nabla X(A)|^4 \sqrt{\frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_2 \cdot \nabla X(A)|^2}{|(-e_2 \cdot \nabla X(A)) \wedge ((e_1 - e_2) \cdot \nabla X(A))|^2}} - 1 \\ & \quad \times \left( \frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_2 \cdot \nabla X(A)|^2}{|(-e_2 \cdot \nabla X(A)) \wedge ((e_1 - e_2) \cdot \nabla X(A))|^2} + 2 \right) \\ &+ \frac{1}{192} \epsilon^4 |e_2 \cdot \nabla X(A)|^4 \sqrt{\frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_1 \cdot \nabla X(A)|^2}{|(-e_1 \cdot \nabla X(A)) \wedge ((e_2 - e_1) \cdot \nabla X(A))|^2}} - 1 \\ & \quad \times \left( \frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_1 \cdot \nabla X(A)|^2}{|(-e_1 \cdot \nabla X(A)) \wedge ((e_2 - e_1) \cdot \nabla X(A))|^2} + 2 \right). \end{aligned}$$

It can be simplified as

$$\begin{aligned}
 & \int_{AOK} |\vec{A}y|^2 dy + \int_{AOJ} |\vec{A}y|^2 dy \\
 & \sim \frac{1}{192} \epsilon^4 |e_1 \cdot \nabla X(A)|^4 \sqrt{\frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_2 \cdot \nabla X(A)|^2}{|(e_1 \cdot \nabla X(A)) \wedge (e_2 \cdot \nabla X(A))|^2} - 1} \\
 & \quad \times \left( \frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_2 \cdot \nabla X(A)|^2}{|(e_1 \cdot \nabla X(A)) \wedge (e_2 \cdot \nabla X(A))|^2} + 2 \right) \\
 & + \frac{1}{192} \epsilon^4 |e_2 \cdot \nabla X(A)|^4 \sqrt{\frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_1 \cdot \nabla X(A)|^2}{|(e_2 \cdot \nabla X(A)) \wedge (e_1 \cdot \nabla X(A))|^2} - 1} \\
 & \quad \times \left( \frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_1 \cdot \nabla X(A)|^2}{|(e_2 \cdot \nabla X(A)) \wedge (e_1 \cdot \nabla X(A))|^2} + 2 \right),
 \end{aligned}$$

as  $\epsilon \rightarrow 0$ . This can be recast as follows:

$$\begin{aligned}
 & \int_{AOK} |\vec{A}y|^2 dy + \int_{AOJ} |\vec{A}y|^2 dy \\
 & \sim \frac{1}{192} \epsilon^4 |e_1 \cdot \nabla X(A)|^4 \sqrt{\frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_2 \cdot \nabla X(A)|^2}{\frac{3}{4} |JX(A)|^2} - 1} \\
 & \quad \times \left( \frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_2 \cdot \nabla X(A)|^2}{\frac{3}{4} |JX(A)|^2} + 2 \right) \\
 & + \frac{1}{192} \epsilon^4 |e_2 \cdot \nabla X(A)|^4 \sqrt{\frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_1 \cdot \nabla X(A)|^2}{\frac{3}{4} |JX(A)|^2} - 1} \\
 & \quad \times \left( \frac{|(e_1 - e_2) \cdot \nabla X(A)|^2 |e_1 \cdot \nabla X(A)|^2}{\frac{3}{4} |JX(A)|^2} + 2 \right)
 \end{aligned}$$

as  $\epsilon \rightarrow 0$ , with the notation  $JX := \det(\nabla X)$ .

The total contribution of the Voronoi cell centered in  $A$  is the sum of the latter term, plus 5 analogous contributions obtained by transforming the 3 unit vectors  $e_{12} := e_1 - e_2, e_1, e_2$  in their images under the action of the cyclic group generated by the rotation of  $\frac{\pi}{3}$ .

Since each term is invariant by the symmetry centered in  $A$ , we find that:

$$\begin{aligned}
 & \int_{V(X(\epsilon(k_1 e_1 + k_2 e_2)), \mathcal{X}_\epsilon)} |y - X(\epsilon(k_1 e_1 + k_2 e_2))|^2 dy \\
 & \sim \frac{\epsilon^4}{48} |e_1 \cdot \nabla X|^4 \Phi(e_1, \nabla X) (3 + \Phi(e_1, \nabla X)^2) (\epsilon(k_1 e_1 + k_2 e_2)) \\
 & + \frac{\epsilon^4}{48} |e_2 \cdot \nabla X|^4 \Phi(e_2, \nabla X) (3 + \Phi(e_1, \nabla X)^2) (\epsilon(k_1 e_1 + k_2 e_2)) \\
 & + \frac{\epsilon^4}{48} |e_{12} \cdot \nabla X|^4 \Phi(e_{12}, \nabla X) (3 + \Phi(e_1, \nabla X)^2) (\epsilon(k_1 e_1 + k_2 e_2))
 \end{aligned}$$

as  $\epsilon \rightarrow 0$ , where

$$\Phi(e, M) := \sqrt{\frac{|MR e|^2 |M R^T e|^2}{\frac{3}{4} |\det(M)|^2} - 1}, \tag{3.1}$$

and where  $R$  is the rotation of an angle  $\frac{\pi}{3}$ .

Then the computation above can be summarized as follows:

$$\int_{V(X(\epsilon(k_1e_1+k_2e_2))|\mathcal{X}_\epsilon)} |y - X(\epsilon(k_1e_1+k_2e_2))|^2 dy \sim \epsilon^4 F(\nabla X(\epsilon(k_1e_1+k_2e_2)))$$

as  $\epsilon \rightarrow 0$ , where

$$F(M) := \frac{1}{48} \sum_{\omega \in \{e_1, e_2, e_{12}\}} |M\omega|^4 \Phi(\omega, M)(3 + \Phi(\omega, M)^2). \tag{3.2}$$

At this point, we recall that  $X$  satisfies property (a). Therefore for each  $\epsilon = 1/n$  with  $n$  a positive integer, the function

$$y \mapsto \text{dist}(y, \mathcal{X}_\epsilon) \text{ is } \mathcal{L}\text{-periodic.}$$

Indeed

$$\text{dist}(y, \mathcal{X}_\epsilon) = y - X(\epsilon k) \Rightarrow \text{dist}(y, \mathcal{X}_\epsilon) = y + l - X(\epsilon(k + nl)) \geq \text{dist}(y + l, \mathcal{X}_\epsilon)$$

for each  $y \in \mathbf{R}^2$  and each  $l \in \mathcal{L}$ . Repeating the same argument with  $y + l$  and  $-l$  instead of  $y$  and  $l$  shows that

$$\text{dist}(y, \mathcal{X}_\epsilon) \geq \text{dist}(y + l, \mathcal{X}_\epsilon) \geq \text{dist}(y, \mathcal{X}_\epsilon)$$

for each  $y \in \mathbf{R}^2$  and  $l \in \mathcal{L}$ , which is precisely the  $\mathcal{L}$ -periodicity condition.

On the other hand, property (a) implies that  $X(\Pi)$  is a fundamental domain for  $\mathbf{R}^2/\mathcal{L}$ . Indeed

$$X(\Pi + l) = X(\Pi) + l, \quad l \in \mathcal{L}$$

so that

$$\bigcup_{l \in \mathcal{L}} X(\Pi) + l = X\left(\bigcup_{l \in \mathcal{L}} \Pi + l\right) = X(\mathbf{R}^2) = \mathbf{R}^2.$$

On the other hand, since  $X$  is one-to-one,

$$(X(\Pi) + l) \cap X(\Pi) = X(\Pi + l) \cap X(\Pi) = X((\Pi + l) \cap \Pi) \subset X(\partial\Pi)$$

is a set of measure 0.

Finally

$$|X(\Pi)| = 1. \tag{3.3}$$

By property (a), the deformation map

$$Y := X - \text{id} : x \mapsto X(x) - x =: Y(x)$$

is  $\mathcal{L}$ -periodic. We recall the following classical observation.

**Lemma 3.1.** *Let  $Y \in C^1(\mathbf{R}^2; \mathbf{R}^2)$  be  $\mathcal{L}$ -periodic. Then*

$$\int_{\Pi} \det(\nabla Y)(x) dx_1 \wedge dx_2 = 0.$$

**Proof.** If  $Y$  is of class  $C^2$ , one has

$$\det(\nabla Y) dx_1 \wedge dx_2 = d(Y_1 dY_2)$$

where  $Y_1(x)$  and  $Y_2(x)$  are the components of the vector  $Y(x)$ . Then, by Stokes' formula

$$\int_{\Pi} \det(\nabla Y)(x) dx_1 \wedge dx_2 = \int_{\Pi} d(Y_1 dY_2) = \int_{\partial \Pi} Y_1 dY_2 = 0$$

because  $Y$  is  $\mathcal{L}$ -periodic.

If  $Y$  is only of class  $C^1$ , let  $\chi_\alpha$  be a regularizing sequence. Then, for each  $\alpha > 0$ , the map  $\chi_\alpha \star Y =: Y_\alpha \in C^2(\mathbf{R}^2; \mathbf{R}^2)$  is still  $\mathcal{L}$ -periodic and  $\nabla Y_\alpha \rightarrow \nabla Y$  uniformly on  $\Pi$  as  $\alpha \rightarrow 0$ . Therefore

$$\int_{\Pi} \det(\nabla Y)(x) dx_1 \wedge dx_2 = \lim_{\alpha \rightarrow 0} \int_{\Pi} \det(\nabla Y_\alpha)(x) dx_1 \wedge dx_2 = 0. \quad \square$$

Thus

$$|X(\Pi)| = \int_{X(\Pi)} dy = \int_{\Pi} |\det(\nabla X(x))| dx = \int_{\Pi} \det(\nabla X(x)) dx$$

since  $X$  is  $C^1$ -close to the identity (property (b)), and

$$\det(\nabla X) = \det(I + \nabla Y) = 1 + \operatorname{div} Y + \det(\nabla Y).$$

Therefore

$$|X(\Pi)| = \int_{\Pi} (1 + \operatorname{div} Y + \det(\nabla Y))(x) dx_1 \wedge dx_2 = 1 + \int_{\partial \Pi} Y \cdot nds = 1$$

by  $\mathcal{L}$ -periodicity of  $Y$ . This proves (3.3).

Set

$$B_R[\mathcal{L}] := \{l \in \mathcal{L} \text{ s.t. } X(\Pi) + l \subset B(0, R)\},$$

and  $\delta := \operatorname{diam}(X(\Pi))$ . Then

$$B(0, R - \delta) \subset \bigcup_{l \in B_R[\mathcal{L}]} (X(\Pi) + l) \subset B(0, R)$$

and since the sets  $X(\Pi) + l$  are pairwise disjoint (up to sets of measure 0) as  $l \in \mathcal{L}$ , we conclude from (3.3) that

$$\pi(R - \delta)^2 = |B(0, R - \delta)| \leq \#B_R[\mathcal{L}] \leq |B(0, R)| = \pi R^2$$

so that

$$\#B_R[\mathcal{L}] \sim \pi R^2 \quad \text{as } R \rightarrow \infty.$$

Thus

$$\begin{aligned} \#B_R[\mathcal{L}] \int_{X(\Pi)} \operatorname{dist}(y, \mathcal{X}_\epsilon)^2 dy &\leq \int_{B(0, R)} \operatorname{dist}(y, \mathcal{X}_\epsilon)^2 dy \\ &\leq \#B_{R+\delta}[\mathcal{L}] \int_{X(\Pi)} \operatorname{dist}(y, \mathcal{X}_\epsilon)^2 dy, \end{aligned}$$

and hence

$$\frac{1}{\pi R^2} \int_{B(0, R)} \operatorname{dist}(y, \mathcal{X}_\epsilon)^2 dy \rightarrow \int_{X(\Pi)} \operatorname{dist}(y, \mathcal{X}_\epsilon)^2 dy \text{ as } R \rightarrow \infty.$$

Thus

$$\begin{aligned} \lim_{R \rightarrow \infty} \frac{1}{\pi R^2} \int_{B(0,R)} \text{dist}(y, \mathcal{X}_\epsilon)^2 dy &= \int_{X(\Pi)} \text{dist}(y, \mathcal{X}_\epsilon)^2 dy \\ &= \sum_{\epsilon \max(|k_1|, |k_2|) < 1/2} \int_{V(X(\epsilon(k_1 e_1 + k_2 e_2))) | \mathcal{X}_\epsilon} |y - X(\epsilon(k_1 e_1 + k_2 e_2))|^2 dy \\ &\sim \epsilon^2 \int_{\Pi} F(\nabla X(x)) dx \end{aligned}$$

as  $\epsilon \rightarrow 0^+$ .

#### 4. Gradient of the functional $\mathcal{F}$

Henceforth we denote

$$\mathfrak{H}_0 := \left\{ Z \in L^2(\mathbf{R}^2/\mathcal{L}; \mathbf{R}^2) \text{ s.t. } Z \text{ is } \mathcal{L}\text{-periodic and } \int_{\Pi} Z(x) dx = 0 \right\}$$

and

$$\text{id} + \mathfrak{H}_0 := \{ \text{id} + Z \text{ s.t. } Z \in \mathfrak{H}_0 \}.$$

The function  $\mathcal{F}$  is obviously defined on  $(\text{id} + \mathfrak{H}_0) \cap \text{Diff}^1(\mathbf{R}^2)$ , and we seek to compute its  $L^2$ -gradient at each  $X$  in  $\text{Diff}^2(\mathbf{R}^2)$ .

Let  $X \in (\text{id} + \mathfrak{H}_0) \cap \text{Diff}^2(\mathbf{R}^2)$  and  $Y \in \mathfrak{H}_0 \cap C^1(\mathbf{R}^2/\mathcal{L}; \mathbf{R}^2)$ ; by the implicit function theorem, we see that  $X + \tau Y$  is in  $(\text{id} + \mathfrak{H}_0) \cap \text{Diff}^2(\mathbf{R}^2)$  for all  $\tau$  sufficiently small. With the expression for  $\mathcal{F}$  obtained in [Theorem 1.1](#), one anticipates that

$$\begin{aligned} \frac{d}{d\tau} \mathcal{F}(X + \tau Y)|_{\tau=0} &= \int_{\Pi} \nabla F(\nabla_x X(x)) \cdot \nabla_x Y(x) dx \\ &= - \int_{\Pi} \text{div}_x(\nabla F(\nabla_x X(x))) \cdot Y(x) dx. \end{aligned} \tag{4.1}$$

In order to verify the second equality above, one only needs to check that  $F$  is of class  $C^2$  on the set of invertible matrices. Notice indeed that the boundary term coming from Green’s formula satisfies

$$\int_{\partial \Pi} \nabla F(\nabla_x X(x)) \cdot Y(x) \otimes n_x ds(x) = 0$$

because  $\nabla_x X(x) = I + \nabla_x Z$  and  $Y$  are both  $\mathcal{L}$ -periodic, while  $n_x$  takes opposite values on segments in  $\partial \Pi$  that are symmetric with respect to the center of  $\Pi$ . That  $F$  is of class  $C^2$  on a neighborhood of  $I$  in  $GL_2(\mathbf{R})$  follows from [\(3.2\)](#). Indeed,  $\det(M) \neq 0$  for all  $M \in GL_2(\mathbf{R})$ , and one has

$$\Phi(e, M)^2 \rightarrow \Phi(e, I) = \frac{1}{3} \quad \text{for all unit vector } e \text{ as } M \rightarrow I.$$

By continuity, there exists an open neighborhood  $\Omega$  of  $I$  in  $GL_2(\mathbf{R})$  such that

$$\Phi(e, M)^2 > \frac{1}{4} \quad \text{for all } (e, M) \in \mathbf{S}^2 \times \Omega.$$

Therefore  $\Phi(e, \cdot)$  is of class  $C^2$  on  $\Omega$  for each unit vector  $e$ , and therefore  $F$  is of class  $C^2$  on  $\Omega$ .

Next we compute  $\nabla F$ . The first step is to compute the directional derivative of  $M \mapsto \Phi(e, M)$  at  $M \in GL_2(\mathbf{R})$  along the direction  $N \in M_2(\mathbf{R})$ . We find that

$$\frac{d}{d\tau} \Phi(e, M + \tau N)|_{\tau=0} = \frac{1}{2\Phi(e, M)} \left[ \frac{2(NRe|MR e)|MR^T e|^2}{\frac{3}{4} \det(M)^2} + \frac{2(NR^T e|MR^T e)|MR e|^2}{\frac{3}{4} \det(M)^2} - \frac{2|MR e|^2|MR^T e|^2 \det(M) \operatorname{trace}(M^{-1}N)}{\frac{3}{4} \det(M)^3} \right].$$

Recalling that

$$(Nu|v) = \operatorname{trace}(N(u \otimes v)), \quad u, v \in \mathbf{R}^2, \quad N \in M_2(\mathbf{R}),$$

and

$$\frac{d}{d\tau} \det(M + \tau N)|_{\tau=0} = \det(M) \operatorname{trace}(M^{-1}N), \quad M \in GL_2(\mathbf{R}), \quad N \in M_2(\mathbf{R}),$$

we obtain

$$\frac{d}{d\tau} \Phi(e, M + \tau N)|_{\tau=0} = \frac{4}{3\Phi(e, M) \det(M)^2} \left[ \operatorname{trace}[N(Re \otimes MR e)]|MR^T e|^2 + \operatorname{trace}[N(R^T e \otimes MR^T e)]|MR e|^2 - |MR e|^2|MR^T e|^2 \operatorname{trace}(M^{-1}N) \right].$$

Defining

$$A(e, M) := \frac{(Re \otimes MR e)}{|MR e|^2} + \frac{(R^T e \otimes MR^T e)}{|MR^T e|^2} - M^{-1}, \tag{4.2}$$

we see that the map  $M \mapsto A(e, M)$  is a tensor-field on  $GL_2(\mathbf{R})$ , homogeneous of degree  $-1$  with respect to  $M$ . The differential of  $M \mapsto \Phi(e, M)$  can be easily expressed in terms of  $A$ : multiplying and dividing each term of the latter equality by  $\Phi(e, M)^2 + 1$ , we get

$$d_M \Phi(e, M)[N] = \frac{\Phi(e, M)^2 + 1}{\Phi(e, M)} \operatorname{trace}(A(e, M)N).$$

In other words, considering the Frobenius inner product defined on  $M_2(\mathbf{R})$  by

$$(M_1|M_2) = \operatorname{trace}(M_1^T M_2),$$

the gradient of the map  $M \mapsto \Phi(e, M)$  at the point  $M \in GL_2(\mathbf{R})$  is

$$\nabla_M \Phi(e, M) = \frac{\Phi(e, M)^2 + 1}{\Phi(e, M)} A(e, M)^T.$$

Therefore

$$48 \nabla F(M) = 4 \sum_{\omega \in \{e_1, e_2, e_{12}\}} |M\omega|^2 \Phi(\omega, M) (3 + \Phi(\omega, M)^2) \omega \otimes (M\omega) + 3 \sum_{\omega \in \{e_1, e_2, e_{12}\}} |M\omega|^4 \frac{(1 + \Phi(\omega, M)^2)^2}{\Phi(\omega, M)} A(\omega, M)^T.$$

Inserting this expression in (4.1), we find that

$$\begin{aligned} \frac{d}{d\tau} \mathcal{F}(X + \tau Y)|_{\tau=0} &= -\frac{1}{12} \sum_{\omega \in \{e_1, e_2, e_{12}\}} \int_{\Pi} \operatorname{div}_x (|\omega \cdot \nabla X|^2 (3 + \Phi^2) \Phi(\omega, \nabla X) (\omega \cdot \nabla X) \otimes \omega) \cdot Y dx \\ &\quad - \frac{1}{16} \sum_{\omega \in \{e_1, e_2, e_{12}\}} \int_{\Pi} \operatorname{div}_x \left( |\omega \cdot \nabla X|^4 \frac{(1 + \Phi(\omega, \nabla X)^2)^2}{\Phi(\omega, \nabla X)} A(\omega, \nabla X) \right) \cdot Y dx. \end{aligned}$$

In other words, the  $L^2$ -gradient of  $\mathcal{F}$  is given by the formula

$$\begin{aligned} \frac{\delta \mathcal{F}(X)}{\delta X(x)} &= -\operatorname{div}_x(\nabla F(\nabla_x X(x))) \\ &= -\frac{1}{12} \sum_{\omega \in \{e_1, e_2, e_{12}\}} \operatorname{div}_x(|\omega \cdot \nabla X|^2(3 + \Phi^2)\Phi(\omega, \nabla X)\omega \otimes (\omega \cdot \nabla X)) \\ &\quad - \frac{1}{16} \sum_{\omega \in \{e_1, e_2, e_{12}\}} \operatorname{div}_x\left(|\omega \cdot \nabla X|^4 \frac{(1 + \Phi(\omega, \nabla X))^2}{\Phi(\omega, \nabla X)} A(\omega, \nabla X)^T\right). \end{aligned} \tag{4.3}$$

Its  $i$ -th coordinate is given by the expression

$$\begin{aligned} \frac{\delta \mathcal{F}(X)}{\delta X_i(x)} &= -\frac{1}{12} \sum_{\omega \in \{e_1, e_2, e_{12}\}} \partial_j(|\omega \cdot \nabla X|^2(3 + \Phi^2)\Phi(\omega, \nabla X)\omega_j \omega_k \partial_k X_i) \\ &\quad - \frac{1}{16} \sum_{\omega \in \{e_1, e_2, e_{12}\}} \partial_j\left(|\omega \cdot \nabla X|^4 \frac{(1 + \Phi(\omega, \nabla X))^2}{\Phi(\omega, \nabla X)} A_{ji}(\omega, \nabla X)\right), \end{aligned} \tag{4.4}$$

with the usual convention of summation on repeated indices.

### 5. The asymptotic energy functional for a slightly deformed hexagonal lattice

In this section we study the functional  $\mathcal{F}(X)$  near  $X = \operatorname{id}$ . More precisely, we seek a rational expression of  $F(M)$  (with  $F$  defined by (3.2)) for  $M \in GL_2(\mathbf{R})$  near  $I$ . In view of Theorem 1.1, this gives a simplified expression of  $\mathcal{F}(X)$  near  $X = \operatorname{id}$ .

Let

$$M_1 = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

be a near-identity matrix. Straightforward computations show that

$$\Phi(e_1, M_1) = \frac{1}{2\sqrt{3}} \sqrt{\frac{(\alpha^2 - 3\beta^2 + \gamma^2 - 3\delta^2)^2}{(\beta\gamma - \alpha\delta)^2}} = \frac{-\alpha^2 + 3\beta^2 - \gamma^2 + 3\delta^2}{2\sqrt{3}(\alpha\delta - \beta\gamma)}. \tag{5.1}$$

Indeed, since  $|M_1 - I| \ll 1$ , one has  $\alpha^2 - 3\beta^2 + \gamma^2 - 3\delta^2 < 0$ .

Next, we observe that

$$\begin{aligned} \Phi(Re, M) &= \sqrt{\frac{|MR^2e|^2|Me|^2}{\frac{3}{4}|\det(M)|^2} - 1} \\ &= \sqrt{\frac{|R^TMR^2e|^2|R^TMRRTe|^2}{\frac{3}{4}|\det(R^TMR)|^2} - 1} = \Phi(e, R^TMR) \end{aligned}$$

for each  $M \in GL_2(\mathbf{R})$  and each unit vector  $e$ . Indeed, the second equality above follows from the obvious identity  $|R\xi| = |R^T\xi| = |\xi|$  for all  $\xi \in \mathbf{R}^2$  since  $R$  is a rotation. Therefore

$$\begin{aligned} \Phi(e_2, M_1) &= \Phi(e_1, M_2) \quad \text{with } M_2 = R^T M_1 R \\ \Phi(e_{12}, M_1) &= \Phi(e_1, M_{12}) \quad \text{with } M_{12} = R M_1 R^T \end{aligned} \tag{5.2}$$

since  $e_2 = Re_1$  and  $e_{12} = R^T e_1$ .

Elementary computations show that

$$M_2 = \frac{1}{4} \begin{pmatrix} \alpha + \sqrt{3}\gamma + \sqrt{3}\beta + 3\delta & -\sqrt{3}\alpha - 3\gamma + \beta + \sqrt{3}\delta \\ -\sqrt{3}\alpha + \gamma - 3\beta + \sqrt{3}\delta & 3\alpha - \sqrt{3}\gamma - \sqrt{3}\beta + \delta \end{pmatrix}$$

and

$$M_{12} = \frac{1}{4} \begin{pmatrix} \alpha - \sqrt{3}\gamma - \sqrt{3}\beta + 3\delta & \sqrt{3}\alpha - 3\gamma + \beta - \sqrt{3}\delta \\ \sqrt{3}\alpha + \gamma - 3\beta - \sqrt{3}\delta & 3\alpha + \sqrt{3}\gamma + \sqrt{3}\beta + \delta \end{pmatrix}$$

Notice that

$$|M_1 - I| \ll 1 \Rightarrow |M_2 - I| = |R^T(M_1 - I)R| \ll 1 \text{ and } |M_{12} - I| = |R(M_1 - I)R^T| \ll 1.$$

Hence we can use formula (5.1) to compute  $\Phi(e_2, M_1)$  and  $\Phi(e_{12}, M_1)$  with the help of and (5.2). We find that

$$\Phi(M_1, e_2) = \frac{\sqrt{3}\alpha^2 - 3\alpha\beta + \sqrt{3}\gamma^2 - 3\gamma\delta}{3(\alpha\delta - \beta\gamma)}, \tag{5.3}$$

and

$$\Phi(M_1, e_{12}) = \frac{\sqrt{3}\alpha^2 + 3\alpha\beta + \sqrt{3}\gamma^2 + 3\gamma\delta}{3(\alpha\delta - \beta\gamma)}. \tag{5.4}$$

Finally, we insert the expressions found in (5.1), (5.3) and (5.4) in formula (3.2), and find that

$$F(M_1) = \frac{1}{96\sqrt{3}} \frac{P(\alpha, \beta, \gamma, \delta)}{\alpha\delta - \beta\gamma} \tag{5.5}$$

where

$$\begin{aligned} P(\alpha, \beta, \gamma, \delta) = & -\alpha^6 + 6\alpha^4\beta^2 - 9\alpha^2\beta^4 - 3\alpha^4\gamma^2 \\ & + 18\alpha^2\beta^2\gamma^2 + 9\beta^4\gamma^2 - 3\alpha^2\gamma^4 + 12\beta^2\gamma^4 - \gamma^6 - 12\alpha^3\beta\gamma\delta \\ & - 36\alpha\beta^3\gamma\delta - 12\alpha\beta\gamma^3\delta + 12\alpha^4\delta^2 + 18\alpha^2\gamma^2\delta^2 \\ & + 6\gamma^4\delta^2 - 36\alpha\beta\gamma\delta^3 + 9\alpha^2\delta^4 - 9\gamma^2\delta^4. \end{aligned} \tag{5.6}$$

We shall simplify this expression, and more precisely give an intrinsic formula for the polynomial  $P$ . Set

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Elementary (although tedious) computations show that

$$P(\alpha, \beta, \gamma, \delta) = \frac{1}{2}(Q_+(\alpha, \beta, \gamma, \delta) + Q_-(\alpha, \beta, \gamma, \delta))$$

with

$$\begin{aligned} Q_+(\alpha, \beta, \gamma, \delta) & := (\alpha^2 + \beta^2 + \gamma^2 + \delta^2) \left( 24(\alpha\delta - \beta\gamma)^2 - (\alpha^2 + \beta^2 + \gamma^2 + \delta^2)^2 \right), \\ Q_-(\alpha, \beta, \gamma, \delta) & := (\alpha^2 - \beta^2 + \gamma^2 - \delta^2) \left( 12(\alpha\beta + \gamma\delta)^2 - (\alpha^2 - \beta^2 + \gamma^2 - \delta^2)^2 \right). \end{aligned}$$

One has

$$\begin{aligned} (\alpha^2 + \beta^2 + \gamma^2 + \delta^2) & = \text{trace}(M_1^T M_1), \\ (\alpha^2 - \beta^2 + \gamma^2 - \delta^2) & = \text{trace}(M_1^T M_1 S), \end{aligned}$$

while

$$\begin{aligned} (\alpha\beta + \gamma\delta)^2 & = (\alpha^2 + \gamma^2)(\beta^2 + \delta^2) - (\alpha\delta - \beta\gamma)^2 \\ & = \text{trace}(M_1^T M_1 \frac{I+S}{2}) \text{trace}(M_1^T M_1 \frac{I-S}{2}) - \det(M_1)^2 \\ & = \frac{1}{4} \left( \text{trace}(M_1^T M_1)^2 - \text{trace}(M_1^T M_1 S)^2 \right) - \det(M_1)^2. \end{aligned}$$

Therefore

$$\begin{aligned} P(\alpha, \beta, \gamma, \delta) & = 6 \det(M_1)^2 \text{trace}(M_1^T M_1 (2I - S)) \\ & \quad + \frac{3}{2} \text{trace}(M_1^T M_1)^2 \text{trace}(M_1^T M_1 S) \\ & \quad - \frac{1}{2} \text{trace}(M_1^T M_1)^3 - 2 \text{trace}(M_1^T M_1 S)^3. \end{aligned}$$

Hence

$$\begin{aligned}
 F(M_1) &= \frac{1}{16\sqrt{3}} \det(M_1) \operatorname{trace}(M_1^T M_1 (2I - S)) \\
 &\quad + \frac{1}{64\sqrt{3}} \frac{\operatorname{trace}(M_1^T M_1)^2 \operatorname{trace}(M_1^T M_1 S)}{\det(M_1)} \\
 &\quad - \frac{1}{192\sqrt{3}} \frac{\operatorname{trace}(M_1^T M_1)^3}{\det(M_1)} - \frac{1}{48\sqrt{3}} \frac{\operatorname{trace}(M_1^T M_1 S)^3}{\det(M_1)}.
 \end{aligned}$$

We finally compute the Taylor expansion of  $48F$  at order 3 near the identity matrix. Setting

$$N = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

we find that

$$\begin{aligned}
 48F(I + \epsilon N) &= \frac{10}{\sqrt{3}} + \frac{20}{\sqrt{3}} \epsilon (a + d) \\
 &\quad + \frac{1}{\sqrt{3}} \epsilon^2 (13a^2 + 3b^2 - 14bc + 3c^2 + 34ad + 13d^2) \\
 &\quad + \frac{1}{\sqrt{3}} \epsilon^3 (a^3 + 9ab^2 - 2abc + 9ac^2 + 23a^2d - 3b^2d - 26bcd - 3c^2d + 11ad^2 + 5d^3) \\
 &\quad + O(\epsilon^4)
 \end{aligned} \tag{5.7}$$

It is interesting to notice that the Taylor expansion of  $F$  around the identity matrix is invariant under the substitutions  $a \leftrightarrow d$  and  $b \leftrightarrow c$  only up to second order. More precisely

$$48F(I + \epsilon N) = \frac{10}{\sqrt{3}} + \frac{20}{\sqrt{3}} \epsilon \operatorname{trace}(N) + \frac{1}{\sqrt{3}} \epsilon^2 \left( 14 \det(N) + 10 \operatorname{trace}(N)^2 + 3 \operatorname{trace}(N^T N) \right) + O(\epsilon^3). \tag{5.8}$$

### 6. Stability and asymptotic convergence for small perturbations

In this section we use a perturbative approach to study stability properties of the energy functional  $\mathcal{F}(X)$  around the identity.

Following formula (4.1), we consider the PDE defining the gradient flow of  $\mathcal{F}$  in the form

$$\partial_t X(t, x) = \operatorname{div}_x (\nabla F(\nabla_x X(t, x))), \quad X(0, x) = X^{in}(x). \tag{6.1}$$

We assume that  $X^{in}$  satisfies properties (a–c), and we seek a (weak) solution of the Cauchy problem (6.1) such that  $X(t, \cdot) \in \operatorname{Diff}^1(\mathbf{R}^2)$  satisfies (properties (a–c) for all  $t \geq 0$ ). In particular, property (c) is preserved by the evolution of (6.1) since the system of PDEs governing  $X$  is in divergence form.

Therefore, we henceforth seek  $X$  of the form

$$X(t, x) = x + \epsilon Y(t, x)$$

with  $0 < \epsilon \ll 1$ , and property (a) implies that  $Y(t, \cdot)$  is a  $\mathcal{L}$ -periodic map from  $\mathbf{R}^2$  to itself.

*Step 1: Convexification of the problem.*

Define the function  $F_0$  on  $GL_2(\mathbf{R})$  as follows:

$$F_0(M) := F(M) - \frac{5}{12\sqrt{3}} \operatorname{trace}(M - I) - \frac{7}{24\sqrt{3}} \det(M - I). \tag{6.2}$$

Thus

$$F(I + \epsilon \nabla_x Y) = F_0(I + \epsilon \nabla_x Y) + \frac{5}{12\sqrt{3}} \epsilon \operatorname{div}_x(Y) + \frac{7}{24\sqrt{3}} \epsilon^2 \det(\nabla_x Y).$$

Therefore

$$\mathcal{F}(\operatorname{id} + \epsilon Y) = \int_{\Pi} F(I + \epsilon \nabla_x Y(x)) dx = \int_{\Pi} F_0(I + \epsilon \nabla_x Y(x)) dx$$

since

$$\int_{\Pi} \operatorname{div}_x(Y)(x)dx = 0 \quad \text{and} \quad \int_{\Pi} \det(\nabla_x Y(x))dx = 0.$$

The first equality is obvious since  $Y$  is  $\mathcal{L}$ -periodic, while the second follows from [Lemma 3.1](#).

With formula [\(5.8\)](#), we see that

$$F_0(I + \epsilon N) = \frac{5}{24\sqrt{3}} + \frac{5}{24\sqrt{3}}\epsilon^2 \operatorname{trace}(N)^2 + \frac{1}{16\sqrt{3}}\epsilon^2 \operatorname{trace}(N^T N) + O(\epsilon^3). \tag{6.3}$$

Formula [\(6.2\)](#) shows that  $F_0 \in C^\infty(GL_2(\mathbf{R}))$  since  $F \in C^\infty(GL_2(\mathbf{R}))$ . Then, formula [\(6.3\)](#) implies that

$$\nabla^2 F_0(I) \cdot (N, N) \geq \frac{1}{8\sqrt{3}} \operatorname{trace}(N^T N). \tag{6.4}$$

Henceforth we denote by  $\|\cdot\|_2$  the Frobenius norm on  $M_2(\mathbf{R})$ , defined by the formula

$$\|A\|_2 = \operatorname{trace}(A^T A)^{1/2}.$$

The inequality [\(6.4\)](#) implies that there exists three positive constants  $0 < \lambda \leq \Lambda$  and  $\rho_0$  such that

$$\lambda \|N\|_2^2 \leq \nabla^2 F_0(A) \cdot (N, N) \leq \Lambda \|N\|_2^2, \quad \text{for all } A \text{ such that } \|A - I\|_2 < \rho_0 \tag{6.5}$$

Choose  $G \in C^2(M_2(\mathbf{R}))$  such that

$$\|A - I\|_2 < \rho_0/2 \Rightarrow G(A) = F_0(A)$$

while

$$\frac{1}{2}\lambda \|N\|_2^2 \leq \nabla^2 G(A) \cdot (N, N) \leq 2\Lambda \|N\|_2^2 \quad \text{for all } A, N \in M_2(\mathbf{R}). \tag{6.6}$$

Instead of [\(6.1\)](#), consider the Cauchy problem

$$\partial_t X(t, x) = \operatorname{div}_x(\nabla G(\nabla_x X(t, x))), \quad X(0, x) = X^{in}(x). \tag{6.7}$$

Let  $X$  be the solution of this Cauchy problem.

For instance, one can apply Theorem 3.2 of [\[4\]](#) to the convex function  $\mathcal{G}$  defined on the Hilbert space  $L^2(\Pi; \mathbf{R}^2)$  by the formula

$$\mathcal{G}(X) = \begin{cases} \int_{\Pi} G(\nabla_x X(x))dx & \text{if } X \in \mathcal{V}, \\ +\infty & \text{if } X \notin \mathcal{V}, \end{cases}$$

where

$$\mathcal{V} := \left\{ X = \operatorname{Id}_{\Pi} + Y|_{\Pi}, \quad Y \in H^1(\mathbf{R}^2/\mathcal{L}; \mathbf{R}^2) \text{ s.t. } \int_{\Pi} Y(x)dx = 0 \right\}.$$

Indeed [\(6.6\)](#) and the fact that  $\nabla F_0(I) = 0$  (which follows from [\(6.3\)](#)) imply that

$$F_0(I) + \frac{1}{4}\lambda \|A - I\|_2^2 \leq G(A) \leq F_0(I) + \Lambda \|A - I\|_2^2,$$

so that

$$\int_{\Pi} G(\nabla_x X(x))dx < \infty \text{ implies } \nabla_x X \in L^2(\Pi; M_2(\mathbf{R})).$$

*Step 2: Stability in  $L^2$ .*

Multiplying both sides of [\(6.1\)](#) by  $X(t, x) - x$  and integrating over  $\Pi$ , one finds that

$$\frac{d}{dt} \frac{1}{2} \int_{\Pi} |X(t, x) - x|^2 dx = - \int_{\Pi} \operatorname{trace}(\nabla G(\nabla_x X(t, x))^T (\nabla_x X(t, x) - I)) dx.$$

Since  $\nabla G(I) = \nabla F_0(I) = 0$  (by (6.3), for each  $M \in M_2(\mathbf{R})$ , one has

$$\begin{aligned} \text{trace}(\nabla G(M)^T(M - I)) &= \text{trace}((\nabla G(M)^T - \nabla G(I)^T)(M - I)) \\ &= \int_0^1 \frac{d}{ds} \text{trace}(\nabla G(I + s(M - I))^T(M - I)) ds \\ &= \int_0^1 \nabla^2 G(I + s(M - I)) \cdot (M - I, M - I) ds \\ &\geq \frac{1}{2} \lambda \|M - I\|_2^2. \end{aligned}$$

Hence

$$\frac{d}{dt} \int_{\Pi} |X(t, x) - x|^2 dx \leq -\lambda \int_{\Pi} \|\nabla_x X(t, x) - I\|_2^2 dx.$$

Since  $x \mapsto X(t, x) - x$  is  $\mathcal{L}$ -periodic by property (a), we deduce from the Poincaré–Wirtinger inequality that

$$C_P \int_{\Pi} |X(t, x) - x|^2 dx \leq \int_{\Pi} \|\nabla_x X(t, x) - I\|_2^2 dx$$

(denoting by  $C_P > 0$  the best constant in the Poincaré–Wirtinger inequality). Therefore

$$\frac{d}{dt} \int_{\Pi} |X(t, x) - x|^2 dx \leq -\lambda C_P \int_{\Pi} |X(t, x) - x|^2 dx,$$

so that

$$\int_{\Pi} |X(t, x) - x|^2 dx \leq e^{-C_P \lambda t} \int_{\Pi} |X^{in} - x|^2 dx. \tag{6.8}$$

*Step 3: Uniform stability.*

Next we prove that the solution  $X$  of the Cauchy problem (6.7) remains close enough to the identity map. This implies the existence and uniqueness for the gradient flow of  $\mathcal{F}$  for initial data sufficiently close to the identity. Indeed, for such initial data, the gradient flow of  $\mathcal{F}$  coincides with the gradient flow of  $\mathcal{G}$ , which is known to exist and be unique since  $G$  is  $C^2$  and uniformly convex. (See Step 1 above for the existence and uniqueness theory for the gradient flow of  $\mathcal{G}$ .)

Assume that

$$\|X^{in} - \text{id}\|_{W^{\sigma,p}(\Pi)} \leq \epsilon_0$$

with  $p > 2$  and  $1 + 2/p < \sigma < 2$ .

**Short time estimate.** By the Theorem on page 192 in [1], there exists  $t_0 > 0$  such that the solution  $X$  of the Cauchy problem (6.7) satisfies<sup>1</sup>

$$\|X(t, \cdot) - \text{id}\|_{W^{\sigma,p}(\Pi)} \leq 2\epsilon_0 \quad \text{for all } t \in [0, t_0].$$

Since  $(\sigma - 1)p > 2$ , by Sobolev embedding on the 2-dimensional torus  $\Pi$  one has

$$\|X(t, \cdot) - \text{id}\|_{C^{1,\alpha}(\Pi)} \leq C\epsilon_0 \quad \text{for all } t \in [0, t_0], \tag{6.9}$$

for some positive  $\alpha \equiv \alpha(\sigma, p)$  and  $C \equiv C(\alpha, \sigma, p)$ .

<sup>1</sup> Theorem on page 192 in [1] considers solutions in bounded domains. However, this result is based on abstract results on evolution equations that apply also to the periodic case.

Local estimate for positive times. Next pick  $0 < t_1 \leq t_0/2$ , and consider the point  $(\bar{x}, \bar{t})$  with  $\bar{t} \geq t_0$ , together with the parabolic cylinder

$$Q_{t_1}(\bar{x}, \bar{t}) := \{(x, t) \in \Pi \times \mathbf{R} \text{ s.t. } t \in [\bar{t} - t_1, \bar{t}] \text{ and } |x - \bar{x}| \leq \sqrt{t_1}\}.$$

Let us now compute

$$\int_{Q_{t_1}(\bar{x}, \bar{t})} |X(t, x) - x|^2 dx dt \leq \int_{\bar{t}-t_1}^{\bar{t}} \int_{\Pi} |X(t, x) - x|^2 dx dt.$$

By (6.8)

$$\begin{aligned} \int_{\bar{t}-t_1}^{\bar{t}} \int_{\Pi} |X(t, x) - x|^2 dx dt &\leq \int_{\bar{t}-t_1}^{\bar{t}} e^{-C_P \lambda t} \int_{\Pi} |X^{in}(x) - x|^2 dx dt \\ &\leq \frac{1}{C_P \lambda} \|X^{in} - \text{id}\|_{L^2(\Pi)}^2. \end{aligned}$$

In particular,

$$\frac{1}{|Q_{t_1}(\bar{x}, \bar{t})|} \int_{Q_{t_1}(\bar{x}, \bar{t})} |X(t, x) - x|^2 dx dt \leq \frac{1}{C_P \lambda \pi t_1^2} \|X^{in} - \text{id}\|_{L^2(\Pi)}^2.$$

Thus, in the parabolic cylinder  $Q_{t_1}(\bar{x}, \bar{t})$ , the map  $X$  is  $L^2$ -close to the identity map, and we seek to improve this result into a similar statement with the  $C^{1,\alpha}$  instead of  $L^2$  topology. This is done by appealing to the local regularity theory of parabolic equations. Specifically, we apply the A-caloric approximation argument in [9], especially Lemma 7.3 in that reference.

Pick any point  $(\hat{x}, \hat{t}) \in Q_{t_0/2}(\bar{x}, \bar{t})$ . At this point, and throughout the next paragraph, we adopt the notation of [9, Lemma 7.3].

Set  $M = 3$  and  $\rho = t_1$ . First, we assume that  $0 < t_1 \leq \min(t_0/2, \rho_0(M))$ , where  $\rho_0(M)$  is defined in formula (7.12) in [9]. Hence assumption (ii) in [9, Lemma 7.3] is satisfied. Next we deduce from the formulas on p. 711 in [9] that

$$\begin{aligned} |D\ell_\rho| &= \left| \frac{4}{t_1^2 |Q_{t_1}(\bar{x}, \bar{t})|} \int_{Q_{t_1}(\bar{x}, \bar{t})} X(t, x) \otimes (x - \hat{x}) dx dt \right| \\ &\leq \left| \frac{4}{t_1^2 |Q_{t_1}(\bar{x}, \bar{t})|} \int_{Q_{t_1}(\bar{x}, \bar{t})} (X(t, x) - x) \otimes (x - \hat{x}) dx dt \right| \\ &\quad + \left| \frac{4}{t_1^2 |Q_{t_1}(\bar{x}, \bar{t})|} \int_{Q_{t_1}(\bar{x}, \bar{t})} x \otimes (x - \hat{x}) dx dt \right| \\ &\leq \frac{4}{t_1^2} \left( \frac{\epsilon_1}{\sqrt{C_P \lambda \pi t_1}} t_1 + \frac{1}{2} t_1^2 \right) = \frac{4\epsilon_1}{\sqrt{C_P \lambda \pi t_1^2}} + 2 \leq M \end{aligned}$$

(where the penultimate inequality follows from the Cauchy–Schwarz inequality) provided that

$$\|X^{in} - \text{id}\|_{L^2(\Pi)} \leq \epsilon_1 \leq \min(\epsilon_0, \frac{1}{4} \sqrt{C_P \lambda \pi t_1^2}).$$

Choosing  $\epsilon_1$  in this way implies that condition (i) in [9, Lemma 7.3] is satisfied (see Remark 7.4 following the proof of Lemma 7.3 in [9]). Reducing  $\epsilon_1$  and  $t_1$  if needed, we can also satisfy

$$\begin{aligned} \tilde{\Psi}_2(\rho) &\leq \frac{1}{t_1^2 |\mathcal{Q}_{t_1}(\bar{x}, \bar{t})|} \int_{\mathcal{Q}_{t_1}(\bar{x}, \bar{t})} |X(t, x) - \ell_{\rho, (\hat{x}, \hat{t})}(x)|^2 dx dt + t_1^{2\beta} \\ &\leq \frac{1}{t_1^2 |\mathcal{Q}_{t_1}(\bar{x}, \bar{t})|} \int_{\mathcal{Q}_{t_1}(\bar{x}, \bar{t})} |X(t, x) - x|^2 dx dt + t_1^{2\beta} \\ &\leq \frac{\epsilon_1^2}{C_P \lambda \pi t_1^4} \|X^{in} - \text{id}\|_{L^2(\Pi)}^2 + t_1^{2\beta} \leq \tilde{\Psi}_0(M) \end{aligned}$$

where  $\tilde{\Psi}_0(M)$  is defined by formula (7.10) of [9] with  $\omega(s) = 2\Lambda\sqrt{s}$  (according to formula (2.7) in [9]), and where  $\beta \in (0, 1)$  is arbitrary. Hence assumption (iii) in [9, Lemma 7.3] is satisfied. Summarizing, the assumptions of Lemma 7.3 in [9] are satisfied provided that

$$\begin{aligned} 0 < t_1 &\leq \min(t_0/2, \rho_0(M), (\tilde{\Psi}(M)/2)^{1/2\beta}), \\ 0 \leq \epsilon_1 &\leq \min(\epsilon_0, \frac{1}{2}\sqrt{C_P \lambda \pi} t_1^2 \min(\frac{1}{2}, \tilde{\Psi}_0(M))). \end{aligned}$$

Applying Lemma 7.3 in [9] shows that there exists a vector  $\Gamma_{\hat{x}, \hat{t}} \in \mathbf{R}^2$  and a positive constant  $\hat{c}$  such that

$$\frac{1}{|\mathcal{Q}_r(\hat{x}, \hat{t})|} \int_{\mathcal{Q}_r(\hat{x}, \hat{t})} |\nabla X(t, x) - \Gamma_{\hat{x}, \hat{t}}|^2 dx dt \leq \hat{c} \left( (2r/t_1)^{2\alpha} \tilde{\Psi}_0(M) + r^{2\beta} \right)$$

for all  $r \in (0, t_1/2)$ . In this inequality  $\alpha \in (\beta, 1)$ , and  $\hat{c} \equiv \hat{c}(\lambda, \Lambda, \alpha, \beta, M) > 0$ . In particular

$$\frac{1}{|\mathcal{Q}_r(\hat{x}, \hat{t})|} \int_{\mathcal{Q}_r(\hat{x}, \hat{t})} |\nabla X(t, x) - \Gamma_{\hat{x}, \hat{t}}|^2 dx dt \leq cr^{2\beta} \quad \text{for all } r \in (0, t_1/2)$$

with

$$c := \hat{c} \left( (2/t_1)^{2\beta} \tilde{\Psi}_0(M) + 1 \right).$$

This means that  $\nabla X$  belongs to a Campanato space, which is known to coincide with the classical Hölder space [8]. Thus

$$\|\nabla X - I\|_{C^{0,\beta}(\mathcal{Q}_{t_0/2}(\bar{x}, \bar{t}))} \leq \bar{c},$$

with  $\bar{c}$  independent of  $\bar{x}$  and  $\bar{t}$ .

By localization, interpolation with (6.8) and Sobolev embedding, we see that

$$\|X(t, \cdot) - \text{id}\|_{L^\infty(B(\bar{x}, \sqrt{t_0}/2))} \leq C_S(\theta) \bar{c}^\theta e^{-(1-\theta)C_P \lambda t/4} \epsilon_0^{1-\theta}, \quad t \in [\bar{t} - t_0, \bar{t}]$$

for all  $\theta \in (\frac{2}{3}, 1)$ , where  $C_S(\theta)$  denotes the Sobolev constant for the continuous embedding

$$W^{\theta, 4/(2-\theta)}(B(\bar{x}, \sqrt{t_0}/2)) \subset L^\infty(B(\bar{x}, \sqrt{t_0}/2)).$$

(Indeed, applying Theorem 6.4.5 (7) in [3] with  $s_0 = 0, p_0 = 2, s_1 = 1$  and  $p_1 = 4$  shows that

$$\|X(t, \cdot) - \text{id}\|_{W^{\theta, 4/(2-\theta)}(B(\bar{x}, \sqrt{t_0}/2))} \leq \bar{c}^\theta e^{-(1-\theta)C_P \lambda t/4} \epsilon_0^{1-\theta},$$

and  $W^{\theta, 4/(2-\theta)}(B(\bar{x}, \sqrt{t_0}/2)) \subset L^\infty(B(\bar{x}, \sqrt{t_0}/2))$  provided that  $\theta > 1 - \theta/2$  by Sobolev's embedding theorem.)

By a classical argument<sup>2</sup>

$$\|\nabla X(t, \cdot) - I\|_{L^\infty(B(\bar{x}, \sqrt{t_0}/2))} \leq \left(\frac{2}{\beta}\right)^{\frac{\beta}{\beta+1}} C_S(\theta)^{\frac{\beta}{1+\beta}} \frac{1}{1+\beta} \bar{c}^{\frac{1+\theta\beta}{1+\beta}} e^{-\frac{(1-\theta)\beta C_P \lambda t}{4(1+\beta)}} \epsilon_0^{\frac{\beta(1-\theta)}{1+\beta}},$$

<sup>2</sup> Let  $f \in C^{1,\beta}(B(0, R))$  for some  $\beta \in (0, 1)$ . Then

$$\| \nabla f \|_{L^\infty(B(0, R))} \leq \left(\frac{2}{\beta}\right)^{\beta/(\beta+1)} \|f\|_{C^{1,\beta}(B(0, R))}^{1/(\beta+1)} \|f\|_{L^\infty(B(0, R))}^{\beta/(\beta+1)}.$$

for  $|\bar{t} - t| \leq t_0$ . With (6.9), this implies that, for all  $t \geq 0$ , one has

$$\|\nabla X(t, \cdot) - I\|_{L^\infty(\Pi)} \leq \max\left(C\epsilon_0, \left(\frac{2}{\beta}\right)^{\frac{\beta}{\beta+1}} C_S(\theta)^{\frac{1}{1+\beta}} \bar{c}^{\frac{1+\theta\beta}{1+\beta}} e^{-\frac{(1-\theta)\beta C_P \lambda t}{4(1+\beta)}} \epsilon_0^{\frac{\beta(1-\theta)}{1+\beta}}\right).$$

*Step 4: Conclusion.*

By choosing  $\epsilon_0$  small enough, we conclude that

$$\|\nabla X(t, \cdot) - I\|_{L^\infty(\Pi)} \leq \rho_0/2, \quad t \geq 0,$$

so that

$$\nabla G(\nabla_x X(t, x)) = \nabla F_0(\nabla_x X(t, x)), \quad t \geq 0, \quad x \in \Pi.$$

Hence  $X$  satisfies

$$\partial_t X(t, x) = \operatorname{div}_x(\nabla F_0(\nabla_x X(t, x))), \quad t > 0, \quad x \in \Pi.$$

On the other hand, (6.2) implies that

$$(\nabla F(M) - \nabla F_0(M)) \cdot N = \frac{1}{8\sqrt{3}} \operatorname{trace}(N) + \frac{7}{24\sqrt{3}} \det(M) \operatorname{trace}(M^{-1}N)$$

so that

$$\nabla F(\nabla_x X(t, x)) - \nabla F_0(\nabla_x X(t, x)) = \frac{1}{8\sqrt{3}} I + \frac{7}{24\sqrt{3}} JX(t, x)(\nabla_x X(t, x))^{-1}{}^T.$$

Since

$$JX(\nabla_x X^{-1})^T = \begin{pmatrix} \partial X_2/\partial x_2 & -\partial X_2/\partial x_1 \\ -\partial X_1/\partial x_2 & \partial X_1/\partial x_1 \end{pmatrix}$$

one has  $\operatorname{div}_x(JX(\nabla_x X^{-1})^T) = 0$ , so that

$$\operatorname{div}_x \nabla F(\nabla_x X(t, x)) = \operatorname{div}_x(\nabla F_0(\nabla_x X(t, x))).$$

In other words,  $X$  is in fact the solution of (6.1).

Finally, for each  $\theta \in (\frac{2}{3}, 1)$ , one has

$$|X(t, \bar{x}) - \operatorname{id}| \leq \max(2, C_S(\theta)\bar{c}^\theta) e^{-(1-\theta)C_P \lambda (t-t_0)/4} \epsilon_0^{1-\theta}, \quad t > 0,$$

and the proof is complete.

**Conflict of interest statement**

There is no conflict of interest.

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Indeed, by the Mean Value Theorem

$$f(x+h) - f(x) = \nabla f(x) \cdot h + (\nabla f(x+sh) - \nabla f(x)) \cdot h$$

for some  $s \in (0, 1)$ , so that

$$|\nabla f(x)| \leq \frac{2\|f\|_{L^\infty(B(0,R))}}{|h|} + |h|^\beta \|\nabla f\|_{C^{0,\beta}(B(0,R))}.$$

Optimizing in  $|h|$  leads to the conclusion.

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