Lattices energies and variational calculus

Laurent Betermin

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Laurent BÉTERMIN

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Directeur de thèse : **Pr. Etienne SANDIER**
Présidente du Jury : **Pr. Sylvia SERFATY**

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Rapporteurs :	**Pr. Xavier BLANC**	Université Paris Diderot
	Pr. Florian THEIL	University of Warwick
Examinateurs :	**Pr. Djalil CHAFAÏ**	Université Paris-Dauphine
	Pr. Yuxin GE	Université Toulouse Paul Sabatier
	Pr. Etienne SANDIER	Université Paris-Est Créteil
	Pr. Sylvia SERFATY	Université Pierre et Marie Curie

Université Paris-Est Créteil, Laboratoire d'Analyse et de Mathématiques Appliquées,
CNRS UMR 8050, 61 avenue du Général de Gaulle, 94010 Créteil Cedex

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Introduction générale

Dans cette thèse, nous étudions différentes questions appartenant à la large classe des problèmes de cristallisation, c'est-à-dire à la minimisation d'énergies discrètes parmi un ensemble de configurations, comme expliqué dans [14]. Plus précisément, nous cherchons à comprendre pourquoi une structure périodique peut être le minimiseur, local ou global, de certaines énergies d'interactions, afin de tenter d'expliquer l'émergence de structures ordonnées, que ce soit dans la nature (cristaux, ADN,...) ou lors d'expériences (supraconductivité, conception de nouveaux matériaux,...). Evidemment, il s'agit d'un problème extrêmement complexe à résoudre, tant théorique qu'expérimental, le nombre de minima locaux pouvant être très grand, ce qui rend le minimum global difficile à atteindre.

Ainsi, nous nous sommes penchés sur trois types de problèmes propices à l'analyse :

— Dans le **Chapitre 1**, renvoyant à [8], nous discutons le fait qu'un réseau de Bravais puisse être un minimum local compact pour une énergie d'interaction créée par un potentiel radial, en nous inspirant du travail de Theil sur la cristallisation bidimensionnelle [99] ;

— Dans les **Chapitres 2 et 3**, renvoyant respectivement à [7] et [10], nous étudions la minimisation d'énergies par point, créées par un potentiel radial, parmi les réseaux de Bravais du plan, à partir d'un résultat de Montgomery sur l'optimalité du réseau triangulaire pour des fonctions thêta [74], dont nous redonnons une preuve détaillée en Annexe ;

— Dans le **Chapitre 4**, renvoyant à [9], nous nous intéressons au développement asymptotique, quand le nombre de points tend vers l'infini, de l'énergie logarithmique sur la sphère en lien avec le 7ème Problème de Smale, à partir des travaux de Sandier et Serfaty sur les gaz de Coulomb [86, 87] et d'avancées récentes en Théorie Logarithmique du Potentiel [52, 53, 15].

L'objectif de cette introduction en trois parties est d'exposer les différents résultats que nous avons obtenus dans chacun de ces contextes tout en rappelant les travaux antérieurs indispensables à la compréhension globale du sujet.

Réseau comme minimum local compact

Dans son travail sur la cristallisation dans $\mathbb{R}^2$ [99], Theil propose une famille de potentiels radials paramétrés $V_\alpha : \mathbb{R}_+ \to \mathbb{R}$ tels qu'il existe $\alpha_0 \in \left]0, \frac{1}{3}\right[$ tel que pour tout $\alpha \in]0, \alpha_0[$, $V_\alpha \in C^2(]1-\alpha, +\infty[)$ et

1. $\lim\limits_{r\to\infty} V_\alpha(r) = 0$;
2. $\min\limits_{r\geq 0} \sum\limits_{p\in A_2^*} V_\alpha(r\|p\|) = \sum\limits_{p\in A_2^*} V_\alpha(\|p\|)$, où $A_2 := \mathbb{Z}(1,0) \oplus \mathbb{Z}(1/2, \sqrt{3}/2)$ est le réseau triangulaire de côté 1, $A_2^* := A_2 \backslash \{0\}$ et $\|\cdot\|$ désigne la norme euclidienne sur $\mathbb{R}^2$;
3. $V_\alpha(r) \geq \dfrac{1}{\alpha}$ pour $r \in [0, 1-\alpha]$;
4. $V''_\alpha(r) \geq 1$ pour $r \in]1-\alpha, 1+\alpha[$;
5. $V_\alpha(r) \geq -\alpha$ pour $r \in [1+\alpha, 4/3]$;
6. $|V''_\alpha(r)| \leq \alpha r^{-7}$ pour $r \in]4/3, +\infty[$.

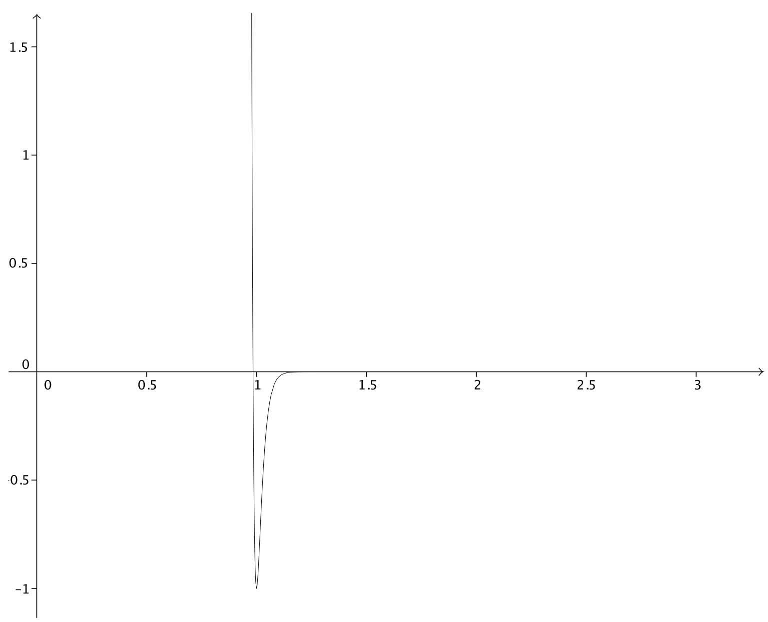


FIGURE 1 – Un exemple de potentiel de Theil V_α

Ainsi, il montre qu'il existe $\alpha_0 > 0$ tel que pour tout $\alpha \in]0, \alpha_0[$ et tout potentiel V_α,

$$\lim_{N\to+\infty} \frac{1}{2N} \min_{(x_i)_i \in \mathbb{R}^{2N}} \sum_{i\neq j} V_\alpha(\|x_i - x_j\|) = \frac{1}{2} \sum_{p\in A_2^*} V_\alpha(\|p\|),$$

c'est-à-dire que le réseau triangulaire A_2 est un minimum global de l'énergie totale d'interaction, au sens de la limite thermodynamique, quand le nombre de points qui interagissent entre eux tend vers l'infini. Ce résultat fait naturellement suite à ceux de Radin [44, 54, 80] portant sur le même type de problème, mais avec des potentiels tronqués à courte portée. Le fait que le paramètre α régisse à la fois la divergence en 0, la largeur du puits autour de la valeur 1 et la décroissance à l'infini du potentiel donne une forme d'interaction qui semble plus stéréotypée que générique quand α est petit. Malgré tout, il s'agit du premier résultat de cristallisation dans $\mathbb{R}^2$, parmi toutes les configurations, pour des interactions à longues portées. On retrouve le même type de potentiels dont le paramètre permet d'ajuster leurs formes à la structure visée dans [36, 41].

Nous nous sommes donc demandé dans [8], et c'est l'objet de notre **Chapitre 1**, si de telles hypothèses sur une famille de potentiels paramétrés pouvaient favoriser la "cristallisation locale" sur un réseau de Bravais [1] donné de $\mathbb{R}^d$. Ainsi, nous avons débarrassé la famille $(V_\alpha)_\alpha$ de toutes ses hypothèses favorisant plutôt la minimalité globale (c'est-à-dire les hypothèses 3. et 5.) et nous avons remplacé les autres par des versions plus générales et/ou locales afin d'obtenir une construction générique de potentiels permettant la minimalité locale compacte suivante.

Soit $L \subset \mathbb{R}^d$ un réseau de Bravais de première distance λ_1, c'est-à-dire

$$\lambda_1 := \min\{\|p\|; p \in L^*\},$$

$\|\cdot\|$ la norme euclidienne sur $\mathbb{R}^d$, $B \subset L$ un sous-ensemble fini et α un réel tel que $\alpha \in]0, \lambda_1/2[$. On dit que B^α, ayant le même cardinal que B, est une perturbation α-compacte de B si

$$\forall b \in B, \exists! b^\alpha \in B^\alpha \text{ tel que } \|b - b^\alpha\| \leq \alpha,$$

et dans ce cas on note $L^\alpha(B) := (L \backslash B) \cup B^\alpha$ le réseau perturbé.

Soit $d \in \mathbb{N}^*$. On dit que $V : \mathbb{R}_+^* \to \mathbb{R}$ est un potentiel d-admissible si V est une fonction C^3 et, pour tout réseau de Bravais $L \subset \mathbb{R}^d$,

$$\sum_{x \in L^*} |V(\|x\|)| + \sum_{x \in L^*} \|x\| |V'(\|x\|)| + \sum_{x \in L^*} \|x\|^2 |V''(\|x\|)| + \sum_{x \in L^*} \|x\|^3 |V'''(\|x\|)| < +\infty.$$

1. C'est-à-dire un réseau du type $L = \bigoplus_{i=1}^d \mathbb{Z} u_i$ où (u_i) est une base de $\mathbb{R}^d$.

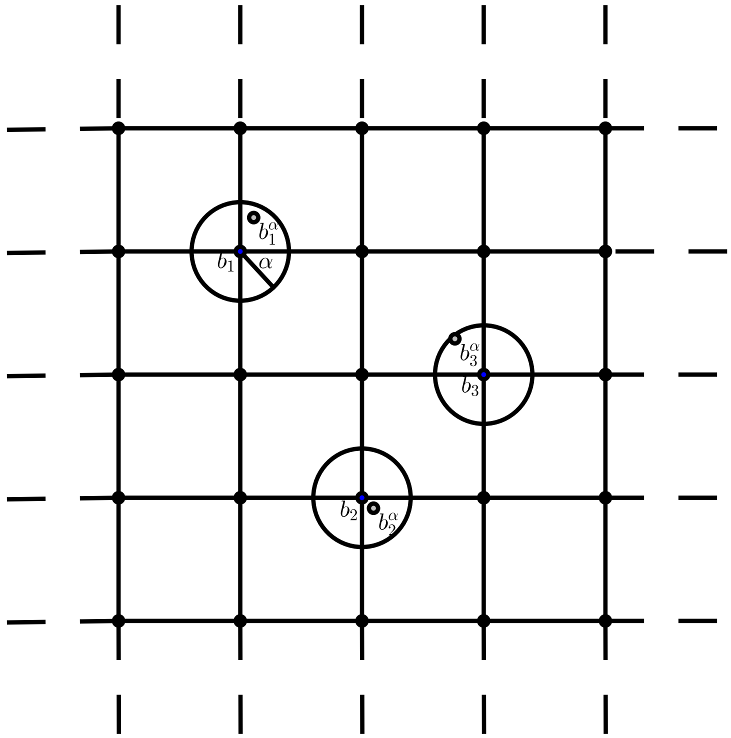


FIGURE 2 – Une perturbation α-compacte de $B = \{b_1, b_2, b_3\}$ avec $L = \mathbb{Z}^2$.

Soit L un réseau de Bravais de $\mathbb{R}^d$ et V un potentiel d-admissible. Soit $N \in \mathbb{N}^*$, on dit que L est un minimum local N-compact pour l'énergie totale créée par V si pour tout sous-ensemble $B \subset L$ tel que $\sharp B \leq N$, il existe $\alpha_0 > 0$ tel que pour tout $\alpha \in [0, \alpha_0)$ et toute perturbation α-compacte B^α de B,

$$\Delta_L^\alpha(V; B) := \sum_{b^\alpha \in B^\alpha} \sum_{\substack{y \in L^\alpha(B) \\ y \neq b^\alpha}} V(\|b^\alpha - y\|) - \sum_{b \in B} \sum_{\substack{x \in L \\ x \neq b}} V(\|b - x\|) \geq 0,$$

c'est-à-dire que l'énergie du réseau perturbé $L^\alpha(B)$ a une énergie totale plus grande que celle de L, dès lors que la perturbation maximale α_0, qui dépend de N, est assez petite.

Ainsi on démontre le **Théorème 1.3.1** du **Chapitre 1** : Soit $L \subset \mathbb{R}^d$ un réseau de Bravais de première distance λ_1 et de deuxième distance

$$\lambda_2 := \min\{\|p\|; p \in L, \|p\| > \lambda_1\}.$$

Soit $V_\theta : \mathbb{R}_+^* \to \mathbb{R}$ un potentiel d-admissible, défini, pour chaque $\theta \in [0, \lambda_1/2)$, par :

1. $\displaystyle\sum_{p \in L^*} \|p\| V_\theta'(\|p\|) = 0$;

2. $\exists r_0 \in [\lambda_1, \lambda_2)$, $\exists \varepsilon > 0$, $\exists p > d+1$ tel que pour tout $r > r_0$, $|V_\theta'''(r)| \leq \theta^{1+\varepsilon} r^{-p-2}$;
3. $V_\theta''(\lambda_1) > 0$ est indépendant de θ ;
4. il existe $M > 0$, indépendant de θ, tel que, pour tout $\lambda_1/2 < r < \lambda_2$, $|V_\theta'''(r)| \leq M$.

Alors pour tout $N \in \mathbb{N}^*$, il existe $\theta_0 > 0$ tel que pour tout $\theta \in [0, \theta_0]$ et tout V_θ, L est un minimum local N-compact pour l'énergie totale créée par V_θ. De plus, dans ce cas, la perturbation maximale α_0 peut être choisie égale à θ. Ainsi, dans le cas où $\theta < 1$, on a $\theta^{1+\varepsilon} < \theta$, c'est-à-dire que la perturbation maximale est plus grande que le coefficient de décroissance de V_θ après la première distance λ_1.

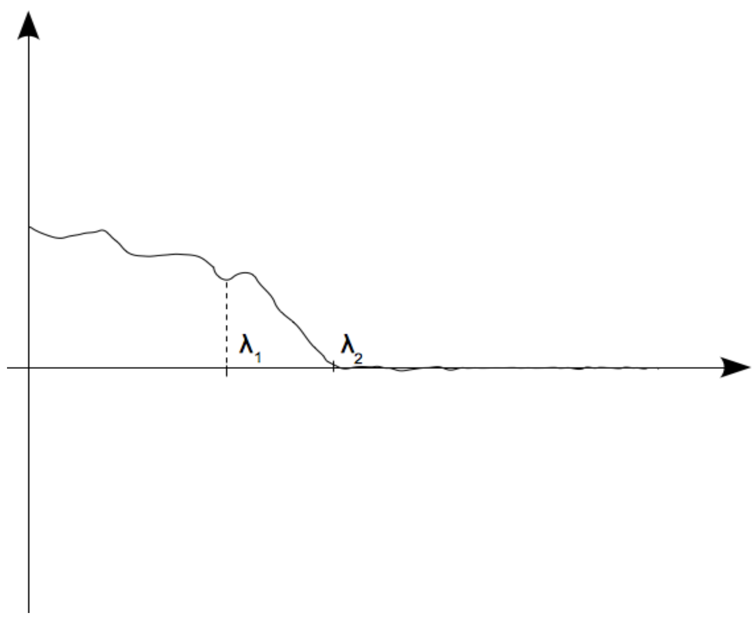


FIGURE 3 – Un exemple de potentiel V_θ

On remarque que l'hypothèse 1. est équivalente au fait que $r = 1$ soit un point critique de $f : r \mapsto \sum_{p \in L^*} V_\theta(r\|p\|)$ et que, juxtaposée aux autres hypothèses, $r = 1$ est un minimum local de f, ou, de manière équivalente, L est un minimum local de l'énergie par point créée par V_θ parmi ses dilatés. Ce type d'hypothèse semble nécessaire à la minimalité locale N-compacte quelque soit N, sous forme de condition de pression nulle[2]. De plus, la méthode utilisée permet de donner une borne inférieure à la perturbation maximale des N points que l'on déplace. En effet, on prouve que, pour tout $0 < \theta < \lambda_1/2$ et tout $0 \leq \alpha \leq \theta$,

$$\Delta_L^\alpha(V_\theta; B) \geq f(\theta) := 2V_\theta''(\lambda_1)\theta^2 - N\left(A\theta^{2+\varepsilon} + C\theta^3 + D\theta^{3+\varepsilon} + E\theta^{4+\varepsilon}\right),$$

2. Voir Remarque 1.4.1

où les constantes A, C, D, E dépendent uniquement des paramètres et pas de θ. Ainsi, il est assez facile de déterminer, au moins numériquement, la première racine positive de f en fonction de N. On voit aussi clairement que plus $V_\theta''(\lambda_1)$ est grand, plus cette racine sera grande et plus on pourra déplacer les N points loin de leurs positions d'origine.

De plus, ce résultat peut être interprété en terme de règle de type "Cauchy-Born" [77, 37]. En effet, si on considère un solide comme étant un réseau L – son intérieur étant un ensemble de N points et le reste étant son bord –, la perturbation linéaire, suffisamment petite, des N points de son intérieur augmente l'énergie d'interaction totale. Ainsi, l'intérieur du solide doit "suivre" son bord pour être dans un état d'énergie minimale, comme illustré dans la Figure 4.

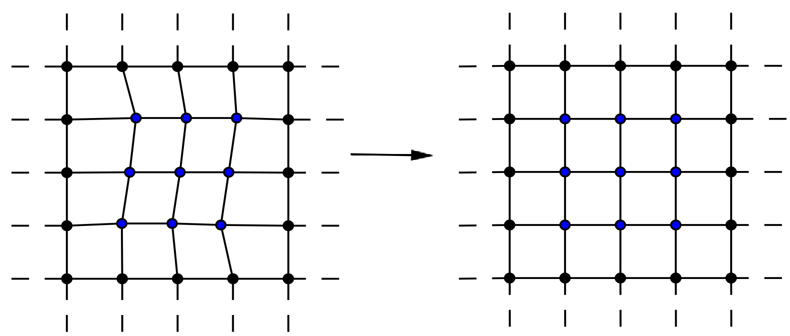


FIGURE 4 – Règle de Cauchy-Born

Minimisation d'énergie parmi les réseaux de Bravais

Si le fait de démontrer la minimalité d'une structure discrète parmi toutes les configurations du plan semble de prime abord difficile, tout autant que de montrer qu'une énergie discrète possède bien un minimiseur global périodique [3], la minimisation d'énergies par point parmi les réseaux de Bravais a connu bon nombre de succès depuis les années 50, et c'est ce type de problème que l'on étudiera au **Chapitre 2**. En effet, Rankin [82], Ennola [39], Cassels [25] et Diananda [35] ont étudié le problème de minimisation, parmi les réseaux de Bravais du plan, de la fonction zêta d'Epstein définie [4], pour $s > 2$, par

$$\zeta_L(s) := \sum_{p\in L^*} \frac{1}{\|p\|^s}, \tag{0.0.1}$$

où $\|\cdot\|$ désigne la norme euclidienne sur $\mathbb{R}^2$, et ils ont prouvé qu'à densité fixée, le minimum est unique, à rotation près, et triangulaire, c'est-à-dire que, pour tout $A > 0$, le réseau

$$\Lambda_A := \sqrt{\frac{2A}{\sqrt{3}}}\left[\mathbb{Z}(1,0) \oplus \mathbb{Z}(1/2, \sqrt{3}/2)\right]$$

est l'unique minimiseur de $L \mapsto \zeta_L(s)$ parmi les réseaux d'aire [5] A.

Il a fallu attendre Montgomery [74] pour qu'un autre pas significatif soit fait dans ce domaine. Il montra que, pour tout $A > 0$, le réseau triangulaire Λ_A est l'unique minimiseur, à rotation près, parmi les réseaux de Bravais d'aire A, des fonctions thêta définies, pour $\alpha > 0$, par

$$\theta_L(\alpha) := \Theta_L(i\alpha) = \sum_{p\in L} e^{-2\pi\alpha\|p\|^2},$$

où Θ_L est la fonction thêta de Jacobi du réseau L. Ce résultat, dont nous redonnons la preuve détaillée dans notre Annexe, est extrêmement important car il permet de montrer l'optimalité du réseau triangulaire Λ_A parmi les réseaux de Bravais d'aire A fixée pour une classe plus large de potentiels d'interactions. Ainsi, comme expliqué par Cohn et Kumar [30], on montre dans la **Proposition 2.3.1** du **Chapitre 2**, en utilisant

3. Mis à part dans certains cas simples d'interactions entre premiers voisins ou dans le cas d'interactions oscillantes comme dans l'article de Süto [96].

4. Cette série converge pour $s > 2$ et on peut définir son prolongement analytique si $s > 0$. Dans la suite, quand $d = 2$, seul le cas $s > 2$ nous intéressera.

5. On dira qu'un réseau de Bravais $L = \mathbb{Z}u \oplus \mathbb{Z}v$ a pour aire A si l'aire de sa cellule fondamentale est $|L| = \|u \wedge v\| = A$.

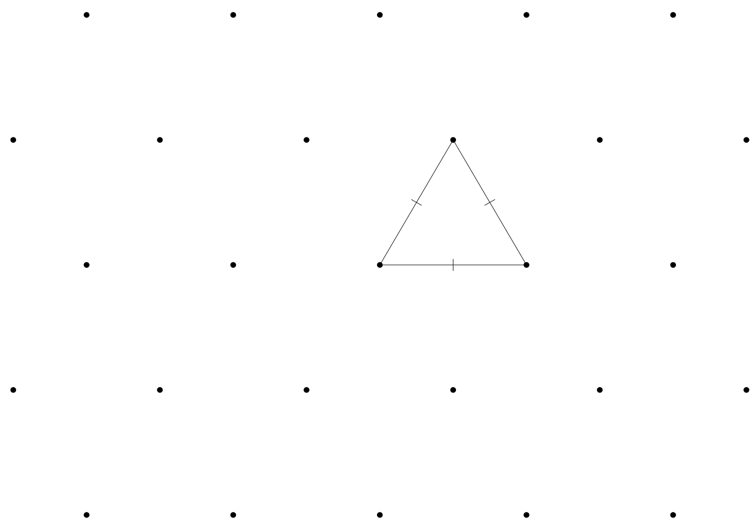


Figure 5 – Réseau triangulaire

à la fois le résultat de Montgomery et un Théorème de Bernstein [6], rappelé dans ce même Chapitre 2, que si $f:\mathbb{R}_+^*\to\mathbb{R}$ est complètement monotone, c'est-à-dire que pour tout $r>0$ et tout $k\in\mathbb{N}$, $(-1)^k f^{(k)}(r)\geq 0$, alors quelque soit $A>0$, Λ_A est l'unique minimiseur, à rotation près, de l'énergie

$$L\mapsto E_f[L]:=\sum_{p\in L^*} f(\|p\|^2),$$

parmi les réseaux de Bravais d'aire fixée A.

Nous pourrions croire que la complète monotonicité de f est une condition trop forte pour la minimalité de Λ_A pour $L\mapsto E_f[L]$ quelque soit $A>0$, mais on montre dans la **Proposition 2.3.4** du **Chapitre 2** que pour la fonction strictement positive, strictement décroissante et strictement convexe V définie par

$$V(r):=\frac{14}{r^2}-\frac{40}{r^3}+\frac{35}{r^4},$$

il existe A_1,A_2 tels que Λ_A ne soit pas un minimiseur de E_V parmi les réseaux de Bravais d'aire fixée $A\in(A_1,A_2)$. Ainsi on peut imaginer [6] que l'optimalité de Λ_A pour tout A est équivalente avec le fait que f soit totalement monotone et obtenir des minimiseurs "exotiques" pour certaines interactions décroissantes, positives et convexes, comme on

6. Ceci est une intuition raisonnable, mais nous n'en donnons pas la preuve.

peut le voir, numériquement, dans les travaux de Marcotte, Stillinger et Torquato [67] portant sur des potentiels tronqués.

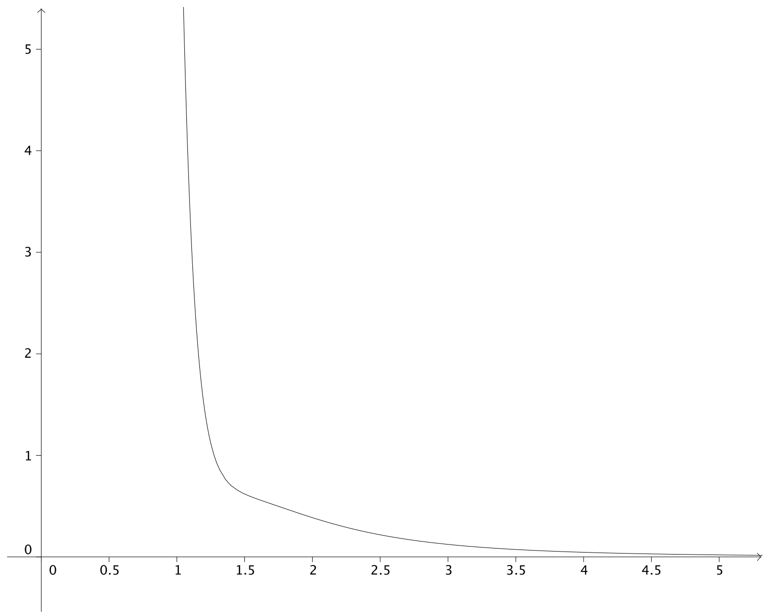


FIGURE 6 – Courbe de V

Dès lors, on peut se demander quels types de résultats on obtient si f n'est pas totalement monotone, et c'est l'objet de notre **Théorème 2.1.2** du **Chapitre 2**. On démontre ainsi deux sortes de résultats :

— La minimalité de Λ_A, à haute densité fixée (c'est-à-dire $A > 0$ suffisamment petit), pour certains potentiels, quand ceux-ci sont équivalents en 0 à une fonction totalement monotone. Nous donnons des bornes non-optimales [7] pour l'aire en dessous de laquelle ces résultats sont vrais en fonction de leurs paramètres ;

— La minimalité globale, parmi tous les réseaux de Bravais du plan, sans restriction de densité, d'un réseau triangulaire pour des énergies par point engendrées par des potentiels du type Attractif-Répulsif et Lennard-Jones, définis respectivement par

$$\varphi_{a,x}^{AR}(r) = a_2\frac{e^{-x_2 r}}{r} - a_1\frac{e^{-x_1 r}}{r} \quad \text{et} \quad V_{a,x}^{LJ}(r) = \frac{a_2}{r^{x_2}} - \frac{a_1}{r^{x_1}},$$

pour une infinité de valeurs [8] des paramètres $(a_1, a_2, x_1, x_2) \in (0, +\infty)^4$ dans le

7. Nous reparlerons de cette non-optimalité plus bas.
8. On donne des exemples explicites de telles valeurs dans l'énoncé du théorème.

premier cas et $(a_1, a_2, x_1, x_2) \in (0, +\infty)^2 \times (1, +\infty)^2$ dans le deuxième cas, et plus particulièrement quand ces potentiels possèdent un puits. De plus, dans le cas des potentiels de type Lennard-Jones, l'aire du minimiseur global $L_{a,x}$ est donnée par

$$|L_{a,x}| = \left(\frac{a_2 x_2 \zeta_{\Lambda_1}(2x_2)}{a_1 x_1 \zeta_{\Lambda_1}(2x_1)} \right)^{\frac{1}{x_2 - x_1}}.$$

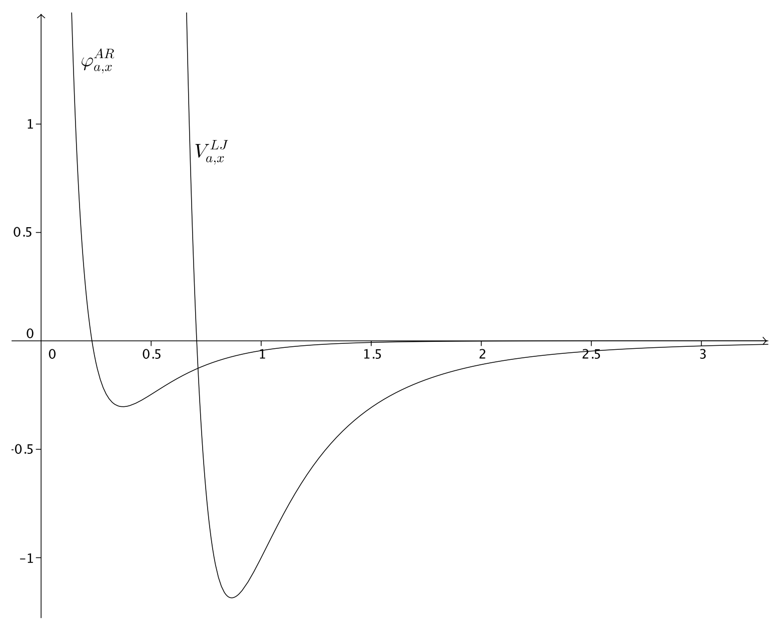


FIGURE 7 – Courbes de $\varphi_{a,x}^{AR}(r) = 2\frac{e^{-6r}}{r} - \frac{e^{-3r}}{r}$ et $V_{a,x}^{LJ}(r) = \frac{1}{r^6} - \frac{2}{r^4}$

Ces résultats découlent en fait d'une représentation intégrale de l'énergie d'un réseau L d'aire A soumis à un potentiel admissible[9] f, que nous prouvons dans notre **Théorème 2.1.1** :

$$E_f[L] = \frac{\pi}{A} \int_1^{+\infty} \left[\theta_L\left(\frac{y}{2A}\right) - 1 \right] \left[y^{-1}\mu_f\left(\frac{\pi}{yA}\right) + \mu_f\left(\frac{\pi y}{A}\right) \right] dy + C_A,$$

où μ_f est la transformée de Laplace inverse de f et C_A est une constante indépendante de L. Ainsi, le fait que

$$g_A(y) := y^{-1}\mu_f\left(\frac{\pi}{yA}\right) + \mu_f\left(\frac{\pi y}{A}\right)$$

9. Ce type de potentiel est choisi tel que E_f soit toujours finie et que f possède une transformée de Laplace inverse.

soit positif pour presque tout $y \geq 1$ assure, par le résultat de Montgomery, que, pour tout réseau de Bravais L d'aire A,

$$E_f[L] - E_f[\Lambda_A] = \frac{\pi}{A}\int_1^{+\infty}\left[\theta_L\left(\frac{y}{2A}\right) - \theta_{\Lambda_A}\left(\frac{y}{2A}\right)\right] g_A(y)dy \geq 0,$$

c'est-à-dire la minimalité de Λ_A. La méthode est donc de trouver la relation la plus optimale possible entre A et les paramètres de f afin que $g_A(y)$ soit positif pour presque tout $y \geq 1$. De plus, dans le cas de potentiels avec un puits, un argument de dilatation [10] permet de donner une borne supérieure pour l'aire d'un réseau qui est un minimum global pour l'énergie. Ainsi, le fait que cette borne supérieure soit plus petite que celle des aires A telles que Λ_A soit l'unique minimiseur à aire fixée nous assure que le minimum global est unique, à rotation près, et triangulaire.

Ces résultats confirment les simulations numériques faites par Torquato et ses coauteurs, par exemple dans [84, 100] ainsi que celui de Theil [99], c'est-à-dire que le minimum global avec un potentiel possédant un puits semble être un réseau triangulaire. Malheureusement, ils ne permettent pas de montrer la minimalité globale, parmi les réseaux de Bravais, d'un réseau triangulaire pour le potentiel classique de Lennard-Jones [11] $(12-6)$ défini par

$$V_{LJ}(r) := \frac{1}{r^6} - \frac{2}{r^3}.$$

En effet, notre méthode n'est pas optimale, c'est-à-dire qu'elle ne permet pas de déterminer toutes les aires A telles que Λ_A soit l'unique minimiseur de $L \mapsto E_f[L]$ parmi les réseaux de Bravais du plan d'aire fixée A. Des résultats numériques donnés dans la **Section 3.3.2** du **Chapitre 3** nous donnent un exemple de cette non-optimalité dans le cas de la minimisation de $L \mapsto E_{V_{LJ}}[L]$. De plus, nous expliquons dans la **Section 2.4.3** du **Chapitre 2** pourquoi notre méthode semble difficile à améliorer.

Dans [10], avec Peng Zhang, nous nous sommes intéressés plus particulièrement à ce potentiel de Lennard-Jones V_{LJ} et son énergie par point, et ce fut d'ailleurs notre première incursion dans ce domaine d'étude [12]. Après avoir montré dans le **Théorème 3.3.1** du **Chapitre 4** la minimalité du réseau triangulaire pour $E_{V_{LJ}}$ parmi les réseaux de Bravais d'aire fixée $0 < A \leq \pi(120)^{-1/3} \approx 0.63693$, en utilisant la positivité de g_A

10. Voir preuve du Théorème 2.1.2.

11. Comme on somme sur les carrés des distances du réseau, les exposants sont 6 et 3 afin de sommer effectivement le potentiel de Lennard-Jones $(12-6)$ sur les réseaux.

12. Les résultats sont, dans cette thèse, présentés dans l'ordre antichronologique car plus naturel.

pour des A assez petits, et, dans la **Proposition 3.3.5**, la non-minimalité du réseau triangulaire pour des A suffisamment grands, résultat qui est en fait plus général comme on le verra dans la **Proposition 2.6.6** du **Chapitre 2**, nous avons tenté de caractériser le minimum global de $E_{V_{LJ}}$ parmi tous les réseaux de Bravais du plan. Nous montrons, dans la **Proposition 3.4.1** et dans la **Proposition 3.4.5** du **Chapitre 3** que, si $L_0 = \mathbb{Z}u \oplus \mathbb{Z}v$ est un minimum global de $E_{V_{LJ}}$, paramétré de telle sorte que $\|u\| \leq \|v\|$ soient ses deux premières distances, alors on a :

— l'énergie minimale vaut $E_{V_{LJ}}(L_0) = -\zeta_{L_0}(6) = -\zeta_{L_0}(12) < 0$;

— la première distance est bornée : $0.74035 < \|u\| < 1$;

— la deuxième distance est bornée : $\|v\| \leq 1$;

— L_0 est caractérisé par $\zeta_{L_0}(6) = \max\{\zeta_L(6); L \text{ tel que } \zeta_L(12) \leq \zeta_L(6)\}$.

De plus, des vérifications numériques, confirmant celles faites par Blanc, Le Bris et Yedder [13] dans le cas du problème à N points, nous incitent fortement à penser que pour tout $A \in (0,1)$, Λ_A est l'unique minimiseur, à rotation près, de $E_{V_{LJ}}$ parmi les réseaux de Bravais d'aire fixée A, et qu'ainsi son minimum global doit être triangulaire d'aire

$$|L_0| = \left(\frac{\zeta_{\Lambda_1}(12)}{\zeta_{\Lambda_1}(6)}\right)^{1/3} \approx 0.84912.$$

Enfin, toujours dans [10], c'est-à-dire notre **Chapitre 3**, **Section 3.5**, nous avons étudié le modèle bidimensionnel de Thomas-Fermi [62] pour les solides. En effet, ce modèle, issu de la Chimie Quantique, présenté dans [13, Section 2] et [12, Section 4], est le suivant : considérons N noyaux représentés par le N-uplet $X_n = (x_1, ..., x_N) \in \mathbb{R}^{2N}$ associés à N électrons de densité totale $\rho \geq 0$. Alors l'énergie de Thomas-Fermi du système est donnée par

$$\begin{aligned} E^{TF}(\rho, X_N) = & \int_{\mathbb{R}^2} \rho^2(x)dx - \frac{1}{2}\iint_{\mathbb{R}^2\times\mathbb{R}^2} \log\|x-y\|\rho(x)\rho(y)dxdy \\ & + \sum_{j=1}^N \int_{\mathbb{R}^2} \log\|x-x_j\|\rho(x)dx - \frac{1}{2}\sum_{j\neq k}\log\|x_j-x_k\|. \end{aligned}$$

On cherche alors à déterminer $I_N^{TF} = \inf_{X_N} E^{TF}(X_N)$ où

$$E^{TF}(X_N) := \inf_{\rho}\left\{E^{TF}(\rho, X_N), \rho \geq 0, \rho \in L^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^2), \int_{\mathbb{R}^2} \rho = N\right\}.$$

Blanc et ses coauteurs [12, 13] ont montré que

$$E^{TF}(X_N) = \sum_{i\neq j} W_{TF}(\|x_i - x_j\|) + NC,$$

où $W_{TF}(r) = \frac{1}{2}K_0(\sqrt{\pi}r)$ avec K_0 la fonction de Bessel modifiée de seconde espèce et C une constante indépendante de la configuration. Ainsi, le problème limite qui est à résoudre est celui donné par la limite thermodynamique

$$\lim_{N\to+\infty} \frac{E^{TF}(X_N)}{N},$$

c'est-à-dire la minimisation parmi les réseaux de Bravais de l'énergie par point

$$E_{TF}(L) = \sum_{p\in L^*} W_{TF}(\|p\|).$$

Blanc, Le Bris et Yedder [13] avaient conjecturé que cette énergie était minimale à toute densité pour le réseau triangulaire, ce que nous avons montré, dans notre **Théorème 3.5.1** du **Chapitre 3**, en écrivant l'énergie en terme de fonction thêta et en utilisant le résultat de Montgomery, remontrant finalement au passage que la fonction $r \mapsto K_0(\sqrt{r})$ est complètement monotone. Ces interactions de type Bessel se retrouvent aussi dans des modèles de mécanique des fluides et de supraconductivité [1, 93].

L'étape suivante, qui est discutée par Cohn et Kumar [30, Section 9], serait de montrer l'optimalité de Λ_A pour E_f, quand f est totalement monotone, parmi tous les réseaux périodiques d'aire A de $\mathbb{R}^2$, et pas uniquement les réseaux de Bravais. Ce type de problème fait l'objet de recherches actives en lien avec le design sphérique, comme par exemple les travaux de Coulangeon et Schürmann [31, 89, 33].

Quant au même type de problème en **dimensions supérieures**, il n'existe pas à ce jour de résultats d'optimalité globale d'un réseau de $\mathbb{R}^d$, $d > 2$, pour la fonction thêta définie classiquement par

$$\theta_L(\alpha) = \sum_{p\in L} e^{-\pi\alpha\|p\|^2},$$

ou pour la fonction zêta d'Epstein d-dimensionnelle (0.0.1), définie pour $s > d$ et prolongeable pour $s > 0$, parmi les réseaux de Bravais de $\mathbb{R}^d$. Cela rend bien évidemment encore plus difficile l'étude d'énergies engendrées par des potentiels plus compliqués, d'autant plus que notre représentation intégrale de E_f est basée sur l'équation fonctionnelle de θ_L suivante, prouvée en Annexe : pour tout réseau de Bravais L d'aire $|L| = 1/2$ et tout $\alpha > 0$,

$$\theta_L(1/\alpha) = \alpha\theta_L(\alpha),$$

valable uniquement pour $d = 2$. En effet, pour $d > 2$, celle-ci est remplacée par

$$\theta_L(\alpha) = \alpha^{-d/2}\theta_{L^*}\left(\frac{1}{\alpha}\right),$$

pour tout réseau L de volume 1 et tout $\alpha > 0$, où $L^\star$ est le réseau dual de L, c'est-à-dire

$$L^\star := \left\{ x \in \mathbb{R}^d ; \forall y \in L, x \cdot y \in \mathbb{Z} \right\}.$$

En dimension $d = 3$, Ennola [40] a prouvé que le réseau cubique à faces centrées [13] est un minimum local pour $L \mapsto \zeta_L(s)$, pour tout $s > 0$. Malheureusement, on ne peut avoir l'optimalité de ce réseau pour toutes les valeurs de $s > 0$ fixées [14], comme expliqué dans [88]. En effet, notons, pour $s > d$, qu'un résultat classique permettant le prolongement analytique de ζ_L nous donne,,

$$F(L, s) := \pi^{-s/2}\Gamma(s/2)\zeta_L(s) = F(L^\star, d/2 - s/2).$$

Ainsi, on a, pour L_3 le réseau cubique à faces centrées et $L_3^\star$ son réseau dual, c'est-à-dire le réseau cubique centré :

$$G(s) := F(L_3, s) - F(L_3^\star, s) = -G(d/2 - s/2),$$

et il y a seulement deux possibilités : $G \equiv 0$ ou G change de signe. Comme les distances du réseau L_3 sont différentes des distances du réseau $L_3^\star$, G ne peut pas être identiquement nulle et change donc de signe. Ainsi, il existe $s_0 > 0$ tel que

$$\zeta_{L_3}(s_0) > \zeta_{L_3^\star}(s_0),$$

c'est-à-dire que L_3 ne peut être le minimum global de $L \mapsto \zeta_L(s)$ pour chaque $s > 0$, contrairement à ce qu'avait conjecturé Ennola [40]. Ainsi, il n'est pas non plus possible que ce réseau soit un minimum de $L \mapsto \theta_L(\alpha)$ pour tout $\alpha > 0$ pour la même raison [15], car pour tout L de volume 1 et tout $s > d$,

$$\zeta_L(s) = \frac{\pi^{s/2}}{\Gamma(s/2)} \int_0^{+\infty} \left(\theta_L(\alpha) - 1\right) \alpha^{s/2-1} dy.$$

De plus, un autre problème, pour la minimisation parmi les réseaux périodiques, vient du fait que l'empilement le plus compact de sphères de même rayon [16] n'est pas unique pour $d = 3$. En effet, le réseau hexagonal compact, qui n'est pas un réseau de Bravais de $\mathbb{R}^3$, vérifie aussi cette propriété.

13. La Figure 8 est recopiée avec l'aimable autorisation de Franz-Josef Haug (Ecole Polytechnique Fédérale de Lausanne)
14. Par contre, cela semble vrai pour $s > 3/2$ d'après [88, Section 1] et [14, Figure 7].
15. Mais cela semble plausible pour $\alpha > 1$, d'après [88, Section 5] et [14, Figure 8].
16. Aussi appelé "best packing".

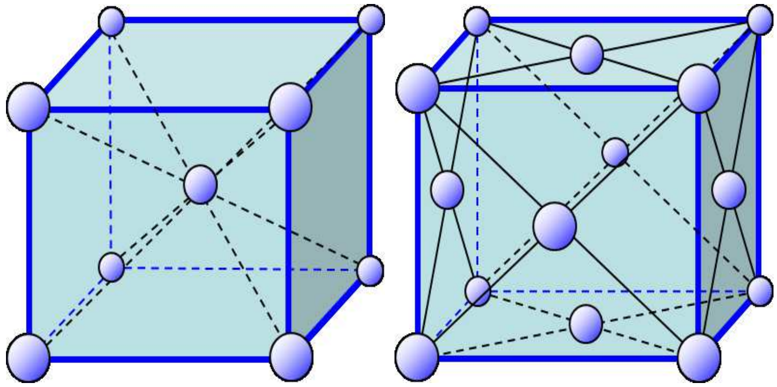


FIGURE 8 – Réseaux Cubique Centré (gauche) et Cubique à Faces Centrées (droite)

Malgré tout, en dimensions $d \in \{2, 4, 8, 24\}$, là où le best packing L_d est connu et unique, Cohn et Kumar ont conjecturé [30, Conjecture 9.4] que L_d est l'unique minimiseur de E_f, avec f complètement monotone, à densité fixée parmi les configurations périodiques, et pas uniquement les réseaux de Bravais. Un bon indice étant le résultat de Sarnak et Strömbergsson [88, Theorem 1] qui montre que L_d est un minimum local strict de $L \mapsto \zeta_L(s)$, $s > 0$, et $L \mapsto \theta_L(\alpha)$, $\alpha > 0$, parmi les réseaux de Bravais de $\mathbb{R}^d$ pour $d \in \{4, 8, 24\}$.

Asymptotique de l'énergie logarithmique sur la sphère

Alors que le problème de réseau minimisant dans $\mathbb{R}^3$ reste largement ouvert malgré quelques tentatives [41, 96, 97], celui de la minimisation de l'énergie logarithmique sur la sphère $\mathbb{S}^2$ fait l'objet d'une attention toute particulière. Notons $\|\cdot\|$ la norme euclidienne dans $\mathbb{R}^3$ et définissons, pour $(y_1, ..., y_n) \in (\mathbb{S}^2)^n$, l'énergie logarithmique de cette configuration par

$$\mathrm{E}_{\log}(y_1, ..., y_n) := -\sum_{i \neq j}^{n} \log \|y_i - y_j\|.$$

et notons $\mathcal{E}_{\log}(n)$ le minimum de cette énergie parmi les configurations de n points sur $\mathbb{S}^2$.

Cette énergie apparaît naturellement, comme expliqué par Saff et Kuijlaars [59] ou par Brauchart et Grabner [21], dans beaucoup de situations physiques. De plus, la recherche de minimiseurs pour $\mathrm{E}_{\log}$ appartient à une classe plus large de problèmes sur la sphère dont fait par exemple partie celui de Thomson, où le logarithme est remplacé par $r \to r^{-1}$, qui est lié à la construction de grandes molécules stables de carbone utiles dans les nanotechnologies (on pense par exemple au buckminsterfullerene C_{60}, voir Figure 9).

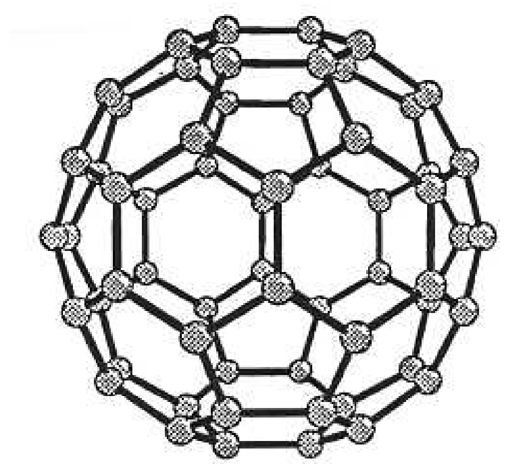


FIGURE 9 – Buckminsterfullerene C_{60}.

En 1998, Smale [92] a d'ailleurs fait figurer, parmi une liste de 18 problèmes importants pour notre siècle, celui [17] de trouver pour chaque $n \geq 2$, une constante universelle $c \in \mathbb{R}$ et une configuration $(y_1, ..., y_n) \in (\mathbb{S}^2)^n$ telles que

$$\mathrm{E}_{\log}(y_1, ..., y_n) - \mathcal{E}_{\log}(n) \leq c \log n,$$

et cela en temps polynomial en n. Cela revient donc à étudier le développement asymptotique de $\min_{\{y_i\} \in \mathbb{S}^2} \mathrm{E}_{\log}(y_1, ..., y_n)$ quand le nombre de points n tend vers l'infini. La Figure 10 donne un exemple d'une configuration de 1000 points proche d'un minimiseur de l'énergie logarithmique.

Grâce aux travaux de Wagner [106] et de Saff et Kuijlaars [60], nous savions que, quand $n \to +\infty$,

$$\mathcal{E}_{\log}(n) = \left(\frac{1}{2} - \log 2 \right) n^2 - \frac{n}{2} \log n + O(n).$$

17. Il s'agit du septième problème de Smale.

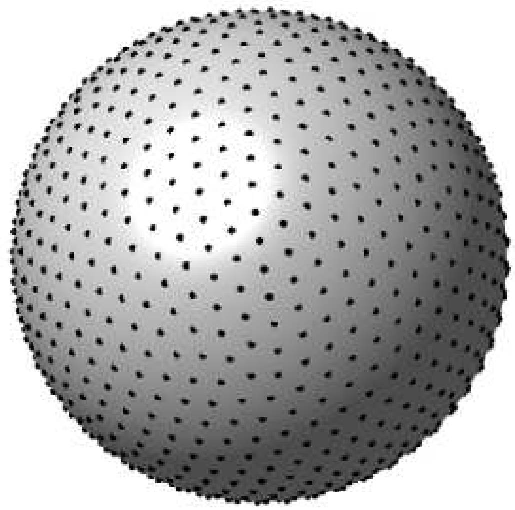


FIGURE 10 – Configuration de 1000 points proche d'un minimiseur de $\mathrm{E}_{\log}$ Bendito et al. [5].

De plus, Rakhmanov, Saff et Zhou [81] ont conjecturé l'existence d'une constante C, indépendante de n, telle que, quand $n \to +\infty$,

$$\mathcal{E}_{\log}(n) = \left(\frac{1}{2} - \log 2\right) n^2 - \frac{n}{2} \log n + Cn + o(n),$$

constante qui est conjecturée être égale à

$$C_{BHS} := 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)}$$

par Brauchart, Hardin et Saff [22], via une autre conjecture sur l'énergie de Riesz sur la sphère.

Ainsi, dans [9], en collaboration avec Etienne Sandier, et c'est l'objet du **Théorème 4.7.5** du **Chapitre 4**, nous avons démontré la conjecture de Rakhmanov, Saff et Zhou, c'est-à-dire l'existence de la constante C, à partir des travaux de Sandier et Serfaty [86, 87] portant sur les gaz de Coulomb bidimensionnels où ils étudient le développement asymptotique, quand le nombre de points n tend vers l'infini, du minimum du Hamiltonien d'un système de n points $(x_1, ..., x_n)$ de $\mathbb{R}^2$ défini par

$$w_n(x_1, ..., x_n) := -\sum_{i \neq j}^{n} \log \|x_i - x_j\| + n\sum_{i=1}^{n} V(x_i),$$

où $\|\cdot\|$ désigne la norme euclidienne sur $\mathbb{R}^2$ et $V : \mathbb{R}^2 \to \mathbb{R}$ est un potentiel confinant suffisamment régulier. Comme on a, pour $\mu_n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$ et $\Delta = \{(x,x); x \in \mathbb{R}^2\}$,

$$w_n(x_1, ..., x_n) = n^2 \left[\iint_{\mathbb{R}^4 \setminus \Delta} \left(\frac{V(x)}{2} + \frac{V(y)}{2} - \log\|x-y\| \right) d\mu_n(x) d\mu_n(y) \right],$$

il est indispensable de connaître la distribution limite minimisant l'énergie suivante, définie sur l'ensemble $\mathcal{M}_1(\mathbb{R}^2)$ des mesures de probabilités sur $\mathbb{R}^2$:

$$I_V(\mu) := \iint_{\mathbb{R}^4} \left(\frac{V(x)}{2} + \frac{V(y)}{2} - \log\|x-y\| \right) d\mu(x) d\mu(y).$$

Dans [87], le potentiel V est supposé fortement confinant, c'est-à-dire que

$$\lim_{\|x\| \to +\infty} \{V(x) - 2\log\|x\|\} = +\infty,$$

et cela implique, par des arguments classiques de Théorie Logarithmique du Potentiel [42, 85] qu'il existe une unique mesure d'équilibre μ_V minimisant I_V et dont le support Σ_V est compact. De plus, si V est assez régulier, alors μ_V est absolument continue par rapport à la mesure de Lebesgue, i.e.

$$d\mu_V(x) = m_V(x) dx.$$

Ainsi, en écrivant $\mu_n = (\mu_n - \mu_V) + \mu_V$ et en utilisant les équations d'Euler-Lagrange [18] associées au problème de minimisation $\min\limits_{\mathcal{M}_1(\mathbb{R}^2)} I_V(\mu)$, de la forme $\zeta(x) = 0$ quasi-partout [19] sur Σ_V et $\zeta(x) \geq 0$ quasi-partout sur $\mathbb{R}^2$, on obtient

$$w_n(x_1, ..., x_n) = n^2 I_V(\mu_V) - \frac{n}{2}\log n + \frac{1}{\pi} W(\nabla H_n', \mathbb{1}_{\mathbb{R}^2}) + 2n \sum_{i=1}^n \zeta(x_i),$$

où $H_n' := -2\pi\Delta^{-1}(\nu_n' - \mu_V')$ avec $x' := \sqrt{n}x$ les coordonnées blow-up, $m_V'(x) := m_V(x/\sqrt{n})$, $d\mu_V'(x') := m_V'(x')dx'$ la mesure dans les coordonnées blow-up et W une énergie dite "renormalisée" définie par

$$W(E, \chi) = \lim_{\eta \to 0} \left(\frac{1}{2} \int_{\mathbb{R}^2 \setminus \cup_{p \in \Lambda} B(p,\eta)} \chi(x) \|E(x)\|^2 dx + \pi \log \eta \sum_{p \in \Lambda} \chi(p) \right),$$

pour toute fonction continue χ et tout champ de vecteurs E vérifiant $\operatorname{div} E = 2\pi(\nu - m)$ et $\operatorname{curl} E = 0$ où $\nu = \sum_{p \in \Lambda} \delta_p$ avec $\Lambda \subset \mathbb{R}^2$ un ensemble discret. On peut voir W comme

18. Aussi appelées inégalités variationnelles de Frostman.

19. C'est-à-dire en dehors d'un ensemble de capacité nulle. La définition de ζ est donnée au Chapitre 4 par (4.4.1).

une énergie d'interaction de type "coulombienne" entre les points de Λ qui apparaît naturellement dans l'étude des interactions entre vortex dans les supraconducteurs de type II dans la théorie de Ginzburg-Landau, comme expliqué dans [86, 87, 90, 91]. C'est d'ailleurs l'analogue de l'énergie de Dirichlet pour un champ de vecteurs dans $L^p_{loc}(\mathbb{R}^2, \mathbb{R}^2)$, $1 < p < 2$, ayant des singularités.

Ainsi, par une méthode de Γ-convergence, Sandier et Serfaty [87] ont montré que, si $(x_1, ..., x_n)$ minimise w_n pour chaque n, alors

$$\lim_{n\to+\infty} \frac{1}{n}\left[\frac{1}{\pi}W(\nabla H_n', \mathbb{1}_{\mathbb{R}^2}) + 2n\sum_{i=1}^{n}\zeta(x_i)\right] = \alpha_V := \frac{1}{\pi}\min_{\mathcal{A}_1} W - \frac{1}{2}\int_{\mathbb{R}^2} m_V(x)\log m_V(x)dx,$$

où $\min_{\mathcal{A}_1} W$, atteint d'après [86, Theorem 1], est le minimum, parmi les configurations de densité moyenne [20] égale à 1, de

$$W(E) = \limsup_{R\to+\infty}\frac{W(E, \chi_{B_R})}{|B_R|},$$

avec χ_{B_R} des fonctions cutoff ayant pour support la boule centrée en 0 et de rayon R. Dès lors, quand $n \to +\infty$, on a l'asymptotique du minimum de w_n donnée par

$$\min_{\{x_i\}\in\mathbb{R}^{2n}} w_n(x_1, ..., x_n) = n^2 I_V(\mu_V) - \frac{n}{2}\log n + \alpha_V n + o(n).$$

Dans [9], notre travail a été de redémontrer cette formule, en utilisant les mêmes techniques que dans [86, 87] – et c'est l'objet du **Théorème 4.6.1** de notre **Chapitre 4** – mais pour un potentiel V faiblement confinant, c'est-à-dire vérifiant

$$\liminf_{\|x\|\to+\infty}\left\{V(x) - \log(1 + \|x\|^2)\right\} > -\infty.$$

Dans ce cas-là, des travaux récents de Hardy et Kuijlaars [52, 53] d'un côté et Bloom, Levenberg et Wielonsky [15] de l'autre ont permis de montrer à la fois l'existence d'une mesure d'équilibre μ_V dont le support peut être $\mathbb{R}^2$ tout entier, mais aussi les équations d'Euler-Lagrange associées [21]. Nous avons donc pu généraliser, dans notre **Théorème 4.6.1**, l'asymptotique démontrée dans [87] à une classe de potentiels plus généraux [22] dont fait partie

$$V(x) = \log(1 + \|x\|^2),$$

20. C'est-à-dire des ensembles Λ tels que pour tout $R > 1$, il existe une constante universelle C vérifiant $\nu(B_R) \leq C|B_R|$ où $|B_R|$ désigne l'aire de la boule centrée en 0 et de rayon R, avec $\operatorname{div} E = 2\pi(\nu - 1)$ et $\operatorname{curl} E = 0$.

21. Ces équations sont identiques à celles du cas où Σ_V est compact.

22. Voir la définition 4.3.2.

et dont la mesure d'équilibre associée, de support $\Sigma_V = \mathbb{R}^2$, est

$$d\mu_V(x) = \frac{dx}{\pi(1+\|x\|^2)^2}.$$

Dès lors, en remarquant, par projection stéréographique, que l'étude de $\mathrm{E}_{\log}$ sur la sphère revient à étudier w_n avec ce potentiel V particulier, on obtient notre **Théorème 4.7.5**, c'est-à-dire l'asymptotique, quand $n \to +\infty$:

$$\mathcal{E}_{\log}(n) = \left(\frac{1}{2} - \log 2\right) n^2 - \frac{n}{2}\log n + \left(\frac{1}{\pi}\min_{\mathcal{A}_1} W + \frac{\log \pi}{2} + \log 2\right) n + o(n),$$

ce qui permet de démontrer la conjecture de Rakhmanov, Saff et Zhou, c'est-à-dire l'existence de

$$C = \frac{1}{\pi}\min_{\mathcal{A}_1} W + \frac{\log \pi}{2} + \log 2,$$

qui est effectivement une constante car $\min_{\mathcal{A}_1} W$ est atteint.

Enfin, Sandier et Serfaty [86] ont conjecturé que le minimum de W parmi les configurations de $\mathcal{A}_1$, c'est-à-dire les configurations de densité moyenne 1, est atteint pour le réseau triangulaire – aussi appelé dans ce contexte réseau d'Abrikosov [23] – Λ_1 de densité 1. En effet, le fait de soumettre un matériau supraconducteur de type II à un champ magnétique le traversant fait apparaître des vortex, quand l'intensité de ce champ est suffisamment fort, qui se placent sur un réseau triangulaire parfait (voir Figure 11).

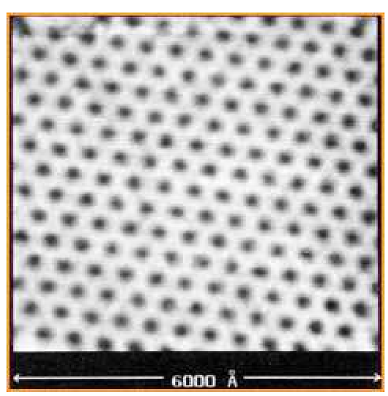


FIGURE 11 – Observation de vortex dans un supraconducteur – Hess et al. [55]

23. Le physicien Abrikosov (1928-) avait prédit dans [1] l'apparition d'une telle structure périodique pour les vortex, ce qui lui valut le Prix Nobel de Physique en 2003, mais en privilégiant le réseau carré, erreur due à la très faible différence d'énergie entre ces deux structures.

Ils ont d'ailleurs prouvé dans [86, Theorem 2] – et nous redonnons, dans notre **Théorème 4.2.3** du **Chapitre 4**, une preuve de ce résultat utilisant l'optimalité de Λ_1 pour la hauteur du tore plat démontrée par Osgood, Phillips et Sarnak [78] – que Λ_1 est l'unique minimiseur, à rotation près, de W parmi les réseaux de Bravais de densité 1, c'est-à-dire

$$\operatorname{argmin}\{W(L); L = \mathbb{Z}u \oplus \mathbb{Z}v, |L| = 1\} = \Lambda_1.$$

Enfin, dans notre **Théorème 4.7.7** du **Chapitre 4**, nous montrons que les conjectures de Sandier-Serfaty et de Brauchart-Hardin-Saff sont équivalentes, c'est-à-dire que

$$\min_{\mathcal{A}_1} W = W(\Lambda_1) \iff C = C_{BHS} = 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)},$$

en utilisant la formule de Chowla-Selberg [28], construisant ainsi un pont entre deux thèmes de Recherche actuels en liant la conjecture des vortex avec le septième problème de Smale.

Chapitre 1

Sufficient Condition for a Compact Local Minimality of a Lattice

Ce chapitre fait référence à la prépublication [8].

Sommaire

1.1 Introduction

As explained by Blanc and Lewin [14], the crystallization problem, that is to say to understand why the particles structures are periodic at low temperature, is difficult and still open in the main cases. Theil [99] exhibited a radial parametrized long-range potential with the same form as the Lennard-Jones potential such that the triangular lattice is the ground state of the total energy in the sense of thermodynamic limit. This kind of potential, parametrized by a real $\alpha > 0$, is larger than α^{-1} close to the origin, corresponding to exclusion Pauli's principle, it has a well centred in 1 and a 2α width, its second derivative at 1 is strictly positive and its decay at infinity is $r \mapsto \alpha r^{-7}$. Thus, as small is α, as close to 1 is the mutual distance between nearest neighbours of the ground state configuration and the interactions between distant points are negligible.

In this chapter, our idea is to present a parametrized potential very close to this one,

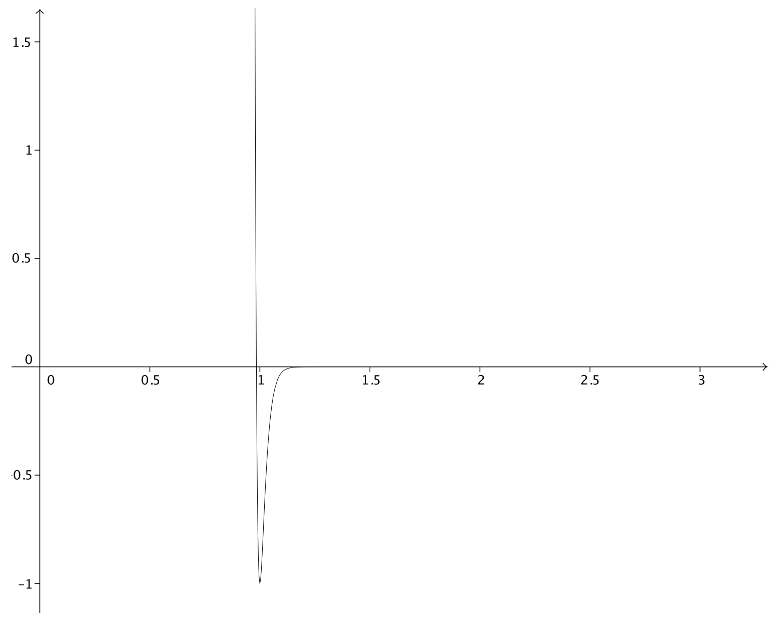


FIGURE 1.1 – Example of Theil's potential

with the most natural possible assumptions, such that a given Bravais lattice L of $\mathbb{R}^d$ is a "N-compact" local minimum for the total energy of interaction. This kind of local minimality is called "N-compact" because, given a maximal number N of points that we want to move a little bit, there exists a maximal perturbation of the points which gives a larger total energy of interaction, in the sense of the difference of energies is positive. Moreover, as small is the parameter, as large the number N can be taken. We strongly inspire Theil's potential, keeping only local assumptions and strong parametrized decay. Furthermore, our work can be related to that of Torquato et al. about targeted self-assembly [84, 100] where they search radial potentials such that a given configuration – more precisely a part of a lattice – is a ground state for the total energy of interaction.

After defining the concepts and our parametrized potentials, we give the theorem, its proof and some important remarks and applications.

1.2 Preliminaries : Bravais lattice and N-compact local minimality

Definition 1.2.1. *Let $d \in \mathbb{N}^*$, $(u_1, ..., u_d)$ be a basis of $\mathbb{R}^d$ and $L = \bigoplus_{i=1}^n \mathbb{Z}u_i \subset \mathbb{R}^d$ be a Bravais lattice. For any $\lambda > 0$, we define $m(\lambda) := \sharp\{L \cap \{\|x\| = \lambda\}\}$ where $\|\cdot\|$ denote the Euclidean norm and $\sharp A$ is the cardinal of set A. Moreover, we call $\lambda_1 := \min\{\|x\|; x \in L^*\}$, where $L^* = L\backslash\{0\}$, and $\lambda_2 := \min\{\|x\|; \|x\| > \lambda_1, x \in L\}$. Furthermore, for a Bravais lattice $L \subset \mathbb{R}^d$, we define the following both lattice sums, for $n > d$,*

$$\zeta_L^*(n) := \sum_{\substack{x\in L \\ \|x\|>\lambda_1}} \|x\|^{-n},$$

$$\bar{\zeta}_L(n) := \sum_{\substack{x\in L \\ \|x\|>\lambda_1}} (\|x\| - \lambda_1)^{-n}.$$

Definition 1.2.2. *Let $L \subset \mathbb{R}^d$ be a Bravais lattice, $B \subset L$ be a finite subset and α be a real such that $0 < \alpha < \lambda_1/2$. We say that B^α, with $\sharp B^\alpha = \sharp B$, is an α-**compact perturbation** of B if*

$$\forall b \in B, \exists! b^\alpha \in B^\alpha \text{ such that } \|b - b^\alpha\| \leq \alpha.$$

Moreover, if B^α is an α-compact perturbation of $B \subset L$, we write $L^\alpha(B) := (L\backslash B) \cup B^\alpha$ the perturbed lattice.

Definition 1.2.3. *Let $d \in \mathbb{N}^*$. We say that $V : \mathbb{R}_+^* \to \mathbb{R}$ is a **d-admissible potential** if V is a C^3 function and, for any Bravais lattice $L \subset \mathbb{R}^d$,*

$$\sum_{x\in L^*} |V(\|x\|)| + \sum_{x\in L^*} \|x\||V'(\|x\|)| + \sum_{x\in L^*} \|x\|^2|V''(\|x\|)| + \sum_{x\in L^*} \|x\|^3|V'''(\|x\|)| < +\infty.$$

Remark 1.2.1. If, for any $k \in \{0, 1, 2, 3\}$, $|V^{(k)}(r)| = O(r^{-p_k})$, $p_k > d + k$, then V is d-admissible.

Definition 1.2.4. *Let L be a Bravais lattice of $\mathbb{R}^d$, V be a d-admissible potential and $N \in \mathbb{N}^*$. We say that L is a **N-compact local minimum for the total V-energy** if for any subset $B \subset L$ such that $\sharp B \leq N$, there exists $\alpha_0 > 0$ such that for any $\alpha \in [0, \alpha_0)$ and any α-compact perturbation B^α of B,*

$$\Delta_L^\alpha(V; B) := \sum_{b^\alpha\in B^\alpha} \sum_{\substack{y\in L^\alpha(B) \\ y\neq b^\alpha}} V(\|b^\alpha - y\|) - \sum_{b\in B} \sum_{\substack{x\in L \\ x\neq b}} V(\|b - x\|) \geq 0.$$

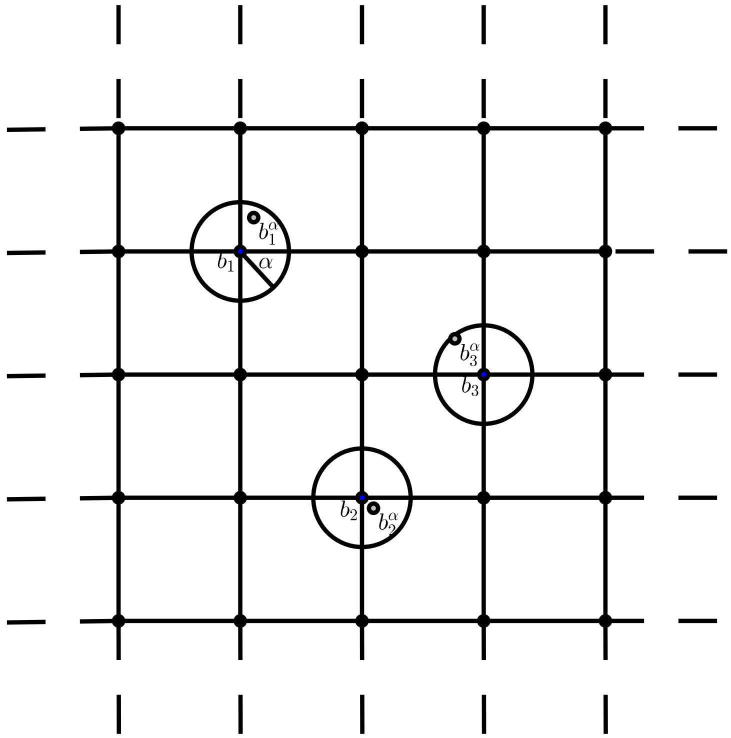


FIGURE 1.2 – An α-compact perturbation of $B = \{b_1, b_2, b_3\}$ with $L = \mathbb{Z}^2$.

1.3 Parametrized potential and main result

Definition 1.3.1. *Let $L \subset \mathbb{R}^d$ be a Bravais lattice. We call **parametrized** L**-potential** every d-admissible function $V_\theta : \mathbb{R}_+^* \to \mathbb{R}$, defined for fixed $\theta \in [0, \lambda_1/2)$, satisfying :*

1. ***Zero pressure condition :** it holds $\displaystyle\sum_{x \in L^*} \|x\| V_\theta'(\|x\|) = 0$;*
2. ***Parametrized fast decay :** $\exists r_0 \in [\lambda_1, \lambda_2)$, $\exists \varepsilon > 0$, $\exists p > d+1$ such that for any $r > r_0$, $|V_\theta'''(r)| \leq \theta^{1+\varepsilon} r^{-p-2}$;*
3. ***Local convexity around first neighbours :** $V_\theta''(\lambda_1) > 0$ is independent of θ ;*
4. ***Bounded third derivative :** there exists $M > 0$, independent of θ, such that, for any $\lambda_1/2 < r < \lambda_2$, $|V_\theta'''(r)| \leq M$.*

Theorem 1.3.1. *Let $L \subset \mathbb{R}^d$ be a Bravais lattice, then for any $N \in \mathbb{N}^*$, there exists $\theta_0 > 0$ such that for every $\theta \in [0, \theta_0]$ and every parametrized L-potential V_θ, L is a N-compact local minimum for the total V_θ-energy. Furthermore, in this case, the maximal perturbation α_0 can be chosen equal to θ.*

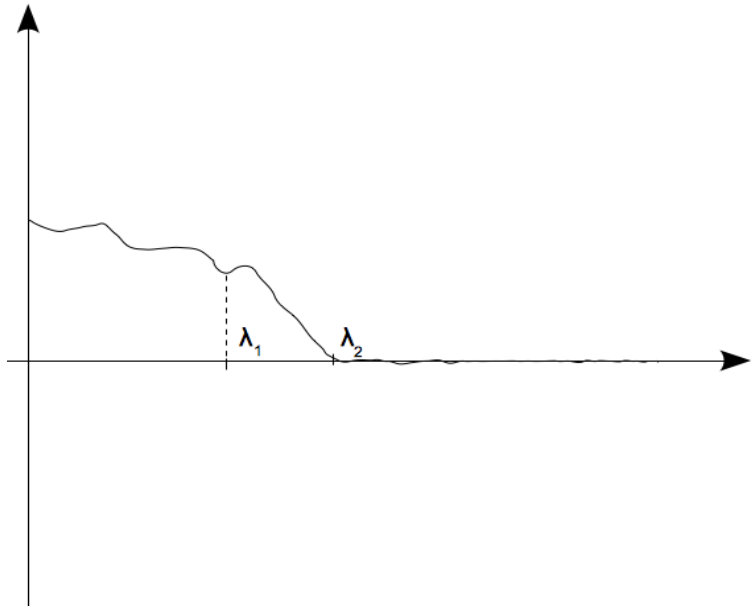


FIGURE 1.3 – Example of potential V_θ

Proof. Let L be a Bravais lattice of $\mathbb{R}^d$. Let $N \in \mathbb{N}^*$ and $B := \{b_1, ..., b_N\}$. Let α_0 be such that $0 \leq \alpha_0 < \lambda_1/2$ and $B^{\alpha_0} = \{b_1^{\alpha_0}, ..., b_N^{\alpha_0}\}$ be a α_0-compact perturbation of B. For any $1 \leq i \leq N$, for any $y \in L^{\alpha_0}(B)$, $y \neq b_i^{\alpha_0}$, and $x \in L$ such that $\|x - y\| \leq \alpha_0$, we define

$$\alpha_{i,x} := \|b_i^{\alpha_0} - y\| - \|b_i - x\|.$$

We assume, without loss of generality, that $\max_{i,x} |\alpha_{i,x}| = 2\alpha_0$, left to decrease α_0. We set $\theta \in [0, \lambda_1/2)$ and V_θ a L-parametrized potential. We have

$$\Delta_L^{\alpha_0}(V_\theta; B) = \sum_{i=1}^N \sum_{\substack{y \in L^{\alpha_0}(B) \\ y \neq b_i^{\alpha_0}}} V_\theta(\|b_i^{\alpha_0} - y\|) - \sum_{i=1}^N \sum_{\substack{x \in L \\ x \neq b_i}} V_\theta(\|b_i - x\|).$$

By Taylor expansion, we get, for any $1 \leq i \leq N$, for any $y \in L^{\alpha_0}(B)$, $y \neq b_i^{\alpha_0}$, and $x \in L$ such that $\|x - y\| \leq \alpha_0$,

$$V_\theta(\|b_i^{\alpha_0} - y\|) \geq V_\theta(\|b_i - x\|) + \alpha_{i,x} V_\theta'(\|b_i - x\|) + \frac{\alpha_{i,x}^2}{2} V_\theta''(\|b_i - x\|) - \frac{|\alpha_{i,x}|^3}{6} \|V_\theta'''\|_{i,x}$$

where $\|V_\theta'''\|_{i,x} := \sup\{|V_\theta'''(r)|; \|b_i - x\| - \alpha_{i,x} < r < \|b_i - x\| + \alpha_{i,x}\}$. Hence we obtain

$$\Delta_L^{\alpha_0}(V_\theta; B) \geq \sum_{i=1}^N \sum_{\substack{x \in L \\ x \neq b_i}} \alpha_{i,x} V_\theta'(\|b_i - x\|) + \frac{1}{2} \sum_{i=1}^N \sum_{\substack{x \in L \\ x \neq b_i}} \alpha_{i,x}^2 V_\theta''(\|b_i - x\|) - \frac{1}{6} \sum_{i=1}^N \sum_{\substack{x \in L \\ x \neq b_i}} |\alpha_{i,x}|^3 \|V_\theta'''\|_{i,x}.$$

Now we cut interactions into two parts : the short range and the long range. For any $1\leq i\leq N$, we set

$$\mathcal{S}_L^i:=\{x\in L; \|x-b_i\|=\lambda_1\}\quad \text{and}\quad \mathcal{L}_L^i:=\{x\in L; \|x-b_i\|>\lambda_1\}.$$

As we assume that for all $r>r_0$, $|V_\theta'''(r)|\leq \theta^{1+\varepsilon}r^{-p-2}$, and V_θ',V_θ'' go to 0 at $+\infty$, we have, by a simple argument, that $|V_\theta'(r)|\leq \theta^{1+\varepsilon}r^{-p}$ and $|V_\theta''(r)|\leq \theta^{1+\varepsilon}r^{-p-1}$ for all $r>r_0$. Therefore we get the following inequalities :

$$\sum_{i=1}^N\sum_{\substack{x\in L\\ x\neq b_i}}\alpha_{i,x}V_\theta'(\|b_i-x\|)\geq V_\theta'(\lambda_1)\left(\sum_{i=1}^N\sum_{x\in\mathcal{S}_L^i}\alpha_{i,x}\right)-2\alpha_0\theta^{1+\varepsilon}\sum_{i=1}^N\sum_{x\in\mathcal{L}_L^i}\frac{1}{\|b_i-x\|^p},$$

$$\frac{1}{2}\sum_{i=1}^N\sum_{\substack{x\in L\\ x\neq b_i}}\alpha_{i,x}^2V_\theta''(\|b_i-x\|)\geq \frac{V_\theta''(\lambda_1)}{2}\left(\sum_{i=1}^N\sum_{x\in\mathcal{S}_L^i}\alpha_{i,x}^2\right)-2\alpha_0^2\theta^{1+\varepsilon}\sum_{i=1}^N\sum_{x\in\mathcal{L}_L^i}\frac{1}{\|b_i-x\|^{p+1}}.$$

As $\displaystyle\sum_{x\in L^*}\|x\|V_\theta'(\|x\|)=0$, we have $\displaystyle V_\theta'(\lambda_1)=-\frac{1}{m(\lambda_1)\lambda_1}\sum_{\substack{x\in L\\ |x|>\lambda_1}}\|x\|V_\theta'(\|x\|)$. As L is a Bravais lattice, for any $1\leq i\leq N$, $\sharp\mathcal{S}_L^i=m(\lambda_1)$ and we obtain

$$\begin{aligned}\left|V_\theta'(\lambda_1)\left(\sum_{i=1}^N\sum_{x\in\mathcal{S}_L^i}\alpha_{i,x}\right)\right|&\leq\frac{1}{m(\lambda_1)\lambda_1}\left(\sum_{x\in\mathcal{L}_L^0}\|x\||V_\theta'(\|x\|)|\right)\left(\sum_{i=1}^N\sum_{x\in\mathcal{S}_L^i}|\alpha_{i,x}|\right)\\ &\leq\frac{2\alpha_0\theta^{1+\varepsilon}N}{\lambda_1}\zeta_L^*(p-1).\end{aligned}$$

As L is a Bravais lattice, we have, for any $b_i\in B\subset L$ and any $p>d$,

$$\sum_{x\in\mathcal{L}_L^i}\frac{1}{\|b_i-x\|^p}=\zeta_L^*(p),$$

and it follows that

$$\sum_{i=1}^N\sum_{\substack{x\in L\\ x\neq b_i}}\alpha_{i,x}V_\theta'(\|b_i-x\|)\geq -2\alpha_0\theta^{1+\varepsilon}N\left(\lambda_1^{-1}\zeta_L^*(p-1)+\zeta_L^*(p)\right).$$

Since $\max\limits_{i,x}|\alpha_{i,x}|=2\alpha_0$, it is clear that $\displaystyle\sum_{i=1}^N\sum_{x\in\mathcal{S}_L^i}\alpha_{i,x}^2\geq 4\alpha_0^2$, and we obtain

$$\frac{1}{2}\sum_{i=1}^N\sum_{\substack{x\in L\\ x\neq b_i}}\alpha_{i,x}^2V_\theta''(\|b_i-x\|)\geq 2V_\theta''(\lambda_1)\alpha_0^2-2N\alpha_0^2\theta^{1+\varepsilon}\zeta_L^*(p+1).$$

Now we remark that $-\dfrac{1}{6}\sum_{i=1}^N\sum_{\substack{x\in L\\x\neq b_i}}|\alpha_{i,x}|^3\|V_\theta'''\|_{i,x}\geq -\dfrac{4}{3}\alpha_0^3\sum_{i=1}^N\sum_{\substack{x\in L\\x\neq b_i}}\|V_\theta'''\|_{i,x}$. Moreover,

$$\begin{aligned}\sum_{i=1}^N\sum_{\substack{x\in L\\x\neq b_i}}\|V_\theta'''\|_{i,x}&=\sum_{i=1}^N\sum_{x\in\mathcal{S}_L^i}\|V_\theta'''\|_{i,x}+\sum_{i=1}^N\sum_{x\in\mathcal{L}_L^i}\|V_\theta'''\|_{i,x}\\&\leq MNm(\lambda_1)+\theta^{1+\varepsilon}\sum_{i=1}^N\sum_{x\in\mathcal{L}_L^i}\frac{1}{(\|b_i-x\|-|\alpha_{i,x}|)^{p+2}}\\&\leq MNm(\lambda_1)+\theta^{1+\varepsilon}N\bar{\zeta}_L(p+2),\end{aligned}$$

because $|\alpha_{i,x}|<\lambda_1$. Finally we get, for any $0\leq\alpha_0<\lambda_1/2$ and every $0\leq\alpha\leq\alpha_0$,

$$\begin{aligned}\Delta_L^\alpha(V_\theta;B)\geq&2V_\theta''(\lambda_1)\alpha_0^2-2N\left[\alpha_0^2\theta^{1+\varepsilon}\zeta_L^*(p+1)+\frac{2}{3}M\alpha_0^3m(\lambda_1)+\frac{2}{3}\alpha_0^3\theta^{1+\varepsilon}\bar{\zeta}_L(p+2)\right.\\&\left.+\alpha_0\theta^{1+\varepsilon}\left(\lambda_1^{-1}\zeta_L^*(p-1)+\zeta_L^*(p)\right)\right].\end{aligned}$$

Given $\theta\in[0,\lambda_1/2)$, if we choose $\alpha_0=\theta$, then there exist positive real A,C,D,E, independent of θ, such that

$$\Delta_L^\theta(V_\theta;B)\geq 2V_\theta''(\lambda_1)\theta^2-N\left(A\theta^{2+\varepsilon}+C\theta^3+D\theta^{3+\varepsilon}+E\theta^{4+\varepsilon}\right).\tag{1.3.1}$$

As $V_\theta''(\lambda_1)>0$ is also independent of θ, there exists $\theta_0\in[0,\lambda_1/2)$, depending on N, sufficiently small such that for any $\theta\in[0,\theta_0]$ and for any $\alpha\in[0,\theta]$, $\Delta_L^\alpha(V_\theta;B)\geq 0$ and then L is a N-compact local minimum for the total V_θ-energy, for any parametrized L-potential V_θ. □

1.4 Remarks

1. Zero pressure condition and local minimality among dilated of L. As explained for instance in [4], if $E_{V_\theta}[L]:=\sum_{x\in L^*}V_\theta(\|x\|)$ is the energy per particle of L, i.e. the free energy at zero temperature, then, by usual thermodynamics formula, we define pressure P and isothermal compressibility κ_T by

$$\begin{aligned}&P:=-\frac{dE_{V_\theta}[L]}{dA}=-\frac{1}{2A}\sum_{x\in L^*}\|x\|V_\theta'(\|x\|),\\&\frac{1}{\kappa_T}:=-A\frac{dP}{dA}=A\frac{d^2E_{V_\theta}[L]}{dA^2}=\frac{1}{4A}\sum_{x\in L^*}\left[\|x\|^2V_\theta''(\|x\|)-\|x\|V_\theta'(\|x\|)\right].\end{aligned}$$

where A is the area of L (i.e. the inverse of the density of points of L). As we want to have L as a N-compact local minimum for arbitrary large N in an infinite volume, it is thermodynamically natural – for instance if L is the cooling of an ideal gas – to suppose $P = 0$ at zero temperature, which gives a kind of justification of the necessity of the zero pressure condition 1. in Definition 1.3.1.

Moreover, we know that $\kappa_T > 0$ (see [95, Section 5.1]), therefore

$$\sum_{x\in L^*} \|x\|^2 V_\theta''(\|x\|) > 0.$$

Actually, that follows here from assumptions on V_θ, if L is a N-compact local minimum for the total V_θ-energy with N sufficiently large. Indeed, by assumption, we have, for θ sufficiently small,

$$\sum_{x\in L^*} \|x\|^2 V_\theta''(\|x\|) \geq m(\lambda_1)\lambda_1 V_\theta''(\lambda_1) - \theta^{1+\varepsilon}\zeta_L^*(p+1) > 0.$$

Now if we consider $f : r \mapsto E_{V_\theta}[rL]$, we get, by $P = 0$ and $\kappa_T \geq 0$, $f'(1) = 0$ and $f''(1) > 0$ and L **is a local minimum of $\tilde{L} \mapsto E_{per}[V_\theta; \tilde{L}]$ among its dilated**, which seems natural if L is a N-compact local minimum for the total V_θ-energy for N sufficiently large. We remark that this hypothesis is assumed in Theil's paper [99].

However, the reverse is false. A Bravais lattice can be a local minimum among its dilated for the energy per point but not a N-compact local minimum for the total energy. For instance, if $d = 1$, $L = \mathbb{Z}$, $N = 1$ and V defined by $V(r) = 0$ for $r \geq 5/2$, $V'(1) = V'(2) = 0$, $V''(1) = -1$ and $V''(2) = 1/3$. We have $\sum_{x\in\mathbb{Z}^*} |x|V'(|x|) = 0$ and $\sum_{x\in\mathbb{Z}^*} |x|^2 V''(|x|) = 2/3 \geq 0$ hence $\mathbb{Z}$ is a local minimum, among its dilated, of the V-energy per point. For $\alpha \geq 0$, we estimate, by Taylor expansion,

$$\begin{aligned}
\Delta^\alpha(V; L) &= \sum_{x\in\mathbb{Z}^*} [V(|x-\alpha|) - V(|x|)] \\
&= V(1-\alpha) + V(1+\alpha) - 2V(1) + V(2-\alpha) + V(2+\alpha) - 2V(2) \\
&= \alpha^2 V''(1) + \alpha^2 V''(2) + \alpha^2\phi(\alpha) = \alpha^2(-2/3 + \phi(\alpha))
\end{aligned}$$

where $\phi(\alpha)$ goes to 0 as $\alpha \to 0$. Hence for $\alpha < \alpha_0$ sufficiently small, $-2/3 + \phi(\alpha) < 0$ and $\mathbb{Z}$ is not a 1-compact local minimum of the total V-energy.

2. Effects of parameters ε, p and $V_\theta''(\lambda_1)$. By (1.3.1), our assumptions on V_θ give indications about the stability of lattice L :

— Range : a larger p or a larger ε allows to take a larger perturbation α_0 for fixed N, i.e. a better "collapse" at infinity implies a stronger stability of the lattice ;

— Second derivative around nearest-neighbours distance : a larger $V_\theta''(\lambda_1)$ also allows a larger perturbation α_0 for fixed N. Typically, a narrow well around λ_1 "catches" the first neighbours of the minimizing configuration at distance λ_1.

3. Difference between the collapse after the first distance and the perturbation. We can see, for $\theta < 1$, that $\theta^{1+\varepsilon} << \theta$, i.e. the collapse is really smaller than the perturbation and this allows to do not assume a local behaviour of V_θ around λ_1 with respect to θ, as in Theil's work. Obviously, if $\theta = 0$ then $V_0(r) = 0$ for any $r > r_0$ and $V_0'(\lambda_1) = 0$, therefore λ_1 is a local minimum of V_0 and the potential is short-range : only the first neighbours interact and the N-compact local minimality is clear for any N with a perturbation α_0 as small as N is large.

4. A kind of Cauchy-Born rule. Our result can be viewed like a justification of a kind of Cauchy-Born rule (see [77, 37]). Indeed, if we consider a solid as a Bravais lattice L where the inside is a finite part of L with cardinal N and the rest is its boundary, a small linear perturbation of the inside, depending on N, increases the total energy of interaction in the solid. That is to say that the inside of the solid follows its boundary to a stable configuration.

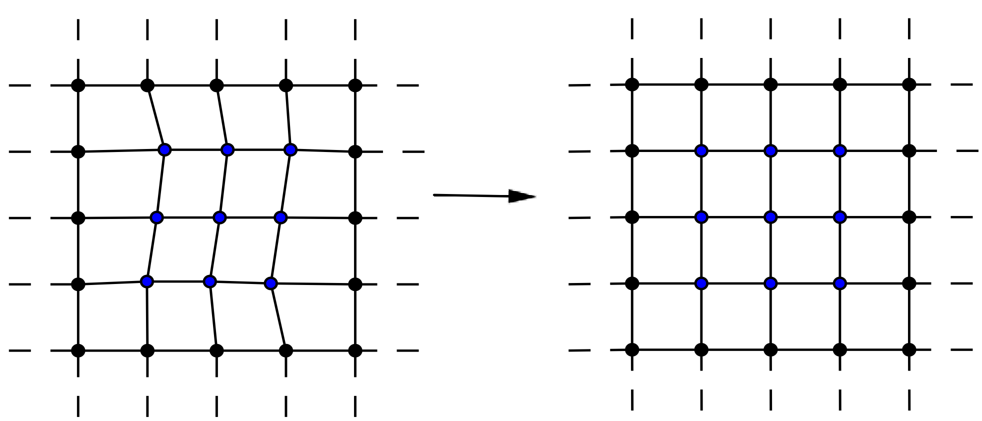


FIGURE 1.4 – A kind of Cauchy-Born rule

5. Numerical example. If we let $d = 2$, $V_\theta''(1) = 1$, $M = 1$, $p = 4\,;\ \varepsilon = 1$ and L is the triangular lattice of length 1, i.e. $L = A_2 = \mathbb{Z}(1,0) \oplus \mathbb{Z}(1/2, \sqrt{3}/2)$, then we get $\zeta_L^*(p-1) \approx 4.9616984$, $\zeta_L^*(p) \approx 1.710774$, $\zeta_L^*(p+1) \approx 0.761895$, $\bar{\zeta}_L(p+2) \approx 15.50957$. Hence, by (1.3.1), we have

$$\Delta_{A_2}^\theta(V_\theta; B) \geq 2\theta^2 \left[1 - N(10.3397\theta^3 + 0.761895\theta^2 + 10.67247\theta^3)\right].$$

For any $k \in \mathbb{N}$, if $N = 10^k$, then the maximal perturbation is a least $\theta_0 \approx 10^{-k-1}$ and the collapse is at least $\theta_0^{1+\varepsilon} \approx 10^{-2k-2}$.
Actually, (1.3.1) is true for any $\theta \in [0, \theta_0]$ if

$$\theta_0 \leq \left(\frac{V_\theta''(\lambda_1)}{\Phi}\right)^{1/\varepsilon} \times N^{-1/\varepsilon}$$

where $\Phi = \zeta_L^*(p+1) + \frac{2}{3}m(\lambda_1)M + \frac{2}{3}\bar{\zeta}_L(p+2) + \lambda_1^{-1}\zeta_L^*(p-1) + \zeta_L^*(p)$, which gives a computable lower bound of a maximal perturbation of a finite set with cardinal N.

Chapitre 2

2D Theta Functions and Crystallization among Lattices

Ce chapitre fait référence à la prépublication [7]. Celle-ci fut écrite après [10], dont les résultats seront présentés au chapitre suivant.

Sommaire

2.1 Introduction and statement of the main results

The two-dimensional crystallization phenomenon – that is to say the formation of periodic structures in matter, most of the time at very low temperatures, – is well known and observed. For instance, similarly to [76], the following may be mentioned : Langmuir monolayers, Wigner crystal [1], rare gas atoms adsorbed on graphite, colloidal suspensions, dusty plasma and, from another point of view, vortices in superconductors. In all these cases, particle interactions are complex (quantum effects, kinetic energy, forces related to the environment) and this implies that the physical and mathematical understanding of this kind of problem is highly complicated. However, we would like to know the precise mechanisms that favour the emergence of these periodic structures in order to predict crystal shapes or to build new materials.

Semiempirical model potential with experimentally determined parameters are widely used in various physical and chemical problems, and for instance in Monte Carlo simulation studies of clusters and condensed matter. A widespread model is the radial potential, also called "two-body potential", which corresponds to interaction only depending on distances between particles. This kind of potential, based on approximations, seems to be effective to show the behaviour of matter at very low temperature, when potential energy dominates the others. There are many examples, that can be found in [56], but they are usually constructed, except for very simple models such as Hard-sphere, with inverse power laws and exponential functions, which are easily calculated with a computer if we consider a very large number of particles. For instance we can cite :

— the Lennard-Jones potential $r \mapsto \dfrac{a_2}{r^{x_2}} - \dfrac{a_1}{r^{x_1}}$, where the attractive term corresponds to the dispersion dipole-dipole (van der Waals : $\sim r^{-6}$) interaction,

1. In a system of interacting electrons, where the coulomb interaction energy between them sufficiently dominates the kinetic energy or thermal fluctuations

initially proposed by Lennard-Jones [61] to study the thermodynamic properties of rare gases and now widely used to study various systems, the best know being for $(x_1, x_2) = (6, 12)$;

— the Buckingham potential $r \mapsto a_1 e^{-\alpha r} - \frac{a_2}{r^6} - \frac{a_3}{r^8}$ proposed by Buckingham [23] and including attractive terms due to the dispersion dipole-dipole ($\sim r^{-6}$) and dipole-quadrupole ($\sim r^{-8}$) interactions, and repulsive terms approximated by an exponential function ;

— the purely repulsive screened Coulomb potential $r \mapsto a\frac{e^{-br}}{r}$, also called "Yukawa potential", proposed by Bohr [16] for short atom-atom distances and used for describing interactions in colloidal suspensions, dusty plasmas and Thomas-Fermi model for solids [13, 10] ;

— the Born-Mayer potential $r \mapsto ae^{-br}$ used by Born and Mayer [17] in their study of the properties of ionic crystals in order to describe the repulsion of closed shells of ions.

Many mathematical works [2] were conducted with various assumptions on particles interaction : hard sphere potentials [54, 80] ; oscillating potentials [96] ; radial (parametrized or not) potentials [103, 99, 36, 109] ; molecular simulations with radial potentials [67, 83, 13] ; three-body (radial and angle parts) potentials [65, 66, 64] ; radial potentials and crystallization among Bravais lattices (Number Theory results and applications) [39, 82, 25, 78, 49, 33, 31, 32, 88, 74, 10] ; vortices, in superconductors, among Bravais lattice configurations [86, 110, 9]. Writing these problems in terms of energy minimization is common to all these studies. Furthermore, in many cases, triangular lattices (also called "Abrikosov lattices" in Ginzburg-Landau theory [1], or sometimes "hexagonal lattices"), which achieves the best-packing configuration in two dimensions, is a minimizer for the corresponding energy.

A clue to understanding this optimality, which is claimed by Cohn and Kumar [30, p. 139] [3], is the fact that triangular lattice minimizes, among Bravais lattices, at fixed density, energies

$$L \mapsto E_f[L] := \sum_{p \in L \backslash \{0\}} f(\|p\|^2)$$

where $\|\cdot\|$ denotes Euclidean norm in $\mathbb{R}^2$ and $f : \mathbb{R}_+^* \to \mathbb{R}$ is a completely monotonic function, i.e. $\forall k \in \mathbb{N}, \forall r \in \mathbb{R}_+^*, (-1)^k f^{(k)}(r) \geq 0$. Moreover, Cohn and Kumar conjectured, in [30, Conjecture 9.4], that the triangular lattice seems to minimize energies

2. We cite only papers about 2D problems.

3. A proof of this assertion will be given in Section 2.3

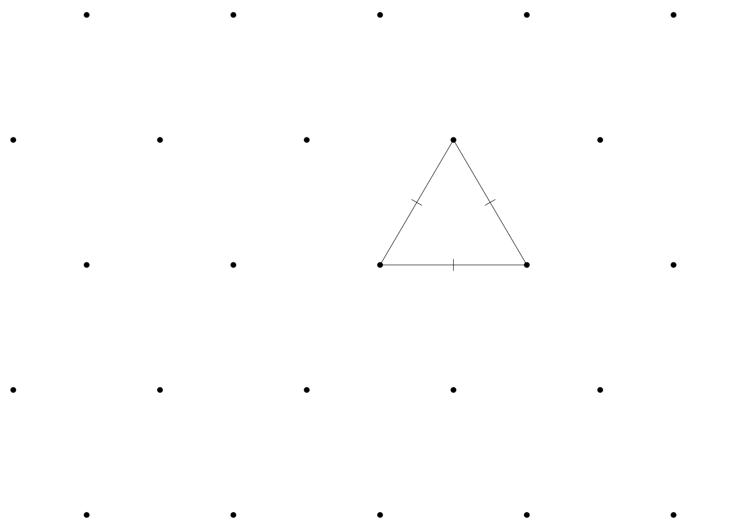


FIGURE 2.1 – Triangular lattice

E_f among complex lattices, i.e. union of Bravais lattices, with a fixed density. Hence, it is not surprising, as for the Lennard-Jones potential we studied in [10], that some non-convex sums of completely monotonic functions give triangular minimizer for their energies at high fixed density. We observed this behaviour in works of Torquato et al. [67, 83]. However, it is important to distinguish mathematical results and physical consistency. Indeed, at very high density i.e. when particles are sufficiently close, kinetic and quantum effects cannot be ignored and our model fails. For instance, Wigner crystal appears if the density is sufficiently low and matter obviously cannot be too condensed. Nevertheless, this kind of result is interesting, whether in Number Theory or in Mathematical Physics and this study of energy among Bravais lattices is the first important step in the search for global ground state, i.e. minimizer among all configurations. For instance, we have recently found in [9] a deep connexion between the behaviour of vortices in the Ginzburg-Landau theory, which is studied by Sandier and Serfaty [86, 87, 90], and optimal logarithmic energy on the unit sphere related to Smale 7th Problem. Thus the optimality of triangular lattice, among Bravais lattices, for a renormalized energy W, which is a kind of Coulomb energy between points in the whole plane, gives important information about optimal asymptotic expansion of spherical logarithmic energy thanks to works by Saff et al. [81, 22].

The aim of this chapter is to prove this minimality of triangular lattice at high density, with the same strategy as in our previous work [10], that is to say the use of Montgomery result [74] about optimality of triangular lattice at a fixed density for theta functions

$$L \mapsto \theta_L(\alpha) := \sum_{p \in L\backslash\{0\}} e^{-2\pi\alpha\|p\|^2},$$

for some general admissible [4] potentials f, summable on lattices and such that their inverse Laplace transforms μ_f exist on $[0, +\infty)$. Hence, as in the classical "Riemann's trick" that we used in [10], we can write an integral representation of energy E_f which we deduce a sufficient condition for minimality of triangular lattice among Bravais lattices of fixed density [5]. This is precisely the aim of our first main theorem, which we now state.

Theorem 2.1.1. *For any admissible potential f, for any $A > 0$ and any Bravais lattice L of area A, there exists a constant C_A, which not depends on L, such that*

$$E_f[L] = \frac{\pi}{A}\int_1^{+\infty} \left[\theta_L\left(\frac{y}{2A}\right) - 1\right]\left[y^{-1}\mu_f\left(\frac{\pi}{yA}\right) + \mu_f\left(\frac{\pi y}{A}\right)\right] dy + C_A \qquad (2.1.1)$$

where μ_f is the inverse Laplace transform of f. Moreover, if

$$y^{-1}\mu_f\left(\frac{\pi}{yA}\right) + \mu_f\left(\frac{\pi y}{A}\right) \geq 0 \quad \text{a.e. on } [1, +\infty) \qquad (2.1.2)$$

then the triangular lattice of area A, i.e. $\Lambda_A = \sqrt{\frac{2A}{\sqrt{3}}}\left[\mathbb{Z}(1,0) \oplus \mathbb{Z}(1/2, \sqrt{3}/2)\right]$, is the unique minimizer of $L \mapsto E_f[L]$, up to rotation, among Bravais lattices of fixed area A.

Sufficient condition (2.1.2) can be applied for some general functions f. More precisely, we will consider the following potentials [6], defined for $r > 0$, which we will explain the interest throughout the chapter :

— Sums of screened coulombian potentials :

$$\varphi_{a,x}(r) = \sum_{i=1}^{n} a_i \frac{e^{-x_i r}}{r},$$

4. A rigorous definition will be given in preliminaries.

5. Actually, as in [10], we will write all our results in terms of area, that is to say the inverse of the density.

6. It is important to distinguish potential f and the function $r \mapsto f(r^2)$ that we sum on lattices to compute E_f.

with $0 < x_1 < x_2 ... < x_n$, $a_i \in \mathbb{R}^*$ for all $1 \leq i \leq n$ and $\displaystyle\sum_{i=1}^n a_i \geq 0$;

— Sums of inverse power laws :

$$V_{a,x}(r) = \sum_{i=1}^n \frac{a_i}{r^{x_i}},$$

with $1 < x_1 < x_2 < ... < x_n$, $a_i \in \mathbb{R}^*$ for all $1 \leq i \leq n$ and $a_n > 0$;

— Potentials with exponential decay :

$$f_{a,x,b,t}(r) = V_{a,x}(r) + \sum_{j=1}^m b_j e^{-t_j\sqrt{r}},$$

with $3/2 < x_1 < x_2 < ... < x_n$, $a_i \in \mathbb{R}_+^*$ for all $1 \leq i \leq n$, $a_n > 0$, $b_j \in \mathbb{R}^*$ and $t_j \in \mathbb{R}_+^*$ for all $1 \leq j \leq m$.

Thus, even though our method is not optimal (see Section 2.4.3), we will give explicit area bounds in Propositions 2.5.1, 2.6.3, 2.6.10 and 2.7.2, with respect to potential parameters, below which minimizer is triangular. Furthermore, we give conditions on parameters, for potentials $\varphi_{a,x}^{AR}$ and $V_{a,x}^{LJ}$ in order to get a triangular global minimizer, i.e. without area constraint, in particular when the potential has a well. This is the aim of our second theorem.

Theorem 2.1.2. *Let functions $\varphi_{a,x}, \varphi_{a,x}^{AR}, V_{a,x}, V_{a,x}^{LJ}$ and $f_{a,x,b,t}$ be defined as before.*

A. Minimality at high density. *If $f \in \{\varphi_{a,x}, V_{a,x}, f_{a,x,b,t}\}$ then there exists $A_0 > 0$ such that for any $0 < A \leq A_0$, Λ_A is the unique minimizer, up to rotation, of $L \mapsto E_f[L]$ among Bravais lattices of fixed area A.*

B. Global optimality without an area constraint. *We have the following two cases*

1. *Let $\varphi_{a,x}^{AR}$ be the attractive-repulsive potential defined by*

$$\varphi_{a,x}^{AR}(r) = a_2\frac{e^{-x_2 r}}{r} - a_1\frac{e^{-x_1 r}}{r},$$

where $0 < a_1 < a_2$ and $0 < x_1 < x_2$. If a_1, a_2, x_1, x_2 satisfy

$$\frac{a_1\left(1+\frac{x_1}{x_2}\pi\right)}{a_2(1+\pi)}e^{\left(1-\frac{x_1}{x_2}\right)\pi} \geq 1 \quad \text{and} \quad \frac{a_1\left(a_1x_2+x_1(a_2-a_1)\pi\right)}{a_2x_2\left(a_1+(a_2-a_1)\pi\right)}e^{\left(1-\frac{x_1}{x_2}\right)\left(\frac{a_2}{a_1}-1\right)\pi} \geq 1, \tag{2.1.3}$$

then the minimizer of $L \mapsto E_{\varphi_{a,x}^{AR}}[L]$ *among all Bravais lattices is unique, up to rotation, and triangular. In particular it is true if* $a_2 = 2a_1$ *and* $x_1 \leq 0.695 x_2$.

2. *Let* $V_{a,x}^{LJ}$ *be the Lennard-Jones type potential defined by*

$$V_{a,x}^{LJ}(r) = \frac{a_2}{r^{x_2}} - \frac{a_1}{r^{x_1}},$$

with $1 < x_1 < x_2$ *and* $(a_1, a_2) \in (0, +\infty)^2$. *We set* $h(t) = \pi^{-t}\Gamma(t)t$. *If we have* $h(x_2) \leq h(x_1)$ *then the minimizer* $L_{a,x}$ *of* $L \mapsto E_{V_{a,x}^{LJ}}[L]$ *among all Bravais lattices is unique, up to rotation, and triangular. Moreover its area is*

$$|L_{a,x}| = \left(\frac{a_2 x_2 \zeta_{\Lambda_1}(2x_2)}{a_1 x_1 \zeta_{\Lambda_1}(2x_1)} \right)^{\frac{1}{x_2 - x_1}}.$$

In particular, it is true if $(x_1, x_2) \in \{(1.5, 2); (1.5, 2.5); (1.5, 3); (2, 2.5); (2, 3)\}$[7].

We proceed as follows, we start below with some preliminaries where we recall Montgomery result about optimality of Λ_A for theta functions θ_L and we give the definition of an admissible potential. Then we prove in Section 2.3 the optimality of Λ_A for every A when f is completely monotonic and we give an example of strictly convex, decreasing and positive potential V such that Λ_A is not a minimizer of E_f for some A. Theorem 2.1.1 is proved in Section 2.4, with some general applications. Furthermore we discuss optimality and improvement of this method. Finally we prove our Theorem 2.1.2 in next sections where we present the interest, in molecular simulation, of studied potentials and we prove some additional results. Throughout the chapter, we give numerical values and examples.

7. See Section 2.6 for numerical values.

2.2 Preliminaries

2.2.1 Bravais lattices, zeta functions and theta functions

We briefly recall our notations [10]. Throughout this chapter, $\|\cdot\|$ will denote the Euclidean norm in $\mathbb{R}^2$. Let $L = \mathbb{Z}u \oplus \mathbb{Z}v$ be a **Bravais lattice** of $\mathbb{R}^2$, then by Engel's theorem (see [38]), we can choose u and v such that $\|u\| \leq \|v\|$ and $(\widehat{u,v}) \in \left[\frac{\pi}{3}, \frac{\pi}{2}\right]$ in order to obtain the uniqueness of the lattice, up to rotations and translations and the fact that the lattice is parametrized by its both first lengths $\|u\|$ and $\|v\|$. Furthermore, if the positive definite quadratic form Q associated to lattice L is given by

$$Q(m,n) := \|mu+nv\|^2 = am^2 + bmn + cn^2,$$

we call $D = b^2 - 4ac < 0$ its discriminant.
We note $|L| = \|u \wedge v\| = \|u\|\|v\|\,|\sin(\widehat{u,v})|$ the **area** [8] of L which is in fact the area of its primitive cell. Let $\Lambda_A = \sqrt{\frac{2A}{\sqrt{3}}}\left[\mathbb{Z}(1,0) \oplus \mathbb{Z}(1/2, \sqrt{3}/2)\right]$ be the **triangular lattice** of area A, then $\|u\|$ is called the **length** of this lattice.

For real $s > 2$, the **Epstein zeta function** of a Bravais lattice L is defined by

$$\zeta_L(s) = \sum_{p \in L^*} \frac{1}{\|p\|^s},$$

where $L^* := L\backslash\{0\}$. As proved in [29, Proposition 10.5.5 and Proposition 10.5.7], we can write $\zeta_L(s)$ in term of L-function or Hurwitz zeta function. More precisely, for $L = \mathbb{Z}^2$ and $L = \Lambda_1$ the triangular lattice of area 1, we have, for any $s > 1$,

$$\zeta_{\mathbb{Z}^2}(2s) = 4L_{-4}(s)\zeta(s) = 4^{-s+1}\zeta(s)\left[\zeta(s,1/4) - \zeta(s,3/4)\right], \tag{2.2.1}$$

$$\zeta_{\Lambda_1}(2s) = 6\left(\frac{\sqrt{3}}{2}\right)^s \zeta(s)L_{-3}(s) = 6\left(\frac{\sqrt{3}}{2}\right)^s 3^{-s}\zeta(s)\left[\zeta(s,1/3) - \zeta(s,2/3)\right], \tag{2.2.2}$$

where ζ is the classical Riemann zeta function $\zeta(s) := \sum_{n=1}^{+\infty} n^{-s}$. Function L_D, defined by

$$L_D(s) := \sum_{n=1}^{+\infty} \left(\frac{D}{n}\right) n^{-s}$$

8. We choose, as in [10], to write results in terms of area and not in terms of density (which is its inverse).

is the Dirichlet L-function associated to quadratic field $\mathbb{Q}(i\sqrt{-D})$, with $\left(\frac{D}{n}\right)$ the Legendre symbol. Furthermore, for $x>0$,

$$\zeta(s,x):=\sum_{n=0}^{+\infty}(n+x)^{-s}$$

is the Hurwitz zeta function. Hence both these special values are easily computable.

Now we recall fundamental Montgomery's Theorem, proved in our annex, about optimality of Λ_A among Bravais lattices for theta functions :

Theorem 2.2.1. (Montgomery, [74]) *For any real number $\alpha>0$ and a Bravais lattice L, let*

$$\theta_L(\alpha):=\Theta_L(i\alpha)=\sum_{p\in L}e^{-2\pi\alpha\|p\|^2}, \tag{2.2.3}$$

*where Θ_L is the Jacobi **theta function** of the lattice L defined for $Im(z)>0$. Then, for any $\alpha>0$, Λ_A is the unique minimizer of $L\to\theta_L(\alpha)$, up to rotation, among Bravais lattices of area A.*

Remark 2.2.2. This result implies that the triangular lattice is the unique minimizer, up to rotation, of $L\mapsto\zeta_L(s)$ among Bravais lattices with density fixed for any $s>2$ which is also proved by Rankin [82], Cassels [25], Ennola [40] and Diananda [35]. Montgomery deduced this fact by the famous "Riemann's trick" (see [98] or [10] for a proof) : for any L such that $D=1$ and any $s>1$,

$$\zeta_L(2s)\Gamma(s)(2\pi)^{-s}=\frac{1}{s-1}-\frac{1}{s}+\int_1^\infty(\theta_L(\alpha)-1)(\alpha^s+\alpha^{1-s})\frac{d\alpha}{\alpha}. \tag{2.2.4}$$

In Section 2.4, we will prove general Riemann's trick (2.1.1), which we call the integral representation of energy, for an admissible potential in order to use Montgomery method in a general case.

Remark 2.2.3. We can find in [75, Appendice A] other proof of minimality of some theta functions based on result of Osgood, Phillips and Sarnak [78, Corollary 1(b) and Section 4] about Laplacian's determinant of flat torus, which has some deep connection with other energies (for instance, see [9, Theorem 2.3]).

2.2.2 Admissible potential, inverse Laplace transform and lattice energies

Definition 2.2.1. *We say that* $f : \{Re(z) > 0\} \to \mathbb{R}$ *is* ***admissible*** *if :*

1. *there exists* $\eta > 1$ *such that* $|f(z)| = O(|z|^{-\eta})$ *as* $|z| \to +\infty$ *;*
2. f *is analytic on* $\{z \in \mathbb{C}; Re(z) > 0\}$ *;*
3. *we have* $\mu_f \not\equiv 0$*, where* μ_f *is the* ***inverse Laplace transform*** *of* f *defined on* $(0, +\infty)$*.*

If f *is admissible, we define, for any Bravais lattice* L *of* $\mathbb{R}^2$*,*

$$E_f[L] := \sum_{p \in L^*} f(\|p\|^2)$$

which is ***the quadratic energy per point of lattice*** L ***created by potential*** f*.*

Remark 2.2.4. As a consequence of [79, Theorem 5.17, Theorem 5.18], we get, by direct application of inversion integral formula :

- There exists an **unique** inverse Laplace transform μ_f [9], which is continuous on $(0, +\infty)$;
- We have $\mu_f(0) = 0$.

Remark 2.2.5. This definition excludes two-dimensional Coulomb potential, defined by $r \mapsto -\log r$, because all its quadratic energies are infinite. However we can define a renormalized energy as in [86] or in [51].

2.2.3 Completely monotonic functions

The class of completely monotonic functions is central in our work. Indeed, as we will see in Section 2.3, these functions have good properties for our problem of minimization among lattices with fixed area thanks to the Montgomery Theorem 2.2.1.

Definition 2.2.2. *A function* $f : (0, +\infty) \to \mathbb{R}_+$ *of type* C^∞ *is said to be* ***completely monotonic*** *if, for any* $k \in \mathbb{N}$ *and any* $r > 0$*,*

$$(-1)^k f^{(k)}(r) \geq 0.$$

9. We will sometimes write $\mathcal{L}$ and $\mathcal{L}^{-1}$ for Laplace and inverse Laplace operators.

Examples 2.2.6. We can find a lot of examples of completely monotonic functions in [69]. Here we give only some interesting classical admissible potentials f :

— $V_x(r) = r^{-x}, x > 1$;

— $V_{a,x}(r) = \displaystyle\sum_{i=1}^{n} a_i r^{-x_i}$ where $a_i > 0$ and $x_i > 1$ for all i ;

— $f_\alpha(r) = e^{-ar^\alpha}, a > 0, \alpha \in (0,1]$, see [69, Corollary 1] ;

— The modified Bessel functions of the second kind, i.e. one of the two solutions of

$$r^2 y'' + ry' - (r^2 + \nu^2)y = 0$$

which goes to 0 at infinity, is $K_\nu(r) = \int_0^{+\infty} e^{-r\cosh t}\cosh(\nu t)dt$, $\nu \in \mathbb{R}$. Moreover, $r \mapsto K_\nu(\sqrt{r})$ is also completely monotonic.

— $V_{SC}(r) = \dfrac{e^{-a\sqrt{r}}}{\sqrt{r}}$, $a > 0$;

— $\varphi_a(r) = \dfrac{e^{-ar}}{r}$, $a > 0$.

Remark 2.2.7. We remark that if $r \mapsto f(r)$ is completely monotonic, it is not generally the case for $r \mapsto f(r^2)$. For instance $r \mapsto e^{-r}$ is completely monotonic, but $r \mapsto e^{-r^2}$ does not check this property.

Now we give the famous connection between completely monotonic function and Laplace transform due to Bernstein [6].

Theorem 2.2.8. ***(Hausdorff-Bernstein-Widder Theorem)***
A function $f : \mathbb{R}_+^* \to \mathbb{R}$ is completely monotonic if and only if it is the Laplace transform of a finite non-negative Borel measure μ on $\mathbb{R}_+$, i.e.

$$f(r) = \mathcal{L}[\mu](r) := \int_0^{+\infty} e^{-rt} d\mu(t).$$

Remark 2.2.9. If f is admissible and completely monotonic, then

$$d\mu(t) = \mu_f(t)dt \quad \text{and} \quad \mu_f(t) \geq 0, \text{ a.e. on } (0,+\infty).$$

Remark 2.2.10. We know that the positivity of the Fourier transform of a radial potential is a key point in crystallization problems. Indeed Nijboer and Ventevogel [103] proved that it is a necessary condition for a periodic ground state and Süto [96] studied potentials f such that $\hat{f}(k) \geq 0$ and $\hat{f}(k) = 0$ for any $\|k\| > R_0$ and proved some interesting crystallization results at high densities. Unfortunately, as Likos [63] explained, this kind of potential, oscillating and with inverse power law decay, seems to be difficult to achieve physically.

Actually it is more common to use Fourier transform in problems of minimization of lattice energy because we have the Poisson summation formula and the natural periodicity of sinus and cosinus. Furthermore, applications of classical formula allows to obtain some interesting results, as in [30, Proposition 9.3]. However we will show in Section 2.4 that inverse Laplace transform also seems well adapted to our problem and gives simple calculations. Indeed, Fourier methods as in [30, 96, 97] are good for more general minimization problems and our method seems to be a better choice for minimization among Bravais lattices because of the integral representation (2.1.1).

2.2.4 Cauchy's bound for positive root of a polynomial

In this part, we recall Cauchy's rule explained in [26, Note III, Scolie 3, page 388] for upper bound of polynomial's positive roots (see also [105] for simple proof).

Theorem 2.2.11. ***(Cauchy's rule)*** *Let P a polynomial of degree $n>0$ defined by*

$$P(X)=\sum_{i=0}^n \alpha_i X^i, \quad \alpha_n>0,$$

where $\alpha_i<0$ for at least one i, $0\leq i\leq n-1$. If λ is the number of negative coefficients, then an upper bound on the values of the positive roots of P is given by

$$M_P:=\max_{i;\alpha_i<0}\left\{\left(\frac{-\lambda\alpha_i}{\alpha_n}\right)^{\frac{1}{n-i}}\right\}$$

Remark 2.2.12. This Theorem stays true for upper bound on the values of the positive zero of any function p defined by

$$p(y)=\sum_{i=1}^n \alpha_i y^{\nu_i}, \quad \alpha_n>0$$

where $0<\nu_1<...<\nu_n$ are real numbers and we obtain

$$M_p:=\max_{i;\alpha_i<0}\left\{\left(\frac{-\lambda\alpha_i}{\alpha_n}\right)^{\frac{1}{\nu_n-\nu_i}}\right\}. \tag{2.2.5}$$

This result will be useful for technical reasons in the following sections, because we will want positive zeros less than 1 to apply our sufficient condition in Theorem 2.1.1 and to prove Theorem 2.1.2.A.

2.3 Completely monotonic functions and optimality of Λ_A

In this part we begin to state a simple fact connecting the positivity of inverse Laplace transform and minimality among lattices at fixed area. Furthermore we will give an example of strictly convex, decreasing, positive potential for which there exists areas so that the triangular lattice is not a minimizer among Bravais lattices with fixed area.

2.3.1 Optimality at any density

The following proposition, claimed by Cohn and Kumar in [30, page 139], is a natural consequence of Montgomery and Hausdorff-Bernstein-Widder Theorems.

Proposition 2.3.1. *Let f be an admissible potential. If f is completely monotonic then, for any $A>0$, Λ_A is the unique minimizer, up to rotation, of*

$$L\mapsto E_f[L]=\sum_{p\in L^*} f(\|p\|^2)$$

among lattices of fixed area A.

Proof. As f is admissible, we can write

$$f(r)=\int_0^{+\infty} e^{-rt}\mu_f(t)dt,$$

and it follows that

$$\begin{aligned}E_f[L]&=\sum_{p\in L^*} f(\|p\|^2)=\sum_{p\in L^*}\int_0^{+\infty} e^{-t\|p\|^2}\mu_f(t)dt=\int_0^{+\infty}\sum_{p\in L^*} e^{-t\|p\|^2}\mu_f(t)dt\\ &=\int_0^{+\infty}\left[\theta_L\left(\frac{t}{2\pi}\right)-1\right]\mu_f(t)dt.\end{aligned}$$

Thus, we get

$$E_f[L]-E_f[\Lambda_A]=\int_0^{+\infty}\left[\theta_L\left(\frac{t}{2\pi}\right)-\theta_{\Lambda_A}\left(\frac{t}{2\pi}\right)\right]\mu_f(t)dt.$$

If f is completely monotonic, by Theorem 2.2.8, $\mu_f(t)\geq 0$ for almost every $t\in(0,+\infty)$. Moreover, by Montgomery Theorem 2.2.1, for any $t>0$ and any Bravais lattice L of area A,

$$\theta_L\left(\frac{t}{2\pi}\right)-\theta_{\Lambda_A}\left(\frac{t}{2\pi}\right)\geq 0,$$

with equality if and only if $L_A = \Lambda_A$, up to rotation. Hence $E_f[L] \geq E_f[\Lambda_A]$ for any L such that $|L| = A$ with equality if and only if $L_A = \Lambda_A$, up to rotation, and Λ_A is the unique minimizer, up to rotation, of the energy among Bravais lattices of fixed area A. $\square$

Remark 2.3.2. We can imagine that the reciprocal is true, i.e. if f is not completely monotonic, then there exists A_0 such that Λ_{A_0} is not a minimizer among Bravais lattices of fixed area A_0. In next subsection, we will give an explicit example correlated with Marcotte, Stillinger and Torquato results [67] about the existence of unusual ground states with convex decreasing positive potential.

Examples 2.3.3. A direct consequence of this theorem is the minimality of triangular lattice among lattices for any fixed area for the following energies :

— $E_{V_x}[L] = \zeta_L(2x)$, $x > 1$ is the first natural example given by Montgomery in [74],

— $E_{V_{a,x}}[L] = \displaystyle\sum_{i=1}^n a_i \zeta_L(2x_i)$ where $a_i > 0$ and $x_i > 1$ for all i,

— $E_{f_\alpha}[L] = \displaystyle\sum_{p \in L^*} e^{-a\|p\|^{2\alpha}}, \alpha \in (0,1]$, in particular $E_{f_{1/2}}[L] = \displaystyle\sum_{p \in L^*} e^{-a\|p\|}$,

— $E_{K_\nu(\sqrt{\cdot})}[L] = \displaystyle\sum_{p \in L^*} K_\nu(\|p\|)$, $\nu \in \mathbb{R}$ which generalizes our study [10] of lattice energy with potential K_0 in Thomas-Fermi model case;

— $E_{V_{SC}}[L] = \displaystyle\sum_{p \in L^*} \frac{e^{-a\|p\|}}{\|p\|}$, $a > 0$, which corresponds to lattice energy for screened Coulomb potential interaction and it can explain the formation of triangular Wigner crystal at low density [48];

— $E_{\varphi_a}[L] = \displaystyle\sum_{p \in L^*} \frac{e^{-a\|p\|^2}}{\|p\|^2}$, $a > 0$.

2.3.2 Repulsive potential and triangular lattice

In this section we give an example of stricly convex decreasing positive radial potential V so that, for some areas, a minimizer of E_V among Bravais lattices of fixed area cannot be triangular. As Ventevogel and Nijboer [102] proved, a convex decreasing positive potential allows to obtain, in one dimension and for any fixed density, a dilated of lattice $\mathbb{Z}$ as unique minimizer among all configurations. Thus the two-dimensional case is deeply different.

Let

$$V(r)=\frac{14}{r^2}-\frac{40}{r^3}+\frac{35}{r^4} \tag{2.3.1}$$

be the potential and

$$E_V[L]=14\zeta_L(4)-40\zeta_L(6)+35\zeta_L(8)$$

be the quadratic energy per point of a Bravais lattice L.

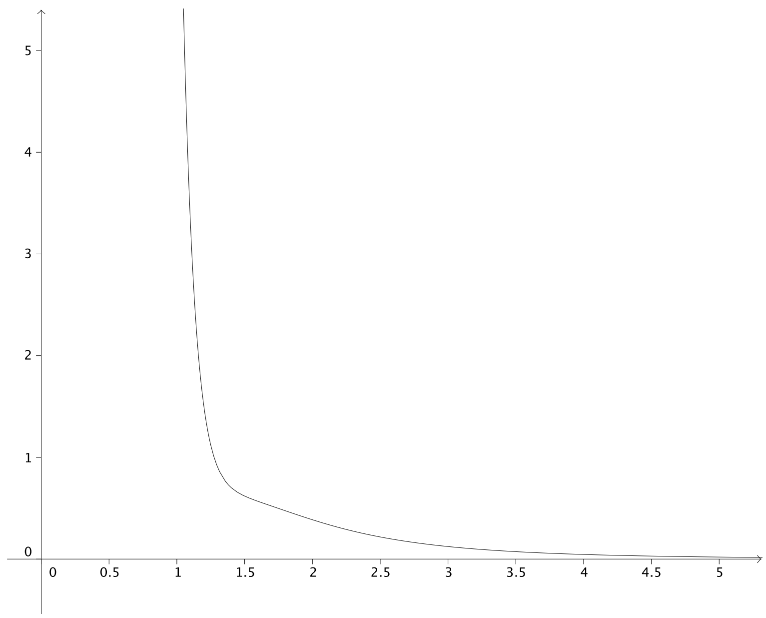


FIGURE 2.2 – Graph of $r\mapsto V(r^2)$

Proposition 2.3.4. ***(Strictly convex potential and non optimality of triangular lattice)*** *Let V be given by (2.3.1), then*

— *V is strictly positive, strictly decreasing and strictly convex on $(0,+\infty)$;*

— *There exist A_1, A_2 such that Λ_A* ***is not a minimizer*** *of E_V among all Bravais lattices of area $A\in(A_1,A_2)$.*

Proof. We have

$$V(r)=\frac{14r^2-40r+35}{r^4}$$

and the discriminant of polynomial $14X^2-40X+35$ is $\Delta_1=-360<0$, hence $V(r)>0$ on $(0,+\infty)$.

We compute

$$V'(r)=\frac{-4(7r^2-30r+35)}{r^5}$$

and the discriminant of $7X^2 - 30X + 35$ is $\Delta_2 = -80 < 0$, therefore $V'(r) < 0$, i.e. V is strictly decreasing on $(0, +\infty)$.
Moreover, we have

$$V''(r) = \frac{4(21r^2 - 120r + 175)}{r^6}$$

and the discriminant of $21X^2 - 120X + 175$ is $\Delta_3 = -300 < 0$, then $V''(r) > 0$ on $(0, +\infty)$, i.e. V is strictly convex on $(0, +\infty)$.
For the second point, we have the following equivalences :

$$\begin{aligned}
&E_V[L] \geq E_V[\Lambda_A] \text{ for any } |L| = A\\
&\iff 14\zeta_L(4) - 40\zeta_L(6) + 35\zeta_L(8) \geq 14\zeta_{\Lambda_A}(4) - 40\zeta_{\Lambda_A}(6) + 35\zeta_{\Lambda_A}(8) \geq 0 \text{ for any } |L| = A\\
&\iff \frac{14}{A^2}\left(\zeta_L(4) - \zeta_{\Lambda_1}(4)\right) + \frac{40}{A^3}\left(\zeta_L(6) - \zeta_{\Lambda_1}(6)\right) + \frac{35}{A^4}\left(\zeta_L(8) - \zeta_{\Lambda_1}(8)\right) \geq 0 \text{ for any } |L| = 1\\
&\iff 14\left(\zeta_L(4) - \zeta_{\Lambda_1}(4)\right)A^2 - 40\left(\zeta_L(6) - \zeta_{\Lambda_1}(6)\right)A + 35\left(\zeta_L(8) - \zeta_{\Lambda_1}(8)\right) \geq 0 \text{ for any } |L| = 1\\
&\iff P_L(A) \geq 0 \text{ for any } |L| = 1
\end{aligned}$$

where the discriminant of

$$P_L(A) = 14\left(\zeta_L(4) - \zeta_{\Lambda_1}(4)\right)A^2 - 40\left(\zeta_L(6) - \zeta_{\Lambda_1}(6)\right)A + 35\left(\zeta_L(8) - \zeta_{\Lambda_1}(8)\right)$$

is

$$\Delta(L) = 1600\left(\zeta_L(6) - \zeta_{\Lambda_1}(6)\right)^2 - 1960\left(\zeta_L(4) - \zeta_{\Lambda_1}(4)\right)\left(\zeta_L(8) - \zeta_{\Lambda_1}(8)\right).$$

For $L = \mathbb{Z}^2$ the square lattice of area 1, we obtain $\Delta(\mathbb{Z}^2) \approx 24.231435 > 0$ then there exist two positive numbers A_1 and A_2 such that $P_{\mathbb{Z}^2}(A) < 0$ for any $A_1 < A < A_2$. Hence, Λ_A is not a minimizer of E_V among Bravais lattices with any fixed area A such that $A_1 < A < A_2$. More precisely we get $A_1 \approx 2.3152307$ and $A_2 \approx 3.759353$. $\square$

Remark 2.3.5. It follows, from the first part of the previous proof, that function $r \mapsto V(r^2)$ is also strictly positive, strictly decreasing and strictly convex on $(0, +\infty)$.

Remark 2.3.6. Actually, the previous proof implies that, for any $A \in (A_1, A_2)$,

$$E_V[\sqrt{A}\mathbb{Z}^2] < E_V[\Lambda_A].$$

Moreover, this interval seems numerically to be optimal, i.e. for any $A \notin [A_1, A_2]$, Λ_A seems to be the unique minimizer, up to rotation, of $L \mapsto E_f[L]$ among Bravais lattices of fixed area A.

2.4 Sufficient condition and first applications

Now we study the case of non completely monotonic potential f, i.e. μ_f is negative on a subset of $(0,+\infty)$ of positive Lebesgue measure.

2.4.1 Integral representation and sufficient condition : Proof of Theorem 2.1.1

Proof. Let L be a Bravais lattice of area A and f be an admissible potential. Firstly we prove the integral representation (2.1.1) of energy $E_f[L]$:

$$E_f[L]:=\sum_{p\in L^*}f(\|p\|^2)=\frac{\pi}{A}\int_1^{+\infty}\left[\theta_L\left(\frac{y}{2A}\right)-1\right]\left(y^{-1}\mu_f\left(\frac{\pi}{yA}\right)+\mu_f\left(\frac{\pi y}{A}\right)\right)dy$$
$$+\frac{\pi}{A}\int_1^{+\infty}\mu_f\left(\frac{\pi}{yA}\right)(y^{-1}-y^{-2})dy.$$

Indeed, for a Bravais lattice L of $\mathbb{R}^2$ with $|L|=1/2$, we have, as in [10], by $t=2\pi u$, $u=y^{-1}$ and Montgomery's identity $\theta_L(y^{-1})=y\theta_L(y)$ (proved in our annex) :

$$\begin{aligned}
&E_f[L]:=\sum_{p\in L^*}f(\|p\|^2)=\sum_{p\in L^*}\int_0^{+\infty}e^{-t\|p\|^2}\mu_f(t)dt=2\pi\sum_{p\in L^*}\int_0^{+\infty}e^{-2\pi u\|p\|^2}\mu_f(2\pi u)dt\\
&=2\pi\int_0^{+\infty}\left[\theta_L(u)-1\right]\mu_f(2\pi u)du\\
&=2\pi\int_0^{1}\left[\theta_L(u)-1\right]\mu_f(2\pi u)du+2\pi\int_1^{+\infty}\left[\theta_L(u)-1\right]\mu_f(2\pi u)du\\
&=2\pi\int_1^{+\infty}\left[\theta_L(y^{-1})-1\right]\mu_f\left(\frac{2\pi}{y}\right)\frac{dy}{y^2}+2\pi\int_1^{+\infty}\left[\theta_L(u)-1\right]\mu_f(2\pi u)du\\
&=2\pi\int_1^{+\infty}\left[y\theta_L(y)-1\right]\mu_f\left(\frac{2\pi}{y}\right)\frac{dy}{y^2}+2\pi\int_1^{+\infty}\left[\theta_L(u)-1\right]\mu_f(2\pi u)du\\
&=2\pi\int_1^{+\infty}\theta_L(y)\mu_f\left(\frac{2\pi}{y}\right)\frac{dy}{y}+2\pi\int_1^{+\infty}\left[\theta_L(u)-1\right]\mu_f(2\pi u)du-2\pi\int_1^{+\infty}\mu_f\left(\frac{2\pi}{y}\right)\frac{dy}{y^2}\\
&=2\pi\int_1^{+\infty}\left[\theta_L(y)-1\right]\left(y^{-1}\mu_f\left(\frac{2\pi}{y}\right)+\mu_f(2\pi y)\right)dy+2\pi\int_1^{+\infty}\mu_f\left(\frac{2\pi}{y}\right)(y^{-1}-y^{-2})dy.
\end{aligned}$$

Now we have, by change of variable $t=y^{-1}$,

$$\left|\int_1^{+\infty}\mu_f\left(\frac{2\pi}{y}\right)(y^{-1}-y^{-2})dy\right|\leq\int_0^1|\mu_f(2\pi t)|\,(t^{-1}-1)dt<+\infty,$$

because μ_f is continuous on $\mathbb{R}_+^*$, $\mu_f(0)=0$ and $t\mapsto t^{-1}$ is integrable in a neighbourhood of 0.

Hence, for L such that $|L|=A$, we have

$$E_f[L]=\sum_{p\in L^*} f(\|p\|^2)=\sum_{p\in \tilde{L}^*} f(2A\|p\|^2)$$

where $L=\sqrt{2A}\tilde{L}$, $|\tilde{L}|=1/2$. By identities $\mu_{f(k.)}=\frac{1}{k}\mu_f\left(\frac{.}{k}\right)$ and $\theta_{\tilde{L}}(s)=\theta_L\left(\frac{s}{2A}\right)$, we get

$$\begin{aligned}E_f[L]=&\frac{\pi}{A}\int_1^{+\infty}\left[\theta_L\left(\frac{y}{2A}\right)-1\right]\left(y^{-1}\mu_f\left(\frac{\pi}{yA}\right)+\mu_f\left(\frac{\pi y}{A}\right)\right)dy\\&+\frac{\pi}{A}\int_1^{+\infty}\mu_f\left(\frac{\pi}{yA}\right)(y^{-1}-y^{-2})dy\end{aligned}$$

and

$$C_A:=\frac{\pi}{A}\int_1^{+\infty}\mu_f\left(\frac{\pi}{yA}\right)(y^{-1}-y^{-2})dy$$

is a finite constant which not depends on L. Now our sufficient condition is clear because, for any Bravais lattice L of area A, we have

$$E_f[L]-E_f[\Lambda_A]=\frac{\pi}{A}\int_1^{+\infty}\left[\theta_L\left(\frac{y}{2A}\right)-\theta_{\Lambda_A}\left(\frac{y}{2A}\right)\right]g_A(y)dy.$$

By Montgomery theorem, $\theta_L(u)-\theta_{\Lambda_A}(u)\geq 0$ for any $u>0$ and any L. Thus, if

$$y^{-1}\mu_f\left(\frac{\pi}{yA}\right)+\mu_f\left(\frac{\pi y}{A}\right)\geq 1\quad\text{for a.e. } y\geq 1,$$

then it follows that

$$E_f[L]-E_f[\Lambda_A]\geq 0,$$

and Λ_A is the unique minimizer of E_f, up to rotation, among lattices of fixed area A. $\square$

2.4.2 Minimization at high density for differentiable inverse Laplace transform

In this part we give two results, in the case of differentiable inverse Laplace transform, which are based on our Theorem 2.1.1.

Proposition 2.4.1. *Let f be an admissible potential such that μ_f is of type C^1 with derivative μ_f'. If*

1. $\mu_f(y) \geq 0$ *on* $\left[\frac{\pi}{A}, +\infty\right)$,
2. $\mu_f'\left(\frac{\pi}{A}y\right) \geq \frac{1}{y^3}\mu_f'\left(\frac{\pi}{Ay}\right)$ *for any* $y \geq 1$,

then Λ_A is the unique minimizer of E_f, up to rotation, among Bravais lattices of fixed area A.

Proof. We write, for any $y \geq 1$,

$$g_A(y) := y^{-1}\mu_f\left(\frac{\pi}{yA}\right) + \mu_f\left(\frac{\pi y}{A}\right) = \frac{u_A(y)}{y}$$

with

$$u_A(y) := \mu_f\left(\frac{\pi}{yA}\right) + y\mu_f\left(\frac{\pi y}{A}\right).$$

Therefore, we get

$$u_A'(y) = \mu_f\left(\frac{\pi y}{A}\right) + \frac{\pi y}{A}\left[\mu_f'\left(\frac{\pi}{A}y\right) - y^{-3}\mu_f'\left(\frac{\pi}{Ay}\right)\right].$$

Assumption 1. implies that $\mu_f\left(\frac{\pi y}{A}\right) \geq 0$ for any $y \geq 1$. Moreover, it is clear that point 2. means that $\mu_f'\left(\frac{\pi}{A}y\right) - y^{-3}\mu_f'\left(\frac{\pi}{Ay}\right) \geq 0$ for any $y \geq 1$, hence $u_A'(y) \geq 0$ for any $y \geq 1$. As

$$u_A(1) = 2\mu_f\left(\frac{\pi}{A}\right) \geq 0,$$

we have $u_A(y) \geq 0$ for any $y \geq 1$ and it follows that

$$g_A(y) \geq 0, \quad \forall y \geq 1,$$

and by Theorem 2.1.1, Λ_A is the unique minimizer, up to rotation, of E_f among Bravais lattices of fixed area A. $\square$

Corollary 2.4.2. *If f is an admissible potential such that its inverse Laplace transform μ_f is convex on $(0, +\infty)$, then there exists $A_0 > 0$ such that for any $A \in (0, A_0)$, Λ_A is the unique minimizer of E_f, up to rotation, among Bravais lattices of fixed area A.*

Proof. As μ_f is convex, there exists $r_0 > 0$ such that, for any $r \geq r_0$, $\mu_f(r) \geq 0$. Moreover, for any $y \geq 1$,

$$\mu_f'\left(\frac{\pi}{A}y\right) \geq \mu_f'\left(\frac{\pi}{Ay}\right)$$

because $\dfrac{\pi}{Ay} \leq \dfrac{\pi y}{A}$ and μ_f is convex. Hence, as $y^{-3} \leq 1$ for any $y \geq 1$, we get both points 1. and 2. of Proposition 2.4.1 for any A such that $0 < A \leq A_0 := \dfrac{\pi}{r_0}$. $\square$

2.4.3 Remarks about our method

As we saw in [10], in Lennard-Jones case, our method is not optimal to finding all areas such that Λ_A is the unique minimizer, up to rotation, of E_f among Bravais lattices of fixed area A. The general and difficult main problem is to find all A such that, for any Bravais lattice L of area A,

$$E_f[L] - E_f[\Lambda_A] = \frac{\pi}{A}\int_1^{+\infty}\left[\theta_L\left(\frac{y}{2A}\right) - \theta_{\Lambda_A}\left(\frac{y}{2A}\right)\right] g_A(y)dy \geq 0,$$

where $g_A(y) := y^{-1}\mu_f\left(\dfrac{\pi}{yA}\right) + \mu_f\left(\dfrac{\pi y}{A}\right)$. We can imagine that even if g_A is not positive almost everywhere on $[1,+\infty)$, the positive part of this integral can compensate the negative one. For instance, if we consider, as in [10], $f(r) = r^{-6} - 2r^{-3}$, then

$$g_A(y) = \frac{\pi^2}{A^2}\left[\frac{\pi^3}{A^3 5!}(y^6 + y^{-5}) - y^3 - y^{-2}\right],$$

and we plot graphs of $y \mapsto \dfrac{\pi^3}{A^3 5!}(y^6 + y^{-5}) - y^3 - y^{-2}$ for $A = 0.8$ (on the left) and $A = 1$ (on the right).

Thus a fine study, with respect to lattices L and real y, of the behaviour of positive function

$$\Delta_L(y) := \theta_L\left(\frac{y}{2A}\right) - \theta_{\Lambda_A}\left(\frac{y}{2A}\right)$$

is necessary. However we find it difficult at this time. Indeed,

- for any Bravais lattice L of area A,

  $$\lim_{y \to +\infty} \Delta_L(y) = 0$$

  and Δ_L exponentially decreases;
- if the complete monotonicity is a necessary condition to optimality of Λ_A for any fixed area A, then function $y \mapsto \Delta_L(y)$ is **not decreasing** on $[1,+\infty)$ for any A

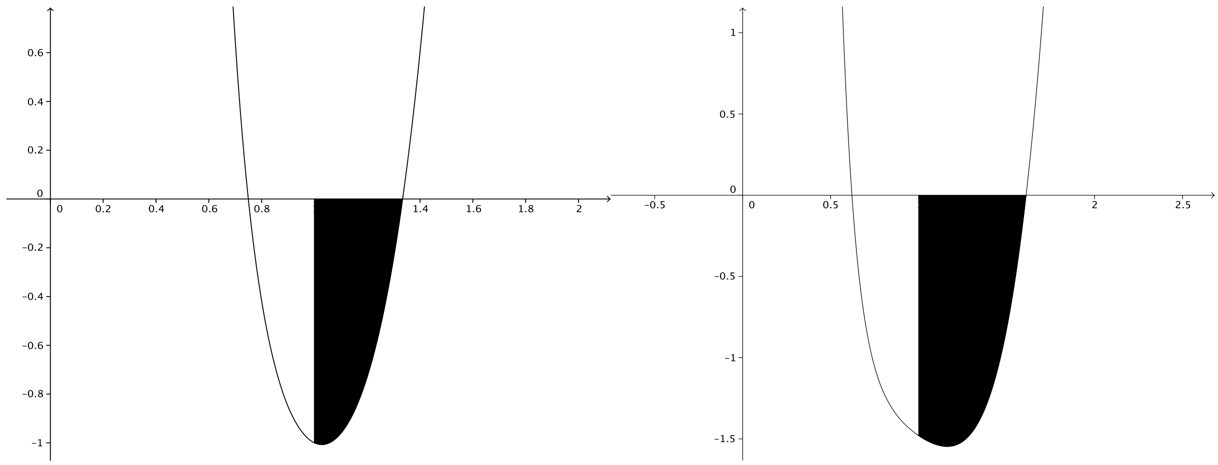


FIGURE 2.3 – Black zone is $\displaystyle\int_1^{y_A} g_A(y)dy$ where y_A is the second zero of g_A, $A \in \{0.8, 1\}$

and any L with area A. Indeed, Δ_L is decreasing on $(1, +\infty)$ if and only if, for any $t \geq 1$, $\Delta_L'(y) \leq 0$, i.e.

$$\begin{aligned}
&\forall A, \forall L, \Delta_L \text{ decreases on } (1,+\infty)\\
&\iff \forall A, \forall L, \forall y \geq 1, -\frac{\pi}{A}\sum_{p\in L^*} \|p\|^2 e^{-\frac{\pi}{A}y\|p\|^2} + \frac{\pi}{A}\sum_{p\in\Lambda_A^*} \|p\|^2 e^{-\frac{\pi}{A}y\|p\|^2} \leq 0\\
&\iff \forall A, \forall L, \forall y \geq 1, \sum_{p\in\Lambda_A^*} \|p\|^2 e^{-\frac{\pi}{A}y\|p\|^2} \leq \sum_{p\in L^*} \|p\|^2 e^{-\frac{\pi}{A}y\|p\|^2}
\end{aligned}$$

which would be not possible, because $r \mapsto re^{-\frac{\pi}{A}yr}$ is never completely monotonic for $y \geq 1$.

Hence comparing $\int_1^{y_A} \Delta_L(y) g_A(y)dy$ and $\int_{y_A}^{+\infty} \Delta_L(y) g_A(y)dy$, where y_A is the second zero of g_A, seems difficult, even improving our method is possible (see [10] for numerical values).

2.5 Sums of screened Coulomb potentials

In this part, we give the first simple example of application of Theorem 2.1.1. We consider non convex sums of screened Coulomb potentials and we prove minimality of Λ_A at high density and global minimality of a triangular lattice among all Bravais lattices for some potentials $\varphi_{a,x}^{AR}$.

2.5.1 Definition and proof of Theorem 2.1.2.A for $\varphi_{a,x}$

Definition 2.5.1. *Let $n \in \mathbb{N}^*$. For coefficients $a = (a_1, ..., a_n) \in (\mathbb{R}^*)^n$ such that $\displaystyle\sum_{i=1}^n a_i \geq 0$ and for $x = (x_1, ..., x_n) \in (\mathbb{R}_+^*)^n$, we define*

$$\varphi_{a,x}(r) := \sum_{i=1}^n a_i \frac{e^{-x_i r}}{r}$$

and we set $\mathcal{K}_a := \left\{ k; \displaystyle\sum_{i=1}^k a_i < 0 \right\}$.

As a proof of Theorem 2.1.2.A for this potential, we purpose to give an explicit bound for the minimality at high density as follows.

Proposition 2.5.1. *Assume $0 < x_1 < ... < x_n$ and let $A > 0$ be such that*

$$A \leq \min\left\{ \min_{k\in\mathcal{K}_a} \left\{ \frac{\pi}{x_{k+1}} \left(-\frac{\sum_{i=1}^n a_i}{\sum_{i=1}^k a_i} \right) \right\}, \frac{\pi}{x_n} \right\},$$

then Λ_A is the unique minimizer of $E_{\varphi_{a,x}}$, up to rotation, among Bravais lattices of fixed area A.

Proof. We compute easily the inverse Laplace transform of $\varphi_{a,x}$, because $\mathcal{L}^{-1}[r^{-1}e^{-x_i r}](y) = \mathbb{1}_{[x_i,+\infty)}(y)$ for any $x_i > 0$ and any $y \geq 0$:

$$\mu_{\varphi_{a,x}}(y) = \sum_{i=1}^n a_i \mathbb{1}_{[x_i,+\infty)}(y).$$

It follows that, for any $y \geq 1$,

$$g_A(y) := \frac{1}{y} \sum_{i=1}^n \mathbb{1}_{[x_i,+\infty)} \left(\frac{\pi}{yA} \right) + \sum_{i=1}^n a_i \mathbb{1}_{[x_i,+\infty)} \left(\frac{\pi y}{A} \right)$$

$$= \frac{1}{y}\sum_{i=1}^n a_i \mathbb{1}_{\left[1,\frac{\pi}{Ax_i}\right]}(y) + \sum_{i=1}^n a_i \mathbb{1}_{\left[\frac{Ax_i}{\pi},+\infty\right)}(y).$$

As, by assumption, $A \leq \dfrac{\pi}{x_n}$, we have, for any $1 \leq i \leq n-1$,

$$\frac{\pi}{Ax_i} \geq \frac{\pi}{Ax_{i+1}} \geq 1.$$

Hence we get

$$g_A(y) = \begin{cases} (1+y^{-1})\displaystyle\sum_{i=1}^n a_i & \text{if } 1 \leq y \leq \frac{\pi}{Ax_n}, \\ \displaystyle\sum_{i=1}^k \frac{a_i}{y} + \sum_{i=1}^n a_i & \text{if } \frac{\pi}{Ax_{k+1}} < y \leq \frac{\pi}{Ax_k}, \text{ for any } 1 \leq k \leq n-1, \\ \displaystyle\sum_{i=1}^n a_i & \text{if } y > \frac{\pi}{Ax_1}. \end{cases}$$

As $\displaystyle\sum_{i=1}^n a_i \geq 0$ and, for any $k \notin \mathcal{K}_a$, $\sum_{i=1}^k a_i \geq 0$, we obtain

$$\forall y \in \left[1, \frac{\pi}{Ax_n}\right] \bigcup_{k\notin\mathcal{K}_a} \left(\frac{\pi}{Ax_{k+1}}, \frac{\pi}{Ax_k}\right] \cup \left(\frac{\pi}{Ax_1}, +\infty\right), \quad g_A(y) \geq 0.$$

Now if $k \in \mathcal{K}_a$, as $A \leq \displaystyle\min_{k\in\mathcal{K}_a}\left\{\frac{\pi}{x_{k+1}}\left(-\frac{\sum_{i=1}^n a_i}{\sum_{i=1}^k a_i}\right)\right\}$, we get, for any $y \in \left(\frac{\pi}{Ax_{k+1}}, \frac{\pi}{Ax_k}\right]$,

$$\sum_{i=1}^k \frac{a_i}{y} + \sum_{i=1}^n a_i \geq \frac{Ax_{k+1}}{\pi}\sum_{i=1}^k a_i + \sum_{i=1}^n a_i \geq 0,$$

and it follows that $g_A(y) \geq 0$ for any $y \geq 1$. By Theorem 2.1.1, Λ_A is the unique minimizer of $E_{\varphi_{a,x}}$, up to rotation, among Bravais lattices of fixed area A. □

2.5.2 Global minimality : Proof of Theorem 2.1.2.B.1

Now we focus on particular "attractive-repulsive" case

— $a = (-a_1, a_2)$ where $0 < a_1 < a_2$;

— $x = (x_1, x_2)$ with $0 < x_1 < x_2$.

Therefore we define, for any $y > 0$,

$$\varphi_{a,x}^{AR}(r) := a_2\frac{e^{-x_2 r}}{r} - a_1\frac{e^{-x_1 r}}{r}.$$

Now, let us prove Theorem 2.1.2.B.1.

Proof. Firstly we study variations of $\varphi_{x,a}$ to prove the existence of global minimizer $L_{a,x}$ among all Bravais lattices and upper bound $\alpha_{a,x}$ for its area. Afterward we prove that inequalities (2.1.3) are equivalent with

$$\alpha_{a,x} \leq \min\left\{\frac{\pi}{x_2}, \frac{\pi}{x_2}\left(\frac{a_2}{a_1}-1\right)\right\}. \tag{2.5.1}$$

Thus, by direct application of Theorem 2.5.1, if $A \leq \min\left\{\frac{\pi}{x_2}, \frac{\pi}{x_2}\left(\frac{a_2}{a_1}-1\right)\right\}$, Λ_A is the unique minimizer among Bravais lattices of fixed area A, therefore $L_{a,x}$ is triangular and unique, up to rotation.

STEP 1 : Variations of function $\varphi_{a,x}$

We have, for any $r>0$,

$$\varphi'_{a,x}(r) = \frac{1}{r^2}\left[a_1(1+x_1r)e^{-x_1r} - a_2(1+x_2r)e^{-x_2r}\right],$$

and it follows that

$$\varphi'_{a,x}(r) \geq 0 \iff g_{a,x}(r) := (x_2-x_1)r + \ln(1+x_1r) - \ln(1+x_2r) + \ln\left(\frac{a_1}{a_2}\right) \geq 0.$$

As, for any $r>0$,

$$g'_{a,x}(r) = \frac{(x_2-x_1)\left(x_1x_2r^2+(x_1+x_2)r\right)}{(1+x_1r)(1+x_2r)} > 0,$$

$g_{a,x}$ is an increasing function on $(0,+\infty)$. We have $a_2>a_1$, therefore $\ln\left(\frac{a_1}{a_2}\right)<0$ and there exists $\alpha_{a,x}$ such that

$$\forall r\in(0,\alpha_{a,x}], g_{a,x}(r)\leq 0, \quad \text{and} \quad \forall r>\alpha_{a,x}, g_{a,x}(r)>0.$$

Thus we get $\varphi_{a,x}$ is a decreasing function on $(0,\alpha_{a,x}]$ and an increasing function on $(\alpha_{a,x},+\infty)$.

STEP 2 : The existence of global minimizer for $E_{\varphi_{a,x}}$

Variations of function $\varphi_{a,x}$ and the fact that $\lim\limits_{\substack{r\to 0\\ r>0}} \varphi_{a,x}(r) = +\infty$ and goes to 0 at infinity implies that global minimizer exists. Indeed, this problem can be viewed like a minimization problem of a three variables (two lengths and an angle) function. By previous limits we can restrict this problem with variables in a compact set, and by continuity this problem has a solution $L_{a,x}$.

STEP 3 : Upper bound for $|L_{a,x}|$ and conclusion
Let $L_{a,x}=\mathbb{Z}u_{a,x}\oplus\mathbb{Z}v_{a,x}$. If $\|u_{a,x}\|>\sqrt{\alpha_{a,x}}$, then a contraction of all distances yields a new lattice with smaller energy because, by STEP 1, $r\mapsto\varphi_{a,x}(r^2)$ is an increasing function on $(\sqrt{\alpha_{a,x}},+\infty)$. Moreover, if $\|v_{a,x}\|>\sqrt{\alpha_{a,x}}$, then a contraction of $\mathbb{R}v_{a,x}$ also gives a lattice with less energy. Thus, we have $\|u_{a,x}\|\leq\|v_{a,x}\|\leq\sqrt{\alpha_{a,x}}$. Now, because $|L_{a,x}|\leq\|u_{a,x}\|\|v_{a,x}\|$, we get [10]

$$|L_{a,x}|\leq\alpha_{a,x}.$$

Now it is not difficult to check that

$$\varphi'_{a,x}\left(\frac{\pi}{x_2}\right)\geq 0\iff\frac{a_1\left(1+\frac{x_1}{x_2}\pi\right)}{a_2(1+\pi)}e^{\left(1-\frac{x_1}{x_2}\right)\pi}\geq 1,$$

and

$$\varphi'_{a,x}\left(\frac{\pi}{x_2}\left(\frac{a_2}{a_1}-1\right)\right)\geq 0\iff\frac{a_1\left(a_1x_2+x_1(a_2-a_1)\pi\right)}{a_2x_2\left(a_1+(a_2-a_1)\pi\right)}e^{\left(1-\frac{x_1}{x_2}\right)\left(\frac{a_2}{a_1}-1\right)\pi}\geq 1,$$

hence (2.5.1) holds and $L_{a,x}$ is unique and triangular by Theorem 2.5.1 as explained at the beginning of the proof.

STEP 4 : Example
If we take $a_2=2a_1$ then

$$\begin{aligned}\frac{a_1\left(a_1x_2+x_1(a_2-a_1)\pi\right)}{a_2x_2\left(a_1+(a_2-a_1)\pi\right)}e^{\left(1-\frac{x_1}{x_2}\right)\left(\frac{a_2}{a_1}-1\right)\pi}&=\frac{a_1\left(1+\frac{x_1}{x_2}\pi\right)}{a_2(1+\pi)}e^{\left(1-\frac{x_1}{x_2}\right)\pi}\\&=\frac{1}{2(1+\pi)}(1+\frac{x_1}{x_2}\pi)e^{\left(1-\frac{x_1}{x_2}\right)\pi}.\end{aligned}$$

Now we set $X=\dfrac{x_1}{x_2}\pi$ and our condition becomes $\dfrac{(1+X)}{2(1+\pi)}e^{-X+\pi}\geq 1$, which is equivalent with

$$g(X):=-X+\log(1+X)-\log(2+2\pi)+\pi\geq 0.$$

10. This argument appears in [10, Proposition 4.1, ii)] and in [72] in order to prove that the distance between two animals in a swarm is less than a specific "confort distance" between them, which minimizes a certain function.

As $g'(X) = -\frac{X}{1+X} \leq 0$ on $\mathbb{R}_+$, then g decreases and there exists $\tilde{X} > 0$ such that $g(\tilde{X}) = 0$. Numerically, we found $\tilde{X} > 2.186$, hence if $X \leq 2.186$, which corresponds to $\frac{x_1}{x_2}\pi \leq 2.186$, i.e. $x_1 \leq \frac{2.186}{\pi}x_2 \approx 0.695825x_2$, then $g(X) \geq 0$. In particular, it is true if $x_1 \leq 0.695x_2$. □

Example 2.5.2. For instance, we can choose $(x_1, x_2) = (1, 2)$. Thus, global minimizer of

$$L \mapsto E_{\varphi_{a,x}}[L] = \sum_{p\in L^*} \varphi_{a,x}(\|p\|^2) = 2a_1 \sum_{p\in L^*} \frac{e^{-2\|p\|^2}}{\|p\|^2} - a_1 \sum_{p\in L^*} \frac{e^{-\|p\|^2}}{\|p\|^2}$$

is unique, up to rotation, and triangular. Hence we can construct potential with arbitrary deep well (using parameter a_1) and with triangular global minimizer.

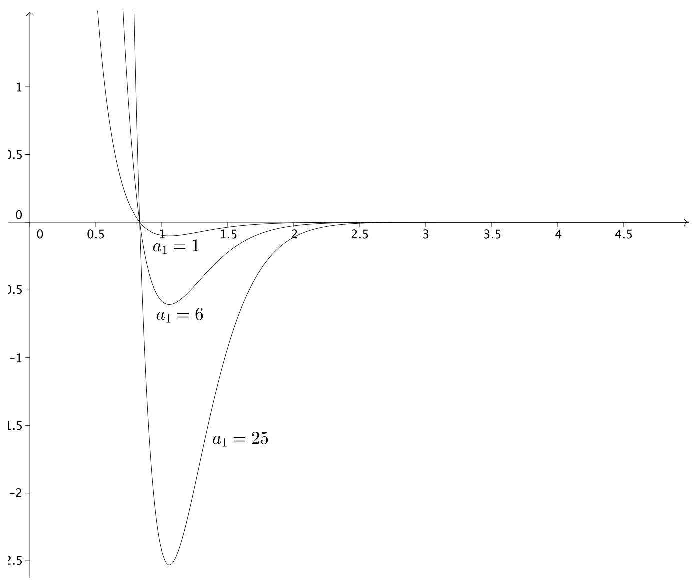


FIGURE 2.4 – Graphs of $r \mapsto \varphi_{a,x}(r^2) = 2a_1\frac{e^{-2r^2}}{r^2} - a_1\frac{e^{-r^2}}{r^2}$ for $a_1 \in \{1, 6, 25\}$

Remark 2.5.3. This kind of potential seems not to be used in molecular simulation but this prediction of triangular ground state could be observed in the future. Furthermore our Theorem 2.1.2.B.1 allows to better understand ground state for parametrized potential with repulsion at short distance and quick decay at large distance, as in [99] where Theil proved global minimality of a triangular lattice among all configurations if the potential's well is sufficiently narrow, i.e. with repulsion and decay sufficiently strong.

2.6 Nonconvex sums of inverse power laws

In this part, we generalize our results [10], which tackled only the classical Lennard-Jones case, for any nonconvex sums of inverse power potentials, that is to say optimality of triangular lattice Λ_A at for high densities and non-optimality of this one for low densities. Furthermore we show that our method allows to obtain global minimizer, i.e. minimizer among all Bravais lattices without constraint of area, of Lennard-Jones type energies with small parameters.

2.6.1 Definition and proof of Theorem 2.1.2.A for $V_{a,x}$

Definition 2.6.1. *Let $n \geq 1$ be an integer and, for $a = (a_1, ..., a_n) \in (\mathbb{R}^*)^n$ such that $a_n > 0$, and $x = (x_1, ..., x_n) \in (\mathbb{R}_+)^n$ such that $1 < x_1 < ... < x_n$, let*

$$V_{a,x}(r) = \sum_{i=1}^{n} \frac{a_i}{r^{x_i}}.$$

We set $I_- := \{i; a_i < 0\}$, $I_+ := \{i; a_i > 0\}$ and $\alpha_i := \dfrac{a_i \pi^{x_i - 1}}{\Gamma(x_i)}$. Moreover we assume that $I_- \neq \emptyset$ (otherwise $V_{a,x}$ is completely monotonic).

Remark 2.6.1. In order to minimize $E_{V_{a,x}}$ among lattices, we should assume $a_n > 0$ because we have $V_{a,x}(r) \sim a_n r^{-x_n}$ as $r \to 0$. Indeed, $V_{a,x}(r) \to +\infty$ as $r \to 0$ and $V_{a,x}(r) \to 0$ as $r \to +\infty$. Therefore there exists minimizer of $E_{V_{a,x}}$ among Bravais lattices with fixed area. If $a_n < 0$, it is sufficient to do $\|u\| \to 0$ to get $E_{V_{a,x}}[L] \to -\infty$ and it follows that a minimizer does not exist.

Example 2.6.2. This kind of potential is widely used in molecular simulation. Indeed, besides Lennard-Jones potentials that we will study in the next subsection, it is sometimes necessary to consider some modifications of it. For instance, the $(12-6-4)$ potential proposed by Mason and Schamp [68], defined by

$$V(r) = \frac{a_3}{r^{12}} - \frac{a_2}{r^6} - \frac{a_1}{r^4},$$

describes the interaction of ions with neutral systems. For instance, in fullerene C_{60}, this potential describes interaction between a carbon atom in the polyatomic ion and a buffer gas helium atom.

An other example, proposed by Klein and Hanley [57, 50] for description of rare gases, more precise than Lennard-Jones, is the potential defined, for $m > 8$, by

$$V(r) = \frac{a_3}{r^m} - \frac{a_2}{r^6} - \frac{a_1}{r^8}.$$

As in the previous section, we give an explicit bounds for the minimality of Λ_A at high density in the following proposition.

Proposition 2.6.3. *If it holds*

$$A \leq \pi \min_{i \in I_-} \left\{ \left(\frac{a_n \Gamma(x_i)}{2\sharp\{I_-\}|a_i|\Gamma(x_n)} \right)^{\frac{1}{x_n - x_i}} \right\}, \tag{2.6.1}$$

then Λ_A is the unique minimizer of $E_{V_{a,x}}$, up to rotation, among Bravais lattices of fixed area A.

Proof. By usual formula, we have

$$\mu_{V_{a,x}}(y) = \sum_{i=1}^n \frac{a_i}{\Gamma(x_i)} y^{x_i - 1},$$

and it follows that

$$\begin{aligned} g_A(y) &:= y^{-1}\mu_{V_{a,x}}\left(\frac{\pi}{yA}\right) + \mu_{V_{a,x}}\left(\frac{\pi y}{A}\right) = \sum_{i=1}^n \frac{\alpha_i}{A^{x_i - 1}}(y^{-x_i} + y^{x_i - 1}) \\ &= y^{-x_n} \sum_{i=1}^n \frac{\alpha_i}{A^{x_i-1}}(y^{x_n - x_i} + y^{x_n + x_i - 1}). \end{aligned}$$

We set

$$p_{a,x}(y) := \sum_{i=1}^n \frac{\alpha_i}{A^{x_i - 1}}(y^{x_n - x_i} + y^{x_n + x_i - 1}).$$

We notice that the term of high order is $\frac{\alpha_n}{A^{x_n - 1}} y^{2x_n - 1}$ with $\alpha_n > 0$ and the number of negative coefficients is $2\sharp\{I_-\}$. Thus, by Cauchy's rule 2.2.11 and more precisely its generalization (2.2.5), an upper bound on the values of the positive zero of $p_{a,x}$ is

$$M_{p_{a,x}} := \max_{i \in I_-} \left\{ \left(\frac{2\sharp\{I_-\}|\alpha_i| A^{x_n - x_i}}{\alpha_n} \right)^{\frac{1}{x_n - x_i}}, \left(\frac{2\sharp\{I_-\}|\alpha_i| A^{x_n - x_i}}{\alpha_n} \right)^{\frac{1}{x_n + x_i - 1}} \right\},$$

because $2x_n - 1 - (x_n - x_i) = x_n + x_i - 1$ and $2x_n - 1 - (x_n + x_i - 1) = x_n - x_i$.
We notice that

$$A \leq \pi \min_{i \in I_-} \left\{ \left(\frac{a_n \Gamma(x_i)}{2\sharp\{I_-\}|a_i|\Gamma(x_n)} \right)^{\frac{1}{x_n - x_i}} \right\} = \min_{i \in I_-} \left\{ \left(\frac{\alpha_n}{2\sharp\{I_-\}|\alpha_i|} \right)^{\frac{1}{x_n - x_i}} \right\}$$

$$\begin{aligned}
&\iff A \leq \left(\frac{\alpha_n}{2\sharp\{I_-\}|\alpha_i|}\right)^{\frac{1}{x_n-x_i}}, \quad \forall i \in I_-\\
&\iff \frac{2A^{x_n-x_i}\sharp\{I_-\}|\alpha_i|}{\alpha_n} \leq 1, \quad \forall i \in I_-\\
&\iff M_{p_{a,x}} \leq 1,
\end{aligned}$$

therefore the assumption implies that the largest zero of $p_{a,x}$ is less than 1. As $\alpha_n > 0$, it follows that $p_{a,x}(y) \geq 0$ for any $y \geq M_{p_{a,x}}$ and then $g_A(y) \geq 0$ for any $y \geq 1$. By Theorem 2.1.1, if (2.6.1) holds, then Λ_A is the unique minimizer of $E_{V_{a,x}}$ among Bravais lattices of fixed area A. $\square$

Remark 2.6.4. This result seems to be natural because for r close to 0, we have $V_{a,x}(r) \sim a_n r^{-x_n}$, and for any A, Λ_A is the unique minimizer of $L \mapsto \zeta_L(2x_n)$ among Bravais lattices of fixed area A. However, if we fix A, $\|u\|$ and $\|v\|$ can be as larger as we want and the behavior of $V_{a,x}$ can be unusual.
Furthermore, in the case

$$V_{a,x}(r) = \frac{a_1}{r^{x_1}} + \frac{a_2}{r^{x_2}} + \frac{a_3}{r^{x_3}}$$

where a_1, a_3 are positive and a_2 negative, our bound (2.6.1) does not depend on a_1. For instance, if $a = (p, -3, 1)$ and $x = (2, 4, 6)$, then, for any p,

$$\pi \min_{i \in I_-} \left\{ \left(\frac{a_n \Gamma(x_i)}{\sharp\{I_-\}|a_i|\Gamma(x_n)} \right)^{\frac{1}{x_n-x_i}} \right\} = \pi \left(\frac{\Gamma(4)}{6\Gamma(6)} \right)^{1/2} \approx 0.2867869$$

which corresponds to triangular lattices of length ≈ 0.5754589.

Example 2.6.5. For our counterexample (2.3.1), i.e. $V(r) = \dfrac{14}{r^2} - \dfrac{40}{r^3} + \dfrac{35}{r^4}$, we have $a = (14, -40, 35)$, $x = (2, 3, 4)$ and $\sharp\{I_-\} = 1$. Hence,

$$\pi \min_{i \in I_-} \left\{ \left(\frac{a_n \Gamma(x_i)}{\sharp\{I_-\}|a_i|\Gamma(x_n)} \right)^{\frac{1}{x_n-x_i}} \right\} = \pi \left(\frac{35\Gamma(3)}{80\Gamma(4)} \right)^{1} = \frac{7\pi}{48} \approx 0.4581488,$$

which corresponds to triangular lattice of length ≈ 0.7273408. Thus, for $A \leq \dfrac{7\pi}{48}$, Λ_A is the unique minimizer of E_V, up to rotation, among Bravais lattices of fixed area A.

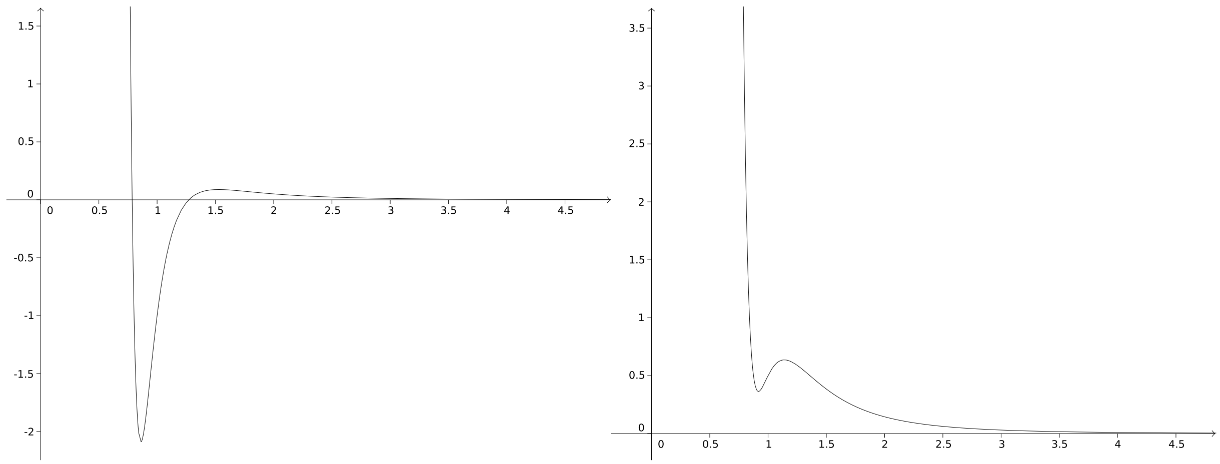


FIGURE 2.5 – Graphs of $V_{a,x}(r^2) = \dfrac{p}{r^4} - \dfrac{3}{r^8} + \dfrac{1}{r^{12}}$ for $p = 1$ (on the left) and $p = 2.5$ (on the right)

2.6.2 Non-optimality of Λ_A at low density

Proposition 2.6.6. *If $a_1 < 0$ and*

$$A \geq \inf_{\substack{L \neq \Lambda_1 \\ |L|=1}} \max_{i \in I_+} \left\{ \left(\frac{\sharp\{I_+\} a_i (\zeta_L(2x_i) - \zeta_{\Lambda_1}(2x_i))}{|a_1|(\zeta_L(2x_1) - \zeta_{\Lambda_1}(2x_1))} \right)^{\frac{1}{x_n - x_i}} \right\}, \tag{2.6.2}$$

that is to say if A is sufficiently large, then Λ_A is not a minimizer of $E_{V_{a,x}}$ among Bravais lattices of fixed area A.

Proof. Let $L_A = \sqrt{A} L_1$ be a Bravais lattice of area A, with $|L_1| = 1$, then

$$\begin{aligned} E_{V_{a,x}}[\Lambda_A] - E_{V_{a,x}}[L_A] &= \sum_{i=1}^n a_i (\zeta_{\Lambda_A}(2x_i) - \zeta_{L_A}(2x_i)) \\ &= \sum_{i=1}^n \frac{a_i}{A^{x_i}} (\zeta_{\Lambda_1}(2x_i) - \zeta_{L_1}(2x_i)) \\ &= A^{-x_n} \sum_{i=1}^n a_i (\zeta_{\Lambda_1}(2x_i) - \zeta_{L_1}(2x_i)) A^{x_n - x_i}. \end{aligned}$$

We set

$$p_{a,x,L_1}(A) := \sum_{i=1}^n a_i (\zeta_{\Lambda_1}(2x_i) - \zeta_{L_1}(2x_i)) A^{x_n - x_i}.$$

As $a_1 < 0$ and, for any $s > 1$,

$$\zeta_{\Lambda_1}(2s) - \zeta_{L_1}(2s) \leq 0,$$

because Λ_1 is the unique minimizer of $L \mapsto \zeta_L(2s)$ among Bravais lattices of area 1, we can apply Cauchy's rule 2.2.11, and more precisely its generalization (2.2.5). The number of negative coefficient of p_{a,x,L_1} is exactly $\sharp\{I_+\}$ and an upper bound on the values of the positive zero of p_{a,x,L_1} for given L_1, is

$$M_{p_{a,x}}(L_1) := \max_{i\in I_+}\left\{\left(\frac{\sharp\{I_+\}a_i(\zeta_{L_1}(2x_i)-\zeta_{\Lambda_1}(2x_i))}{|a_1|(\zeta_{L_1}(2x_1)-\zeta_{\Lambda_1}(2x_1))}\right)^{\frac{1}{x_n-x_i}}\right\}.$$

Hence, for any L such that $|L|=1$, if $A\geq M_{p_{a,x}}(L)$, then $p_{a,x,L}(A)\geq 0$. We conclude that if (2.6.2) holds, then $E_{V_{a,x}}[\Lambda_A]-E_{V_{a,x}}[L_A]\geq 0$ and Λ_A cannot be a minimizer of $E_{V_{a,x}}$ among Bravais lattices of fixed area A. $\square$

Remark 2.6.7. To compute explicitly a lower bound for A such that Λ_A is not a minimizer of energy $E_{V_{a,x}}$, we can take $L=\mathbb{Z}^2$ in (2.6.2) and use equalities (2.2.1) and (2.2.2) (see next subsection for computations in Lennard-Jones case).

2.6.3 Lennard-Jones type potentials : proofs of Theorems 2.1.2.A and 2.1.2.B.2 and numerical results

Now we want to study more precisely the class of Lennard-Jones type potential. In [10] we studied classical $(12-6)$ Lennard-Jones potential $V_{LJ}(r)=r^{-12}-2r^{-6}$, such that its minimizer is 1, and we proved that the minimizer of its energy among lattices with fixed area A is triangular for small A and it cannot be triangular for large A. Here we prove that our method gives interesting results for this kind of potential.

Let $1<x_1<x_2$ and $a_1,a_2\in(0,+\infty)$, we define **Lennard-Jones type potentials** by

$$V_{a,x}^{LJ}(r) := \frac{a_2}{r^{x_2}}-\frac{a_1}{r^{x_1}},\quad \forall r>0.$$

Example 2.6.8. We can cite various Lennard-Jones type potentials used in molecular simulation or in the study of social aggregation (see [72]), besides the classical V_{LJ}. For instance the $(12-10)$ potential

$$V(r)=\frac{a_2}{r^{12}}-\frac{a_1}{r^{10}}$$

describes hydrogen bonds (see [45]).
A $(6-4)$ potential

$$V(r)=\frac{a_2}{r^{6}}-\frac{a_1}{r^{4}}$$

is also used for finding energetically favourable regions in protein binding sites (see [46] for details).

Lemma 2.6.9. *Let $1 < x_1 < x_2$, then function $r \mapsto V_{a,x}^{LJ}(r^2)$ is decreasing on the interval* $\left[0, \left(\frac{a_2 x_2}{a_1 x_1}\right)^{\frac{1}{2(x_2-x_1)}}\right)$ *and increasing on* $\left[\left(\frac{a_2 x_2}{a_1 x_1}\right)^{\frac{1}{2(x_2-x_1)}}, +\infty\right)$.

Proof. The first derivative of this function is $r \mapsto -2a_2 x_2 r^{-2x_2-1} + 2a_1 x_1 r^{-2x_1-1}$ and

$$(V_{a,x}^{LJ})'(r) \geq 0 \iff r \geq \left(\frac{a_2 x_2}{a_1 x_1}\right)^{\frac{1}{2(x_2-x_1)}}.$$

□

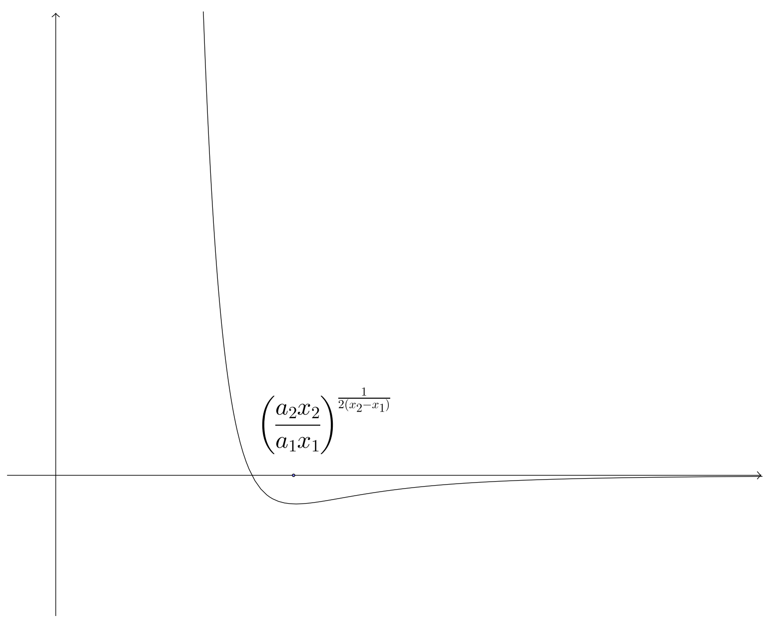


FIGURE 2.6 – Graph of $r \mapsto V_{a,x}^{LJ}(r^2)$

Obviously, the form of potential $V_{a,x}^{LJ}$ implies that minimizer among lattices exists. Indeed, if we fix the area, one of the distance in the lattice cannot be too small otherwise lattice energy goes to infinity (see [10, Proposition 2.3] for details).

As in our previous work [10], the following upper bound for area, such that triangular lattice is the unique minimizer for our energy, is not optimal but the best for our method. Moreover, this upper bound is better than we apply Cauchy's rule (Proposition 2.6.3) but the method is specific for this kind of potential.

Proposition 2.6.10. ***(Lennard-Jones at high density)*** *If* $A \leq \pi \left(\frac{a_2 \Gamma(x_1)}{a_1 \Gamma(x_2)}\right)^{\frac{1}{x_2-x_1}}$, *then Λ_A is the unique minimizer of $E_{V_{a,x}^{LJ}}$, up to rotation, among lattices of area A fixed.*

Proof. We have, by the proof of Theorem 2.6.3, for any $y \geq 1$,

$$g_A(y) = \frac{\alpha_2}{A^{x_2-1}}\left(y^{-x_2} + y^{x_2-1}\right) - \frac{\alpha_1}{A^{x_1-1}}\left(y^{-x_1} + y^{x_1-1}\right) = \frac{y^{-x_2}}{A^{x_1-1}}\tilde{g}_A(y),$$

where $\tilde{g}_A(y) = \frac{\alpha_2}{A^{x_2-x_1}}y^{2x_2-1} - \alpha_1 y^{x_2+x_1-1} - \alpha_1 y^{x_2-x_1} + \frac{\alpha_2}{A^{x_2-x_1}}$. We compute

$$\begin{aligned}\tilde{g}_A'(y) &= \frac{(2x_2-1)\alpha_2}{A^{x_2-x_1}}y^{2x_2-2} - \alpha_1(x_2+x_1-1)y^{x_2+x_1-2} - \alpha_1(x_2-x_1)y^{x_2-x_1-1}\\ &= y^{x_2-x_1-1}u_A(y),\end{aligned}$$

where $u_A(y) = \frac{(2x_2-1)\alpha_2}{A^{x_2-x_1}}y^{x_2+x_1-1} - \alpha_1(x_2+x_1-1)y^{2x_1-1} - \alpha_1(x_2-x_1)$. Moreover

$$u_A'(r) = (x_2+x_1-1)y^{2x_1-2}\left[\frac{(2x_2-1)\alpha_2}{A^{x_2-x_1}}y^{x_2-x_1} - \alpha_1(2x_1-1)\right].$$

We remark that we have

$$u_A'(\bar{y}) = 0 \iff \bar{y} = \left(\frac{\alpha_1(2x_1-1)A^{x_2-x_1}}{\alpha_2(2x_2-1)}\right)^{\frac{1}{x_2-x_1}} = \frac{A}{\pi}\left(\frac{a_1\Gamma(x_2)}{a_2\Gamma(x_1)}\right)^{\frac{1}{x_2-x_1}}\left(\frac{2x_1-1}{2x_2-1}\right)^{\frac{1}{x_2-x_1}}.$$

If $A \leq \pi\left(\frac{a_2\Gamma(x_1)}{a_1\Gamma(x_2)}\right)^{\frac{1}{x_2-x_1}}$ then $\bar{y} < 1$ and $u_A'(y) > 0$ on $[1;+\infty)$, i.e. u_A is an increasing function on $[1;+\infty)$. Furthermore we have

$$u_A(1) = (2x_2-1)\left[\frac{\alpha_2}{A^{x_2-x_1}} - \alpha_1\right] = (2x_2-1)\left[\frac{a_2\pi^{x_2-1}}{A^{x_2-x_1}\Gamma(x_2)} - \frac{a_1\pi^{x_2-1}}{\Gamma(x_1)}\right] \geq 0$$

and $\tilde{g}_A'$ is positive on $[1,+\infty)$. Thus $\tilde{g}_A$ is increasing on $[1,+\infty)$ and, always by assumption,

$$g_A(1) = 2\left(\frac{\alpha_2}{A^{x_2-x_1}} - \alpha_1\right) \geq 0.$$

Hence $g_A(y) \geq 0$ on $[1,+\infty)$ and by Theorem 2.1.1, Λ_A is the unique minimizer of $E_{V_{a,x}^{LJ}}$, up to rotation, among Bravais lattices of fixed area A. □

Remark 2.6.11. This bound is optimal for our method because we have $g_A(1) = 0$ for $A = \pi\left(\frac{a_2\Gamma(x_1)}{a_1\Gamma(x_2)}\right)^{\frac{1}{x_2-x_1}}$ and $A \mapsto g_A(1)$ is a decreasing function.

Example 2.6.12. For $V(r) = \frac{1}{r^6} - \frac{2}{r^3}$, which corresponds to Lennard-Jones energy in our case in [10], we find

$$\pi\left(\frac{a_2\Gamma(x_1)}{a_1\Gamma(x_2)}\right)^{\frac{1}{x_2-x_1}} = \pi\left(\frac{\Gamma(3)}{2\Gamma(6)}\right)^{1/3} = \frac{\pi}{120^{1/3}}.$$

Now we prove that for small parameters, the global minimizer among all Bravais lattices – without area constraint – of the energy is unique and triangular. We follow some ideas from our previous paper [10] which cannot be apply for classical Lennard-Jones potential $V_{LJ}(r) = r^{-12} - 2r^{-6}$.

Lemma 2.6.13. ***(Upper bound for global minimizer's area)*** *Let $L_{a,x}$ be a global minimizer of $E_{V_{a,x}^{LJ}}$ among all Bravais lattices, then*

$$|L_{a,x}| \leq \left(\frac{a_2 x_2}{a_1 x_1}\right)^{\frac{1}{x_2 - x_1}}.$$

Proof. Same argument of STEP 3 in the proof of Theorem 2.1.2.B.1.

□

Thus we can prove **Theorem 2.1.2.B.2**. We recall that function h is defined by

$$h(t) = \pi^{-t}\Gamma(t)t.$$

Proof. Let $L_{a,x}$ be a global minimizer of $E_{V_{a,x}^{LJ}}$. We have

$$h(x_2) \leq h(x_1) \iff \pi\left(\frac{a_2\Gamma(x_1)}{a_1\Gamma(x_2)}\right)^{\frac{1}{x_2-x_1}} \geq \left(\frac{a_2 x_2}{a_1 x_1}\right)^{\frac{1}{x_2-x_1}},$$

then by Lemma 2.6.13 we get

$$|L_{a,x}| \leq \pi\left(\frac{a_2\Gamma(x_1)}{a_1\Gamma(x_2)}\right)^{\frac{1}{x_2-x_1}}$$

and by Proposition 2.6.10, the minimizer among lattices of fixed area $|L_{a,x}|$ is unique and triangular. Hence the global minimizer of the energy is unique and triangular. Furthermore, let

$$f(r) := E_{V_{a,x}^{LJ}}[r\Lambda_1] = a_2\zeta_{\Lambda_1}(2x_2)r^{-2x_2} - a_1\zeta_{\Lambda_1}(2x_1)r^{-2x_1},$$

then we have $f'(r) = -2a_2x_2\zeta_{\Lambda_1}(2x_2)r^{-2x_2-1} + 2a_1x_1\zeta_{\Lambda_1}(2x_1)r^{-2x_1-1}$ and

$$f'(r) \geq 0 \iff r \geq \left(\frac{a_2x_2\zeta_{\Lambda_1}(2x_2)}{a_1x_1\zeta_{\Lambda_1}(2x_1)}\right)^{\frac{1}{2(x_2-x_1)}}.$$

Hence the minimizer of $E_{V_{a,x}^{LJ}}$ among triangular lattices is $\Lambda_{|L_{a,x}|}$ with

$$|L_{a,x}| = \left(\frac{a_2x_2\zeta_{\Lambda_1}(2x_2)}{a_1x_1\zeta_{\Lambda_1}(2x_1)}\right)^{\frac{1}{x_2-x_1}}.$$

□

Remark 2.6.14. For an easy numerical computation of global minimizer's area, we can use formula (2.2.2) to obtain

$$|L_{a,x}| = \frac{1}{2\sqrt{3}}\left(\frac{a_2 x_2 \zeta(x_2)(\zeta(x_2,1/3)-\zeta(x_2,2/3))}{a_1 x_1 \zeta(x_1)(\zeta(x_1,1/3)-\zeta(x_1,2/3))}\right)^{\frac{1}{x_2-x_1}}.$$

Remark 2.6.15. We can apply the previous Theorem to $x=(2,3)$, and $r\mapsto V_{a,x}^{LJ}(r^2)$ is a $(6-4)$ potential. Moreover we can choose a_1 and a_2 such that the well is as deep as we want (see Figure 2.7).

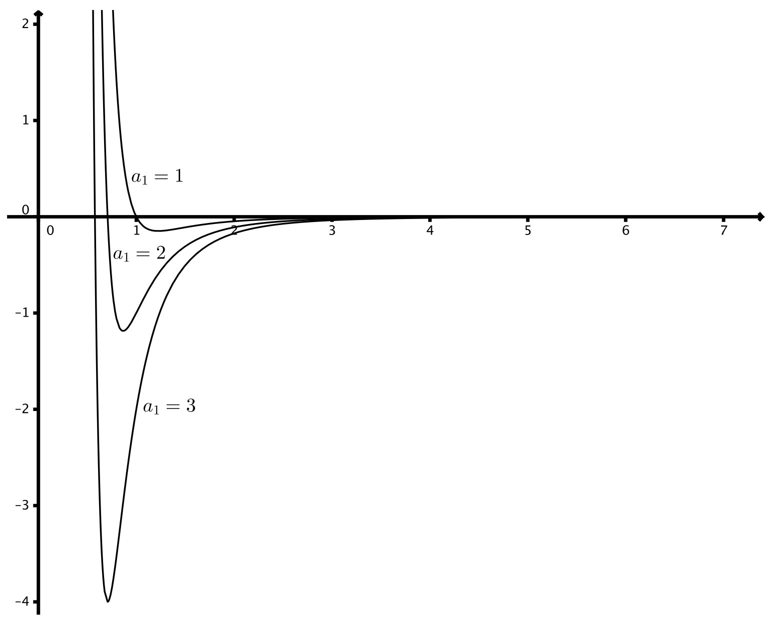


FIGURE 2.7 – Graphs of $r\mapsto \dfrac{1}{r^6}-\dfrac{a_1}{r^4}$ for $a_1\in\{1,2,3\}$

Now we explain a method to choose x_1, x_2 in order to have a triangular global minimizer and we give several numerical values.

Lemma 2.6.16. ***(Variations of h)*** *Function h is decreasing on $[1,\psi^{-1}(\log\pi)-1)$ and increasing on $[\psi^{-1}(\log\pi)-1,+\infty)$ where $\psi(x):=\dfrac{\Gamma'(x)}{\Gamma(x)}$ is the digamma function defined on $(0,+\infty)$.*

Proof. We have $h'(t)=\pi^{-t}\left[\Gamma(t)+t\Gamma'(t)-t\log\pi\Gamma(t)\right]$ and

$$h'(t)\geq 0 \iff \psi(t)+\frac{1}{t}\geq \log\pi.$$

We use the famous identity $\psi(t) + \frac{1}{t} = \psi(1+t)$ for any $t > 0$ and we obtain, because ψ is increasing on $(0, +\infty)$,

$$h'(t) \geq 0 \iff t \geq \psi^{-1}(\log \pi) - 1.$$

□

Remark 2.6.17. We compute $\psi^{-1}(\log \pi) - 1 \approx 2.6284732$ and we define M 1 such that $h(M) = h(1)$. We have $M \approx 4.6022909$. Thus, if we want apply the previous theorem, it is clear that $x_1 < \psi^{-1}(\log \pi) - 1$ and $x_2 < M$. Moreover, if we choose $x_1 \in (1, \psi^{-1}(\log \pi) - 1)$, we can choose $x_2 \in (x_1, M_{x_1})$ where $M_{x_1} \neq x_1$ is such that $h(M_{x_1}) = h(x_1)$.

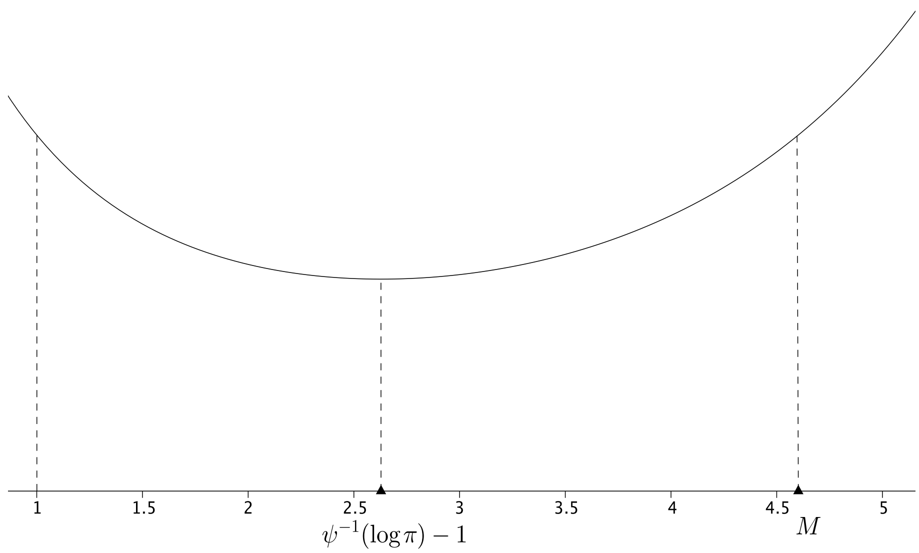


FIGURE 2.8 – Graph of h

Unfortunately we can only choose x_2 and x_1 such that $1 < x_1 < x_2 < 4.6022909$ and Lennard Jones case ($x_2 = 6$ and $x_1 = 3$) is not covered by our Theorem 2.1.2.B.2.

We compute in Table 2.1, for different values of (x_1, x_2) satisfying $h(x_2) < h(x_1)$ and for $a = (1, 1)$, the following numbers :

— the value of the minimizer of $y \mapsto V_{a,x}^{LJ}(y^2)$, i.e.

$$y_{a,x}^{\min} := \left(\frac{x_2}{x_1}\right)^{\frac{1}{2(x_2 - x_1)}},$$

x_2 \ x_1	1.1	1.5	2
1.5	$(1.47, 0.64, 2.78)$		
2	$(1.39, 0.80, 1.82)$	$(1.33, 0.95, 1.27)$	
2.5	$(1.34, 0.90, 1.45)$	$(1.29, 1.02, 1.10)$	$(1.25, 1.10, 0.96)$
3	$(1.30, 0.95, 1.27)$	$(1.26, 1.06, 1.03)$	$(1.22, 1.11, 0.93)$
3.5	$(1.27, 0.99, 1.19)$	$(1.24, 1.08, 1.00)$	
4	$(1.25, 1.01, 1.14)$		

TABLE 2.1 – Some values of $(y_{a,x}^{\min}, r_{a,x}, d_{a,x})$

— the value of the length of triangular global minimizer $L_{a,x}$, that is to say

$$r_{a,x} := \sqrt{\frac{2|L_{a,x}|}{\sqrt{3}}},$$

— the density[11] of $L_{a,x}$, i.e.

$$d_{a,x} := |L_{a,x}|^{-1}.$$

Obviously, we have non-optimality of Λ_A if A is sufficiently large, given by Proposition 2.6.6 :

Proposition 2.6.18. ***(Lennard-Jones at low density)*** *Triangular lattice Λ_A is a minimizer of $E_{V_{a,x}^{LJ}}$ among lattices of area A fixed if and only if*

$$A \leq \inf_{|L|=1, L\neq \Lambda_1} \left(\frac{a_2(\zeta_L(2x_2) - \zeta_{\Lambda_1}(2x_2))}{a_1(\zeta_L(2x_1) - \zeta_{\Lambda_1}(2x_1))} \right)^{\frac{1}{x_2-x_1}},$$

i.e. if A is sufficiently large, Λ_A is not a minimizer of $E_{V_{a,x}^{LJ}}$ among lattices of fixed area A.

Proof. We apply directly Proposition 2.6.6 with $\sharp\{I_+\} = 1$ and we remark that

$$\inf_{\substack{L\neq\Lambda_1 \\ |L|=1}} \max_{i\in I_+} \left\{ \left(\frac{\sharp\{I_+\} a_i(\zeta_L(2x_i) - \zeta_{\Lambda_1}(2x_i))}{|a_1|(\zeta_L(2x_1) - \zeta_{\Lambda_1}(2x_1))} \right)^{\frac{1}{x_n - x_i}} \right\} = \inf_{|L|=1, L\neq\Lambda_1} \left(\frac{a_2(\zeta_L(2x_2) - \zeta_{\Lambda_1}(2x_2))}{a_1(\zeta_L(2x_1) - \zeta_{\Lambda_1}(2x_1))} \right)^{\frac{1}{x_2-x_1}}.$$

□

11. Here we exceptionally give values of densities – and not areas – more used in molecular simulations.

x_2 \ x_1	1.1	1.5	2	3	4	5	6	7	8	9
1.5	0.05									
2	0.14	0.31								
2.5	0.21	0.37	0.43							
3	0.27	0.41	0.47							
3.5	0.31	0.45	0.50	0.58						
4	0.35	0.48	0.53	0.61						
5	0.42	0.53	0.58	0.65	0.71					
6	0.47	0.58	0.63	0.69	0.74	0.78				
7	0.52	0.62	0.66	0.72	0.77	0.80	0.83			
8	0.56	0.65	0.69	0.75	0.79	0.82	0.84	0.86		
9	0.60	0.68	0.72	0.77	0.81	0.84	0.86	0.88	0.89	
10	0.62	0.70	0.74	0.79	0.83	0.85	0.87	0.89	0.90	0.91

TABLE 2.2 – Non-optimal critical densities for non-optimality of triangular lattice.

Remark 2.6.19. More precisely we can find an explicit computable bound (but not optimal) if we take $L=\mathbb{Z}^2$ and use (2.2.1) and (2.2.2). We give, in Table 2.2, densities d_0 such that for any $0<d<d_0$, $E_{V_{a,x}^{LJ}}[d^{-1/2}\mathbb{Z}^2]\leq E_{V_{a,x}^{LJ}}[d^{-1/2}\Lambda_1]$, i.e. square lattice have less energy than triangular lattice, with $a_1=a_2=1$.

2.7 Potentials with exponential decay

2.7.1 Definition and proof of Theorem 2.1.1.A for $f_{a,x,b,t}$

Definition 2.7.1. *Let $a=(a_1,...,a_n)\in(\mathbb{R}^*)^n$ with $a_n>0$, $x=(x_1,...,x_n)$ be such that $3/2<x_1<x_2<...<x_n$, $b=(b_1,...,b_m)\in(\mathbb{R}^*)^m$ and $t=(t_1,...,t_m)\in(\mathbb{R}_+^*)^m$, we define*

$$f_{a,x,b,t}(r):=\sum_{i=1}^n a_i r^{-x_i}+\sum_{j=1}^m b_j e^{-t_j\sqrt{r}}.$$

We set $I_-:=\{i;a_i<0\}$ and $B:=\sum_{j=1}^m |b_j|t_j$.

Remark 2.7.1. As explained in [58], Fumi and Tosi [43] proposed a potential for interaction between ions Na^+ and Cl^- defined by

$$V(r) = \frac{a_1}{r} + b_1 e^{-t_1 r} - \frac{a_2}{r^6} - \frac{a_3}{r^8}.$$

Obviously, potential $r \mapsto \dfrac{a_1}{r}$ is not admissible but the form of V is close to $f_{a,x,b,t}$.

Let us prove Theorem 2.1.2.A for this potential.

Proposition 2.7.2. *If it holds*

$$A \leq \min\left\{\pi \min_{i\in I_-}\left\{\left(\frac{a_n\Gamma(x_i)}{(2\sharp\{I_-\}+2)|a_i|\Gamma(x_n)}\right)^{\frac{1}{x_n-x_i}}\right\}, \left(\frac{a_n\pi^{x_n+1}}{(\sharp\{I_-\}+1)B\Gamma(x_n)}\right)^{\frac{1}{x_n+1/2}}\right\} \tag{2.7.1}$$

then Λ_A is the unique minimizer of $E_{f_{a,x,b,t}}$, up to rotation, among Bravais lattices of fixed area A.

Proof. As we have, by classical formula, for $a>0$,

$$\mathcal{L}^{-1}[e^{-\sqrt{a.}}](y) = \frac{\sqrt{a}}{2\sqrt{\pi}} y^{-3/2} e^{-\dfrac{a}{4y}},$$

taking $a = t_j^2$ for any $1 \leq j \leq m$ and setting $\alpha_i = \dfrac{a_i \pi^{x_i-1}}{\Gamma(x_i)}$, we obtain, for any $y>0$,

$$\mu_{f_{a,x,b,t}}(y) = \sum_{i=1}^n \alpha_i y^{x_i-1} + \sum_{j=1}^m \frac{b_j t_j}{2\sqrt{\pi}} y^{-3/2} e^{-\frac{t_j^2}{4y}} \geq \sum_{i=1}^n \alpha_i y^{x_i-1} - \frac{B}{2\sqrt{\pi}} y^{-3/2}.$$

It follows that

$$\begin{aligned} g_A(y) &:= y^{-1}\mu_{f_{a,x,b,t}}\left(\frac{\pi}{yA}\right) + \mu_{f_{a,x,b,t}}\left(\frac{\pi y}{A}\right) \\ &\geq \sum_{i=1}^n \frac{\alpha_i}{A^{x_i-1}}(y^{-x_i} + y^{x_i-1}) - \frac{BA^{3/2}}{2\pi^2}\sqrt{y} - \frac{BA^{3/2}}{2\pi^2 y^{3/2}} \\ &= y^{-x_n}\left[\sum_{i=1}^n \frac{\alpha_i}{A^{x_i-1}}(y^{x_n-x_i} + y^{x_n+x_i-1}) - \frac{BA^{3/2}}{2\pi^2} y^{x_n+1/2} - \frac{BA^{3/2}}{2\pi^2} y^{x_n-3/2}\right]. \end{aligned}$$

We set

$$p_{a,x,b,t}(y) := \sum_{i=1}^n \frac{\alpha_i}{A^{x_i-1}}(y^{x_n-x_i} + y^{x_n+x_i-1}) - \frac{BA^{3/2}}{2\pi^2} y^{x_n+1/2} - \frac{BA^{3/2}}{2\pi^2} y^{x_n-3/2},$$

and we notice that, for any $1 \leq i \leq n$,

$$\begin{aligned} x_n - x_i &\neq x_n + 1/2, \\ x_n - x_i &\neq x_n - 3/2, \\ x_n + x_i - 1 &\neq x_n + 1/2, \\ x_n + x_i - 1 &\neq x_n - 3/2, \end{aligned}$$

because $x_i > 3/2$. Hence the higher order term is $\frac{\alpha_n}{A^{x_n-1}} y^{2x_n-1}$ with $\alpha_n > 0$, and the number of negative terms is $2\sharp\{I_-\}+2$. Thus, by Cauchy's rule (2.2.5), an upper bound on the values of the positive zero of $p_{a,x,b,t}$ is

$$\begin{aligned} M_{p_{a,x,b,t}} := \max\Bigg\{ &\max_{i\in I_-}\left\{\left(\frac{(2\sharp\{I_-\}+2)|\alpha_i|A^{x_n-x_i}}{\alpha_n}\right)^{\frac{1}{x_n+x_i-1}}\right\}, \max_{i\in I_-}\left\{\left(\frac{(2\sharp\{I_-\}+2)|\alpha_i|A^{x_n-x_i}}{\alpha_n}\right)^{\frac{1}{x_n-x_i}}\right\}, \\ &\left(\frac{B(2\sharp\{I_-\}+2)A^{x_n+1/2}}{2\pi^2\alpha_n}\right)^{\frac{1}{x_n-3/2}}, \left(\frac{B(2\sharp\{I_-\}+2)A^{x_n+1/2}}{2\pi^2\alpha_n}\right)^{\frac{1}{x_n+1/2}}\Bigg\}. \end{aligned}$$

Now we have

$$\begin{aligned} &A \leq \min\left\{\pi \min_{i\in I_-}\left\{\left(\frac{a_n\Gamma(x_i)}{(2\sharp\{I_-\}+2)|a_i|\Gamma(x_n)}\right)^{\frac{1}{x_n-x_i}}\right\}, \left(\frac{2a_n\pi^{x_n+1}}{(2\sharp\{I_-\}+2)B\Gamma(x_n)}\right)^{\frac{1}{x_n+1/2}}\right\} \\ &\iff \forall i \in I_-, A \leq \pi\left(\frac{a_n\Gamma(x_i)}{(2\sharp\{I_-\}+2)|a_i|\Gamma(x_n)}\right)^{\frac{1}{x_n-x_i}} \quad \text{and} \quad A \leq \left(\frac{2a_n\pi^{x_n+1}}{(2\sharp\{I_-\}+2)B\Gamma(x_n)}\right)^{\frac{1}{x_n+1/2}} \\ &\iff \forall i \in I_-, \frac{(2\sharp\{I_-\}+2)|\alpha_i|A^{x_n-x_i}}{\alpha_n} \leq 1 \quad \text{and} \quad \frac{B(2\sharp\{I_-\}+2)A^{x_n+1/2}}{2\pi^2\alpha_n} \leq 1 \\ &\iff M_{p_{a,x,b,t}} \leq 1. \end{aligned}$$

Therefore, if $y \geq 1 \geq M_{p_{a,x,b,t}}$, then $p_{a,x,b,t}(y) \geq 0$ and it follows that $g_A(y) \geq 0$. By Theorem 2.1.1, Λ_A is the unique minimizer of $E_{f_{a,x,b,t}}$ among Bravais lattices of fixed area A. $\square$

Corollary 2.7.3. *If $I_- = \emptyset$ and*

$$A \leq \left(\frac{a_n\pi^{x_n+1}}{B\Gamma(x_n)}\right)^{\frac{1}{x_n+1/2}}$$

then Λ_A is the unique minimizer of $E_{f_{a,x,b,t}}$ among Bravais lattices of fixed area A.

Remark 2.7.4. Obviously, for any A_0, there exists B sufficiently small such that for any $A \in (0, A_0]$, Λ_{A_0} is the unique minimizer of the energy among Bravais lattices of fixed area A. We will study a simple particular case in next subsection in order to illustrate this fact. Furthermore we skipped the completely monotonic case but in the next following part we will give explicit condition for complete monotonicity in a simple case (see Proposition 2.7.6).

2.7.2 Example : opposite of Buckingham type potential

In this part we study the opposite of Buckingham type potential. Indeed, we cannot study Buckingham potential

$$V_B(r) = a_1 e^{-\alpha r} - \frac{a_2}{r^6} - \frac{a_3}{r^8}$$

because $\lim_{r\to 0} V_B(r) = -\infty$ and $\lim_{r\to+\infty} V_B(r) = 0$ and it is sufficient to do $\|u\| \to 0$ in order to have $E_{V_B}[L] \to -\infty$. Hence we choose to treat simple general approximation of its opposite, well-adapted to our problem of minimization among Bravais lattices. Moreover we simplify notations in order to have only two parameters :

Definition 2.7.2. *For $a = (a_1, a_2) \in (0, +\infty)^2$ and for $x = (x_1, x_2) \in (0, +\infty) \times (3/2, +\infty)$, we define, for $r > 0$,*

$$f_{a,x}(r) = a_2 r^{-x_2} - a_1 e^{-x_1\sqrt{r}}.$$

Lemma 2.7.5. ***(Variations of potential** $r \mapsto f_{a,x}(r^2)$**)** We have the following two cases :*

1. *if $(2x_2+1)\left[\ln\left(\frac{2x_2+1}{x_1}\right) - 1\right] \leq \ln\left(\frac{2a_2x_2}{a_1x_1}\right)$, then $r \mapsto f_{a,x}(r^2)$ is decreasing on $(0, +\infty)$;*
2. *if $(2x_2+1)\left[\ln\left(\frac{2x_2+1}{x_1}\right) - 1\right] > \ln\left(\frac{2a_2x_2}{a_1x_1}\right)$ then there exist $r_m, r_M \in (0, +\infty)$ such that $r_m < \frac{2x_2+1}{x_1} < r_M$ and $r \mapsto f_{a,x}(r^2)$ is decreasing on intervals $(0, r_m)$ and $(r_M, +\infty)$ and increasing on (r_m, r_M).*

Proof. We have $f(r) := f_{a,x}(r^2) = a_2 r^{-2x_2} - a_1 e^{-x_1 r}$ and

$$f'(r) = -\frac{2a_2x_2}{r^{2x_2+1}} + a_1x_1e^{-x_1r}.$$

Thus, we get

$$f'(r) \geq 0 \iff e^{-x_1r}r^{2x_2+1} \geq \frac{2a_2x_2}{a_1x_1} \iff g(r) \geq 0,$$

where

$$g(r) = -x_1 r + (2x_2+1)\ln r - \ln\left(\frac{2a_2x_2}{a_1x_1}\right).$$

As $g'(r) = \dfrac{-x_1r + 2x_2 + 1}{r}$, g is increasing on $\left(0, \frac{2x_2+1}{x_1}\right)$ and decreasing on $\left(\frac{2x_2+1}{x_1}, +\infty\right)$. Moreover $g(r)$ goes to $-\infty$ as $r \to 0$ or $r \to +\infty$. Hence if $g\left(\frac{2x_2+1}{x_1}\right) \leq 0$, i.e.

$$(2x_2+1)\left[\ln\left(\frac{2x_2+1}{x_1}\right) - 1\right] \leq \ln\left(\frac{2a_2x_2}{a_1x_1}\right),$$

then $g(r) \leq 0$ and $f'(r) \leq 0$ on $(0,+\infty)$, i.e. f is decreasing on $(0,+\infty)$. Furthermore, if $g\left(\frac{2x_2+1}{x_1}\right) > 0$, then there exist r_m, r_M such that $r_m < \frac{2x_2+1}{x_1} < r_M$ and f is decreasing on intervals $(0, r_m)$ and $(r_M, +\infty)$ and increasing on (r_m, r_M).

$\square$

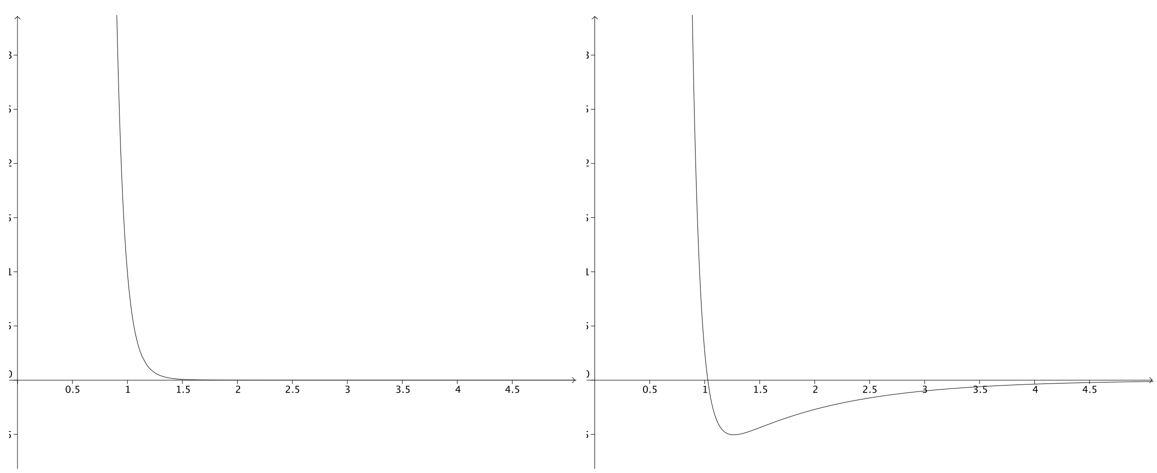


FIGURE 2.9 – Graph of $r \mapsto f_{a,x}(r^2)$ for $a = (1,1)$, $x = (5,6)$ on the left and $a = (1,2)$, $x = (1,6)$ on the right.

Proposition 2.7.6. *We have the following two cases :*

— *If it holds*

$$(x_2 + 1/2)\left[1 + \ln\left(\frac{x_1^2}{4x_2+2}\right)\right] \geq \ln\left(\frac{a_1x_1\Gamma(x_2)}{2\sqrt{\pi}a_2}\right),$$

then for any $A > 0$, Λ_A is the unique minimizer of $E_{f_{a,x}}$, up to rotation, among Bravais lattices of fixed area A.

— *If it holds*

$$A \leq \left(\frac{a_2\pi^{x_2+1}}{a_1x_1\Gamma(x_2)}\right)^{\frac{1}{x_2+1/2}} \quad \textit{and} \quad (x_2+1/2)\left[1+\ln\left(\frac{x_1^2}{4x_2+2}\right)\right] < \ln\left(\frac{a_1x_1\Gamma(x_2)}{2\sqrt{\pi}a_2}\right),$$

then Λ_A is the unique minimizer of $E_{f_{a,x}}$, up to rotation, among Bravais lattices with fixed area A. Moreover, for any $a \in (0,+\infty)^2$, $x_2 > 3/2$, $A_0 > 0$ and any x_1 such that

$$0 < x_1 \leq C_{A_0} := \frac{a_2\pi^{x_2+1}}{a_1 A_0^{x_2+1/2}\Gamma(x_2)},$$

Λ_A is the unique minimizer of $E_{f_{a,x}}$, up to rotation, among Bravais lattices of fixed area $A \in (0, A_0]$.

Proof. By classical formula, we get

$$\mu_{f_{a,x}}(y) = \frac{a_2}{\Gamma(x_2)}y^{x_2-1} - \frac{a_1x_1}{2\sqrt{\pi}}y^{-3/2}e^{-\frac{x_1^2}{4y}}.$$

Our theorem is a consequence of Proposition 2.3.1 because

$$\forall y > 0, \mu_{f_{a,x}}(y) \geq 0 \iff (x_2+1/2)\left[1+\ln\left(\frac{x_1^2}{4x_2+2}\right)\right] \geq \ln\left(\frac{a_1x_1\Gamma(x_2)}{2\sqrt{\pi}a_2}\right).$$

Indeed, we have

$$\begin{aligned}\forall y > 0, \mu_{f_{a,x}}(y) \geq 0 &\iff \forall y > 0, e^{x_1^2/4y}y^{x_2+1/2} \geq \frac{a_1x_1\Gamma(x_2)}{2\sqrt{\pi}a_2}\\ &\iff \forall y > 0, \frac{x_1^2}{4y} + (x_2+1/2)\ln y - \ln\left(\frac{a_1x_1\Gamma(x_2)}{2\sqrt{\pi}a_2}\right) \geq 0.\end{aligned}$$

We set

$$g(y) = \frac{x_1^2}{4y} + (x_2+1/2)\ln y - \ln\left(\frac{a_1x_1\Gamma(x_2)}{2\sqrt{\pi}a_2}\right),$$

and we have $g'(y) = -\frac{x_1^2}{4y^2} + \frac{x_2+1/2}{y}$. It follows that g is decreasing on $\left(0, \frac{x_1^2}{4x_2+2}\right)$ and increasing on $\left(\frac{x_1^2}{4x_2+2}, +\infty\right)$. As g goes to $+\infty$ as y goes to 0 or $+\infty$, it is clear that

$$\begin{aligned}\forall y > 0, g(y) \geq 0 &\iff g\left(\frac{x_1^2}{4x_2+2}\right) \geq 0\\ &\iff (x_2+1/2)\left[1+\ln\left(\frac{x_1^2}{4x_2+2}\right)\right] \geq \ln\left(\frac{a_1x_1\Gamma(x_2)}{2\sqrt{\pi}a_2}\right).\end{aligned}$$

Now, if $f_{a,x}$ is not completely monotonic, we apply directly Proposition 2.7.2 to obtain second point.
Third point is clear because for any $(a_1,a_2)\in(0,+\infty)^2$ and any $x_2>3/2$,

$$x_1\mapsto\left(\frac{a_2\pi^{x_2+1}}{a_1x_1\Gamma(x_2)}\right)^{\frac{1}{x_2+1/2}}$$

is an increasing function which goes to infinity as $x_1\to 0$. □

Example 2.7.7. For instance, we can choose $a=(1,1)$, $x_2=6$ and $A_0=1$. Thus we get

$$C_1=\frac{\pi^{13}}{11!}\approx 0.0727432$$

and for any $x_1\le C_1$, Λ_1 is the unique minimizer of $E_{f_{a,x}}$ among Bravais lattices of unit fixed area.
Moreover the form of the potential $y\mapsto f_{a,x}(y^2)$ is such that the decay to 0 at infinity is slow as x_1 goes to 0.

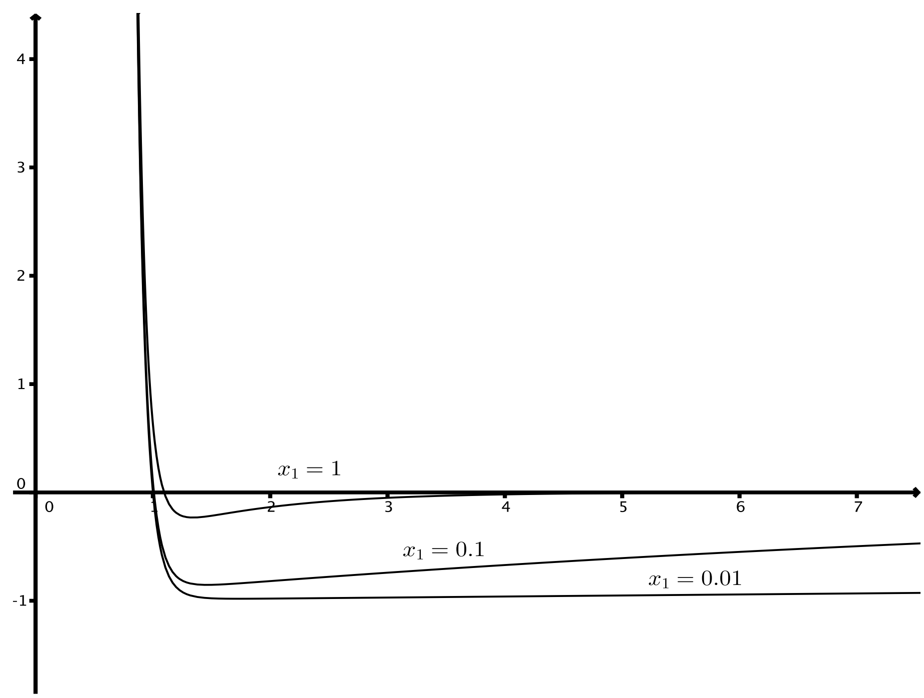


FIGURE 2.10 – Graph of $y\mapsto f_{a,x}(y^2)=\dfrac{1}{y^{12}}-e^{-x_1y}$ for $x_1\in\{0.01,0.1,1\}$

Remark 2.7.8. Our argument used in proofs of Theorem 2.1.2, based on variations of potential, can't be applied for our potentials $f_{a,x}$.

Chapitre 3

Minimization of Energy per Particle among Bravais lattices in $\mathbb{R}^2$: Lennard-Jones (12-6) and Thomas-Fermi cases

Ce chapitre fait référence à [10], écrit en collaboration avec Peng Zhang et publié dans *Communications in Contemporary Mathematics* en 2014, restitué tel quel et antérieur à [7] dont les résultats sont présentés au chapitre précédent.

Sommaire

3.1 Introduction

Understanding the structure of matter at low temperature has been a challenge for many years. In this case, one of the simplest models is to consider identical points as particles interacting in a Lennard-Jones potential. This model is deterministic, therefore we do not consider either entropy nor other quantum effects. The problem is to find the configuration of the points which minimize the total interaction energy, called the Lennard-Jones energy. Radin, in [44], studied this problem in one dimension and showed that, in the case of infinite points, the minimizer is periodic. His method is not adaptable in higher dimensions and he studied, in [54, 80] the case of short range interactions and proved the first result of crystallization in two dimensions for a hard-sphere model. In the meantime, Ventevogel and Nijboer gave in [102, 104, 103] more general results in one dimension for Lennard-Jones energy per particle. Indeed, they showed that a unique lattice of the form $a_0\mathbb{N}$ minimizes the Lennard-Jones energy and that all lattices $a\mathbb{N}$ with $a \leq a_0$ minimize this energy when the density of points $\rho = a^{-1}$ is fixed. Our paper gives some results in the spirit of the latter paper.

After a numerical investigation of Yedder, Blanc, Le Bris, in [13], about the minimization of the Lennard-Jones and the Thomas-Fermi energy in $\mathbb{R}^2$, it seemed that the triangular lattice, also called "hexagonal lattice" – which is composed of equilateral triangles – is the minimum configuration for Lennard-Jones energy among any lattices and for Thomas-Fermi energy with nuclei density fixed. Some time after, Theil, in [99], gave the first proof of crystallization in two dimensions for a "Lennard-Jones like" potential, with a minimum less than one but very close to one and long range interaction. He showed that the global minimizer of the total energy is triangular. His method was adapted by E and Li, in [36], for a three-body potential with long range interactions in order to obtain a honeycomb lattice as global minimizer – see also the works of Mainini, Piovano and Stefanelli in [65, 66] about the crystallization in square and honeycomb lattices for three-body potentials with short range interactions – and by Theil and Flatley in three dimensions in [41].

Furthermore Montgomery, in [74], proved that the triangular lattice is the unique minimizer of theta functions among Bravais lattices with fixed density and hence the unique minimizer of the Epstein zeta function, thanks to the link between these two functions. As the Lennard-Jones potential is a linear sum of Epstein zeta functions, it is natural to study the problem of minimization of the Lennard-Jones energy among

Bravais lattices with and without fixed density. However, there are few results about minimization in the general case of periodic systems. For example, Cohn and Kumar described in [30] a method and a conjecture for completely monotonic functions. It is interesting to observe that this kind of problem is connected with the theory of spherical design due to Delsarte, Goethals and Seidel in [34] and linked to the layers of a lattice, among others, by Venkov and Bachoc in [101, 3] and by Coulangeon et al. in [31, 33, 32].

In this paper, our main results are :

THEOREM :

— *Let $V_{LJ}(r) = r^{-12} - 2r^{-6}$ be the Lennard-Jones potential, then the minimizer of the energy $E_{LJ}(L) = \sum_{p\in L\backslash\{0\}} V_{LJ}(\|p\|)$ among all Bravais lattices of $\mathbb{R}^2$ with fixed density sufficiently large is triangular and unique, up to rotation.*

— *A minimizer of E_{LJ} among all Bravais lattices with fixed density sufficiently small cannot be triangular.*

— *Let $L_0 = \mathbb{Z}u \oplus \mathbb{Z}v$ be a global minimizer of E_{LJ} among all Bravais lattices with $\|u\| \leq \|v\|$, then $0.74035 < \|u\| \leq \|v\| \leq 1$.*

— *Moreover, we have $\zeta_{L_0}(6) = \max\{\zeta_L(6); L$ such that $\zeta_L(12) \leq \zeta_L(6)\}$.*

— *Let $W_{TF} : \mathbb{R}_+^* \to \mathbb{R}$ be the solution of $-\Delta h + \pi h = \delta_0$ which goes to 0 at infinity, then the minimizer of the Thomas-Fermi energy $E_{TF}(L) = \sum_{p\in L\backslash\{0\}} W_{TF}(\|p\|)$ among all Bravais lattices of $\mathbb{R}^2$ with density fixed is triangular and unique, up to rotation.*

This chapter is structured as follows : in Section 3.2, we introduce the notations ; in Section 3.3, we show that the minimizer of the Lennard-Jones energy per particle among Bravais lattices with fixed density, if the density is sufficiently large, it is triangular and unique. Moreover we give numerical results and a conjecture for the minimization with density fixed and we have arguments in order to explain why the global minimizer, among Bravais lattices without fixed density, is triangular ; in Section 3.4, we use proof of Blanc in [11] to find a lower bound for the interparticle distance of the global minimizer, and finally in Section 3.5 we study the same kind of problem for the Thomas-Fermi model only when the density is fixed and we prove that the triangular lattice is the unique minimizer of the Thomas-Fermi energy per particle in $\mathbb{R}^2$.

3.2 Preliminaries

A Bravais lattice (also called a "simple lattice") of $\mathbb{R}^2$ is given by $L = \mathbb{Z}u \oplus \mathbb{Z}v$ where (u,v) is a basis of $\mathbb{R}^2$. By Engel's theorem (see [38]), we can choose u and v so that $\|u\| \leq \|v\|$ and $(\widehat{u,v}) \in \left[\frac{\pi}{3}, \frac{\pi}{2}\right]$ in order to obtain the unicity of the lattice, up to a rotation. We note $|L| = \|u \wedge v\| = \|u\|\|v\|\, |\sin(\widehat{u,v})|$ the area of L which is in fact the area of the lattice primitive cell and $L^* := L\backslash\{0\}$. The **positive definite quadratic form associated with the Bravais lattice** L is, for $(m,n) \in \mathbb{Z}^2$,

$$Q_L(m,n) = \|mu + nv\|^2 = \|u\|^2 m^2 + \|v\|^2 n^2 + 2\|u\|\|v\| \cos(\widehat{u,v}) mn.$$

For a positive definite quadratic form $q(m,n) = am^2 + bmn + cn^2$, we define its **discriminant** $D = b^2 - 4ac < 0$. Hence for Q_L, we obtain :

$$-D = 4\|u\|^2\|v\|^2 - 4\|u\|^2\|v\|^2 \cos^2(\widehat{u,v}) = 4\|u\|^2\|v\|^2 \sin^2(\widehat{u,v}) = 4|L|^2.$$

In this chapter, the term "lattice" will mean a "Bravais lattice", and we define, for $s > 2$, the **Epstein zeta function of the lattice** L by

$$\zeta_L(s) := \sum_{p \in L^*} \frac{1}{\|p\|^s} = \sum_{(m,n) \neq (0,0)} \frac{1}{Q_L(m,n)^{s/2}}.$$

Let $\Lambda_A = \sqrt{\frac{2A}{\sqrt{3}}} \left[\mathbb{Z}(1,0) \oplus \mathbb{Z}(1/2, \sqrt{3}/2)\right]$ be the **triangular lattice of area** A, also called the hexagonal lattice. Its **length** is the norm of its vector u, i.e. the minimum distance strictly positive of Λ_A, $\|u\| = \sqrt{2A/\sqrt{3}}$. We notice, for any $s > 2$, that

$$\zeta_{\Lambda_A}(s) = \frac{\zeta_{\Lambda_1}(s)}{A^{s/2}} \tag{3.2.1}$$

and this relation of scaling is true for any lattice L of area A.
We recall the result of Montgomery, proved in our annex, about theta functions :

Theorem 3.2.1. (Montgomery, [74]) *For any real number $\alpha > 0$ and a Bravais lattice L, let*

$$\theta_L(\alpha) := \Theta_L(i\alpha) = \sum_{m,n \in \mathbb{Z}} e^{-2\pi\alpha Q_L(m,n)},$$

where Θ_L is the ***Jacobi theta function of the lattice*** *L defined for $Im(z) > 0$. Then, for any $\alpha > 0$, Λ_A is the unique minimizer of $L \to \theta_L(\alpha)$ among lattices of area A, up to rotation.*

Remark 3.2.2. The same kind of results were obtained by Nonnenmacher and Voros in [75]. The previous theorem implies that the triangular lattice is the unique minimizer, up to rotation, of $L \mapsto \zeta_L(s)$ among lattices with density fixed for any $s > 2$ which is also proved by Rankin (in [82]).

We consider the classical Lennard-Jones potential

$$V_{LJ}(r) = \frac{1}{r^{12}} - \frac{2}{r^6}$$

whose minimum is obtained at $r = 1$, and for $L = \mathbb{Z}u \oplus \mathbb{Z}v$ a Bravais lattice of $\mathbb{R}^2$, we let

$$E_{LJ}(L) := \sum_{p \in L^*} V_{LJ}(\|p\|) = \zeta_L(12) - 2\zeta_L(6)$$

be the **Lennard-Jones energy of lattice** L. By (3.2.1) this energy among lattices of area A can be viewed as energy $L \mapsto E_{LJ}(\sqrt{A}L)$ over lattices of area 1 and we parametrize L with its length $\|u\|$ and $\|v\|$ by

$$Q_L(m,n) = \|u\|^2 m^2 + \|v\|^2 n^2 + 2mn\sqrt{\|u\|^2\|v\|^2 - 1}.$$

It follows that we can write Lennard-Jones energy among lattices of area A as

$$(\|u\|, \|v\|) \mapsto \sum_{(m,n) \neq (0,0)} V_{LJ}\left(\sqrt{A}\sqrt{\|u\|^2 m^2 + \|v\|^2 n^2 + 2mn\sqrt{\|u\|^2\|v\|^2 - 1}}\right). \quad (3.2.2)$$

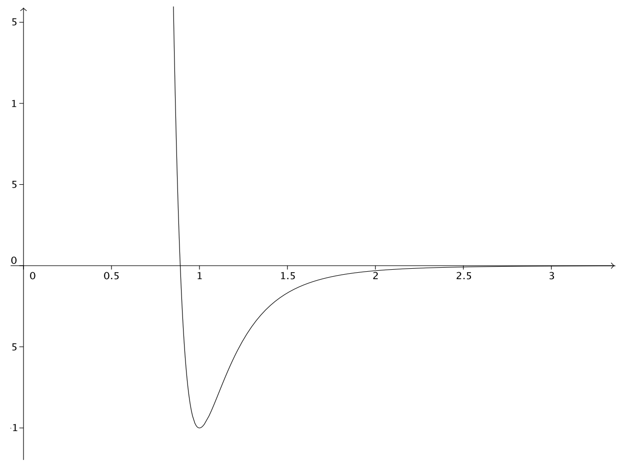


FIGURE 3.1 – Graph of the Lennard-Jones potential V_{LJ}

The aim of this chapter is to study the following two minimization problems, up to rotation :

$$
\begin{aligned}
&(P_A): \text{ Find the minimizer of } E_{LJ} \text{ among lattices } L \text{ with fixed } |L| = A;\\
&(P): \text{ Find the minimizer of } E_{LJ} \text{ among lattices.}
\end{aligned}
$$

Proposition 3.2.3. *The minimum of E_{LJ} among lattices is achieved.*

Proof. We parametrize a lattice L by $x = \|u\|$, $y = \|v\|$ and $\theta = (\widehat{u,v})$, therefore

$$
\begin{aligned}
&f(x,y,\theta) := E_{LJ}(L)\\
&= \sum_{(m,n)\neq(0,0)} \left(\frac{1}{(x^2m^2 + y^2n^2 + 2xymn\cos\theta)^6} - \frac{2}{(x^2m^2 + y^2n^2 + 2xymn\cos\theta)^3} \right).
\end{aligned}
$$

First case : minimization without fixed area. If L is the solution of (P) then x and y cannot be too small, otherwise the energy is too large and a proof of a lower bound for x is given in Section 3.4. Moreover $y \leq 1$ because if $y > 1$ then a contraction of the line $\mathbb{R}v$ gives smaller energy. Therefore we have $x, y \in [m, M]$ and $\theta \in [\pi/3, \pi/2]$. The function $(x,y,\theta) \mapsto f(x,y,\theta)$ is continuous on $[m,M] \times [m,M] \times [\pi/3, \pi/2]$ hence its minimum is achieved.
Second case : minimization with fixed area. We can parametrize L with only two variables x and y – as in (3.2.2) – such that when $x \to 0$ then $y \to +\infty$. As L should be a Bravais lattice, it is clear that the minimum of f is achieved. $\square$

3.3 Minimization among lattices with fixed area

3.3.1 A sufficient condition for the minimality of E_{LJ} : Montgomery's method

Our idea is to write E_{LJ} in terms of θ_L and to use Theorem 3.2.1 in order to find a sufficient condition for the minimality of the triangular lattice among Bravais lattices with a fixed area.

Theorem 3.3.1. *If $A^3 \leq \dfrac{\pi^3}{120}$, then Λ_A is the unique solution of (P_A).*

Proof. As it is explained in [74] or [98], we can write the Epstein zeta function in terms of a theta function. Indeed, we have the following identity, where the discriminant of Q_L is $D = 1$:

$$\text{for } \mathrm{Re}(s) > 1, \zeta_L(2s)\Gamma(s)(2\pi)^{-s} = \frac{1}{s-1} - \frac{1}{s} + \int_1^\infty (\theta_L(\alpha) - 1)(\alpha^s + \alpha^{1-s})\frac{d\alpha}{\alpha}. \quad (3.3.1)$$

Thus, for $|L| = A$, we write $E_{LJ}(L) = \zeta_L(12) - 2\zeta_L(6)$ as an integral

$$\int_1^{+\infty} g_A(\alpha)\left(\theta_L\left(\frac{\alpha}{2A}\right) - 1\right)\frac{d\alpha}{\alpha},$$

up to a constant independent of L and we find A so that $g_A(\alpha) \geq 0$ for any $\alpha \geq 1$. As Λ_A is the unique minimizer of $\theta_L(\alpha)$ for any $\alpha > 0$, we have for any L such that $|L| = A$:

$$E_{LJ}(L) - E_{LJ}(\Lambda_A) = \int_1^{+\infty}\left(\theta_L\left(\frac{\alpha}{2A}\right) - \theta_{\Lambda_A}\left(\frac{\alpha}{2A}\right)\right) g_A(\alpha)\frac{d\alpha}{\alpha} \geq 0$$

and Λ_A is the unique solution of (P_A).
In fact (3.3.1) it is the classic "Riemann's trick" and here we will briefly recall its proof : as

$$\Gamma(s)(2\pi)^{-s}Q_L(m,n)^{-s} = \int_0^\infty t^{s-1}e^{-t}(2\pi)^{-s}Q_L(m,n)^{-s}dt$$

for $\mathrm{Re}(s) > 1$, and by putting $t = 2\pi Q_L(m,n)y$, we obtain

$$\Gamma(s)(2\pi)^{-s}Q_L(m,n)^{-s} = \int_0^\infty e^{-2\pi y Q_L(m,n)}y^{s-1}dy.$$

Summing over $(m,n) \neq (0,0)$ and using the identity $\theta_L(1/\alpha) = \alpha\theta_L(\alpha)$ for any $\alpha > 0$, proved by Montgomery in [74], we obtain

$\Gamma(s)(2\pi)^{-s}\zeta_L(2s)$

$$
\begin{aligned}
&= \int_0^{\infty} (\theta_L(y)-1)y^{s-1}dy \\
&= \int_0^{1} (\theta_L(y)-1)y^{s-1}dy + \int_1^{\infty} (\theta_L(y)-1)y^{s-1}dy \\
&= \int_1^{\infty} (\theta_L(1/\alpha)-1)\alpha^{-1-s}d\alpha + \int_1^{\infty} (\theta_L(\alpha)-1)\alpha^{s-1}d\alpha \\
&= \int_1^{\infty} (\alpha\theta_L(\alpha)-1)\alpha^{-1-s}d\alpha + \int_1^{\infty} (\theta_L(\alpha)-1)\alpha^{s-1}d\alpha \\
&= \int_1^{\infty} \theta_L(\alpha)\alpha^{-s}d\alpha - \int_1^{\infty} \alpha^{-1-s}d\alpha + \int_1^{\infty} (\theta_L(\alpha)-1)\alpha^{s-1}d\alpha \\
&= \int_1^{\infty} (\theta_L(\alpha)-1)\alpha^{-s}d\alpha + \int_1^{\infty} (\theta_L(\alpha)-1)\alpha^{s-1}d\alpha + \int_1^{\infty} \alpha^{-s}d\alpha - \int_1^{\infty} \alpha^{-1-s}d\alpha \\
&= \int_1^{\infty} (\theta_L(\alpha)-1)\alpha^{-s}d\alpha + \int_1^{\infty} (\theta_L(\alpha)-1)\alpha^{s-1}d\alpha + \frac{1}{s-1} - \frac{1}{s} \\
&= \int_1^{\infty} (\theta_L(\alpha)-1)(\alpha^{s}+\alpha^{1-s})\frac{d\alpha}{\alpha} + \frac{1}{s-1} - \frac{1}{s}.
\end{aligned}
$$

Now if $|L| = A$, by the equality $D = (2A)^2$ there are two identities :

$$(2\pi)^{-6}(2A)^6\Gamma(6)\zeta_L(12) = \frac{1}{5} - \frac{1}{6} + \int_1^{+\infty} \left(\theta_L\left(\frac{\alpha}{2A}\right)-1\right)(\alpha^6+\alpha^{1-6})\frac{d\alpha}{\alpha}$$

$$(2\pi)^{-3}(2A)^3\Gamma(3)\zeta_L(6) = \frac{1}{2} - \frac{1}{3} + \int_1^{+\infty} \left(\theta_L\left(\frac{\alpha}{2A}\right)-1\right)(\alpha^3+\alpha^{1-3})\frac{d\alpha}{\alpha}$$

and we find

$$\zeta_L(12) = \frac{(2\pi)^6}{30(2A)^6 5!} + \int_1^{+\infty} \left(\theta_L\left(\frac{\alpha}{2A}\right)-1\right)\frac{(2\pi)^6}{(2A)^6 5!}(\alpha^6+\alpha^{-5})\frac{d\alpha}{\alpha}$$

$$\zeta_L(6) = \frac{(2\pi)^3}{6(2A)^3 2!} + \int_1^{+\infty} \left(\theta_L\left(\frac{\alpha}{2A}\right)-1\right)\frac{(2\pi)^3}{(2A)^3 2!}(\alpha^3+\alpha^{-2})\frac{d\alpha}{\alpha}.$$

Therefore, for any L of area A,

$$E_{LJ}(L) = C_A + \frac{\pi^3}{A^3}\int_1^{+\infty} \left(\theta_L\left(\frac{\alpha}{2A}\right)-1\right) g_A(\alpha)\frac{d\alpha}{\alpha}$$

where $g_A(\alpha) := \frac{\pi^3}{A^3 5!}(\alpha^6+\alpha^{-5}) - (\alpha^3+\alpha^{-2})$, and C_A is a constant depending on A but independent of L. Now we want to prove that if $\pi^3 \geq 120A^3$ then $g_A(\alpha) \geq 0$ for any $\alpha \geq 1$. First, we remark that

$$g_A(1) \geq 0 \iff \frac{\pi^3}{A^3 5!} - 1 \geq 0 \iff \pi^3 \geq 120A^3.$$

Secondly, we compute $g_A'(\alpha) = \dfrac{\pi^3}{A^3 5!}(6\alpha^5 - 5\alpha^{-6}) - (3\alpha^2 - 2\alpha^{-3})$, and if $\pi^3 \geq 120A^3$ then

$$g_A'(1) = \frac{\pi^3}{A^3 5!} - 1 \geq 0.$$

Finally, we compute $g_A''(\alpha) = \dfrac{\pi^3}{A^3 5!}(30\alpha^4 + 30\alpha^{-7}) - (6\alpha + 6\alpha^{-4})$. As $\dfrac{\pi^3}{A^3 5!} \geq 1$ and $\alpha \geq 1$,

$$\frac{\pi^3}{A^3 5!}(30\alpha^4+30\alpha^{-7})-(6\alpha+6\alpha^{-4}) \geq 30\alpha^4+30\alpha^{-7}-6\alpha-6\alpha^{-4} \geq 24\alpha+30\alpha^{-7}-6\alpha^{-4} \geq 0.$$

Thus, we have shown that, for any A so that $\pi^3 \geq 120A^3$, $g_A''(\alpha) \geq 0$ for any $\alpha \geq 1$, $g_A'(1) \geq 0$ and $g_A(1) \geq 0$. Hence $g_A(\alpha) \geq 0$ for any $\alpha \geq 1$ if $\pi^3 \geq 120A^3$. $\square$

Remark 3.3.2. We have $\left(\dfrac{\pi^3}{120}\right)^{1/3} \approx 0.63693$, hence for $A \leq 0.63692$, Λ_A is the unique solution of (P_A).

Remark 3.3.3. We prove below (see Proposition 3.3.5) that when A is sufficiently large then Λ_A is no longer a solution of (P_A). However, our bound $\pi^3 \geq 120A^3$ is likely not to be optimal. If it were, by the Proposition 3.4.3 and its remark, then the triangular lattice is not the solution to (P).

This result explains that the behaviour of the potential is important for the interaction between the first neighbours because in this case the reverse power part r^{-12} is the strongest interaction.

Remark 3.3.4. The three-dimensional case is an open problem. Indeed, there is no result related to the minimization of theta and Epstein functions among Bravais lattices of $\mathbb{R}^3$ with fixed volume. Sarnak and Strömbergsson recalled in [88] that Ennola had shown in [40] the local minimality of the face centred cubic lattice for $\zeta_L(s)$ and for any $s > 0$. They also prove that the face centred cubic lattice cannot be the minimizer of $\zeta_L(s)$ for all $s > 0$. Hence the problem of minimization of Lennard-Jones energy among lattices of $\mathbb{R}^3$, and of course in higher dimensions, seems to be very difficult.

3.3.2 A necessary condition for the minimality of the triangular lattice for E_{LJ}

Proposition 3.3.5. *Λ_A is a solution of (P_A) if and only if* $A \leq \inf_{\substack{|L|=1\\ L\neq\Lambda_1}} \left(\dfrac{\zeta_L(12)-\zeta_{\Lambda_1}(12)}{2(\zeta_L(6)-\zeta_{\Lambda_1}(6))}\right)^{1/3}$.
Hence if A is sufficiently large, Λ_A is not a solution of (P_A).

Proof. We have the following equivalences

$$\begin{aligned}
& E_{LJ}(\Lambda_A) \leq E_{LJ}(L) \text{ for any } L \text{ such that } |L| = A \\
\iff & \zeta_{\Lambda_A}(12) - 2\zeta_{\Lambda_A}(6) \leq \zeta_L(12) - 2\zeta_L(6) \text{ for any } L \text{ such that } |L| = A \\
\iff & 2(\zeta_L(6) - \zeta_{\Lambda_A}(6)) \leq \zeta_L(12) - \zeta_{\Lambda_A}(12) \text{ for any } L \text{ such that } |L| = A \\
\iff & \frac{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))}{A^3} \leq \frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{A^6} \text{ for any } L \text{ such that } |L| = 1
\end{aligned}$$

by the scaling property (3.2.1). We recall that $\zeta_L(6) > \zeta_{\Lambda_1}(6)$ for any L of area A so that $L \neq \Lambda_1$, as a consequence of Theorem 3.2.1 and the Riemann's trick (3.3.1). Then we obtain

$$\begin{aligned}
& E_{LJ}(\Lambda_A) \leq E_{LJ}(L) \text{ for any } L \text{ such that } |L| = A \\
\iff & A \leq \inf_{\substack{|L|=1 \\ L \neq \Lambda_1}} \left(\frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3}.
\end{aligned}$$

□

It is difficult to study the minimum of function $L \mapsto \left(\frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3}$ among lattices $L \neq \Lambda_1$ such that $|L| = 1$. However, we can numerically look for a lower bound. This function can be parametrized with two variables – here the lengths $\|u\|$ and $\|v\|$ of the lattice L as in (3.2.2) – and we can plot the level sets of it. We notice that the large differences between the values of the function only give a domain where the function is minimum.

Indeed, its minimum seems to be around lattice L of area 1 such that $\|u\| = \|v\| = 1.014$ and for this one, we have $\left(\frac{\zeta_L(12) - \zeta_{\Lambda_1}(12)}{2(\zeta_L(6) - \zeta_{\Lambda_1}(6))} \right)^{1/3} \approx 1.1378475$, hence numerically the minimum of this function is between 1.13 and 1.14.

Actually Figure 3.3 gives the Lennard-Jones energy – viewed as a function of two variables $\|u\|$ and $\|v\|$ over the lattices of area one (see (3.2.2)) – for $(\|u\|, \|v\|) \in [1, 1.08]^2$. The triangular lattice Λ_1 corresponds to the point $\left(\sqrt{2/\sqrt{3}}, \sqrt{2/\sqrt{3}}\right) \approx (1.075, 1.075)$ and the square lattice $\mathbb{Z}^2$ corresponds to the point $(1, 1)$. In fact it is clear that the point associated with the triangular lattice is a critical point of this energy, because the triangular lattice is the unique minimizer of Epstein zeta function among lattices of area A. Moreover we can prove that the square lattice is also a critical point, by using an other parametrization as $(\|u\|, \theta)$. We numerically obtain :

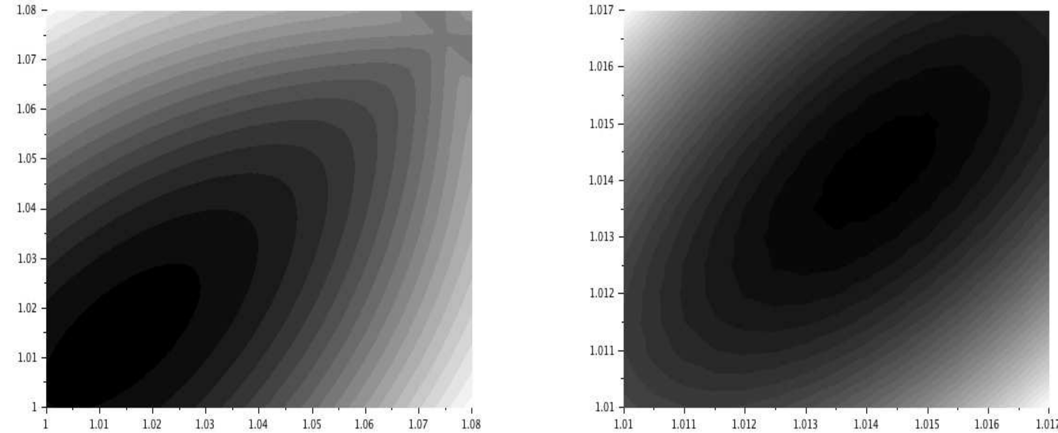
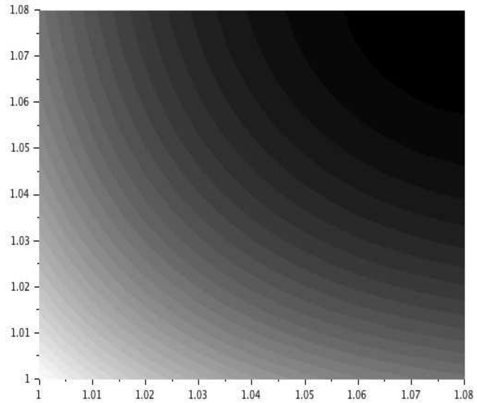


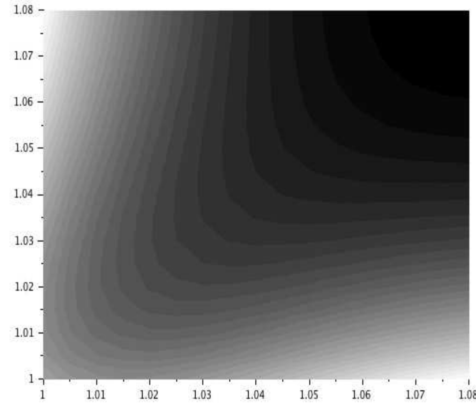
FIGURE 3.2 – Level sets of $(\|u\|,\|v\|)\mapsto \left(\dfrac{\zeta_L(12)-\zeta_{\Lambda_1}(12)}{2(\zeta_L(6)-\zeta_{\Lambda_1}(6))}\right)^{1/3}$ (black = minimum, white = maximum)

- For $A=1$, Λ_1 seems to be its minimizer and $\mathbb{Z}^2$ is a local maximizer.
- For $A=1.13$, Λ_1 seems to be its minimizer but $\mathbb{Z}^2$ seems to be not a local maximizer.
- For $A=1.14$, $\mathbb{Z}^2$ seems to be its minimizer because we estimate $E_{LJ}(\sqrt{1.14}\Lambda_1)\approx -4.435$ is larger than $E_{LJ}(\sqrt{1.14}\mathbb{Z}^2)\approx -4.437$.
- For $A=1.16$, $\mathbb{Z}^2$ seems to be its minimizer.
- For $A=1.2$, $\mathbb{Z}^2$ seems to be its minimizer and Λ_1 is a local maximizer.
- For $A=2$ (and more), $\mathbb{Z}^2$ seems to be its minimizer and Λ_1 is a local maximizer.

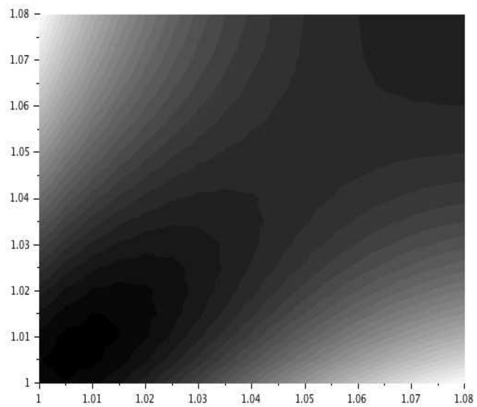
Hence, we can write the following conjecture based on our numerical study of $L\mapsto E_{LJ}(\sqrt{A}L)$ among all lattices with area 1 :
Conjecture : *If A is sufficiently large, the square lattice is the unique solution of (P_A).*



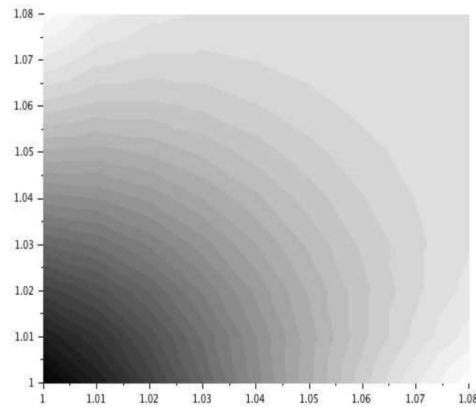
A=1



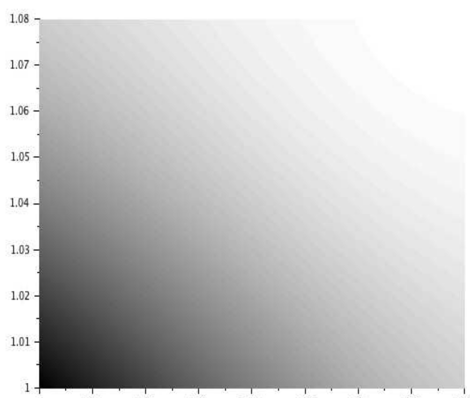
A=1.13



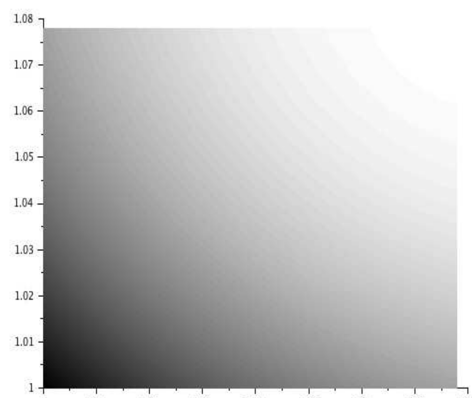
A=1.14



A=1.16



A=1.2



A=2

FIGURE 3.3 – Level sets of $(\|u\|, \|v\|) \mapsto E_{LJ}(\sqrt{A}L)$ for some interesting values of A. (black = min , white = max)

3.4 Global minimization of E_{LJ} among lattices

Now we study the problem (P). We give high properties for the global minimizer among lattices and some indications of its shape.

3.4.1 Characterization of the global minimizer

Proposition 3.4.1. *If $L_0 = \mathbb{Z}u \oplus \mathbb{Z}v$ is a solution of (P) then*
i) $E_{LJ}(L_0) = -\zeta_{L_0}(6) = -\zeta_{L_0}(12) < 0$,
ii) $\|u\| < 1$ *and* $\|v\| \leq 1$,
iii) $\zeta_{L_0}(6) = \max\{\zeta_L(6); L \text{ such that } \zeta_L(12) \leq \zeta_L(6)\}$.

Proof. *i)* We consider the function $f(r) = E_{LJ}(rL_0) = r^{-12}\zeta_{L_0}(12) - 2r^{-6}\zeta_{L_0}(6)$. As L_0 is a global minimizer of E_{LJ}, $r = 1$ is the critical point of f and

$$f'(r) = -12r^{-13}\zeta_{L_0}(12) + 12r^{-7}\zeta_{L_0}(6),$$

hence

$$f'(1) = 0 \iff \zeta_{L_0}(12) = \zeta_{L_0}(6)$$

and $E_{LJ}(L_0) = \zeta_{L_0}(12) - 2\zeta_{L_0}(6) = -\zeta_{L_0}(6) = -\zeta_{L_0}(12)$.

ii) As $\zeta_{L_0}(12) = \zeta_{L_0}(6)$, it is clear that $\|u\| < 1$ because if $r > 1$ then $r^{-12} < r^{-6}$. If $\|v\| > 1$, a little contraction of $\mathbb{R}v$ yields a new lattice L_1 such that $E_{LJ}(L_1) < E_{LJ}(L_0)$ because some of the distances of the lattice decrease while $\|u\|$ is constant, therefore the energy decreases.
iii) $-\zeta_{L_0}(6) = E_{LJ}(L_0) \leq E_{LJ}(L) \iff \zeta_L(6) - \zeta_{L_0}(6) \leq \zeta_L(12) - \zeta_L(6)$ and if L is a lattice such that $\zeta_L(12) \leq \zeta_L(6)$, we get $\zeta_L(6) \leq \zeta_{L_0}(6)$. □

Corollary 3.4.2. *The triangular lattice of length 1 cannot be the solution of (P) though the minimum of the potential V_{LJ} is achieved for $r = 1$.*

Proposition 3.4.3. *The minimizer of E_{LJ} among triangular lattices is Λ_{A_0} such that*

$$A_0 = \left(\frac{\zeta_{\Lambda_1}(12)}{\zeta_{\Lambda_1}(6)}\right)^{1/3}.$$

Proof. As in the above proof, we define the function $f(r) = E_{LJ}(r\Lambda_1)$ and we compute its first derivative $f'(r) = -12r^{-13}\zeta_{\Lambda_1}(12) + 12r^{-7}\zeta_{\Lambda_1}(6)$. It follows that :

$$f'(r) \geq 0 \iff r \geq \left(\frac{\zeta_{\Lambda_1}(12)}{\zeta_{\Lambda_1}(6)}\right)^{1/6} =: r_0$$

hence $\Lambda_{A_0} = r_0\Lambda_1$, with $A_0 = r_0^2 = \left(\frac{\zeta_{\Lambda_1}(12)}{\zeta_{\Lambda_1}(6)}\right)^{1/3}$, is the minimizer of E_{LJ} among all triangular lattices. $\square$

Remark 3.4.4. We compute $A_0 \approx 0.84912$, therefore the length of this lattice is $\|u\| \approx 0.99019$. Moreover we notice that $E_{LJ}(\Lambda_{A_0}) = -\zeta_{\Lambda_{A_0}}(6) \approx -6.76425$ (it will be useful for the next part).
Because $A_0 > 0.63692$, Theorem 3.3.1 is not sufficient to prove that Λ_{A_0} is the solution of (P) but a numerical investigation of $L \mapsto E_{LJ}(\sqrt{A_0}L)$ among all lattices of area 1 seems to indicate that the solution of (P_{A_0}) is triangular and unique. Moreover it is not

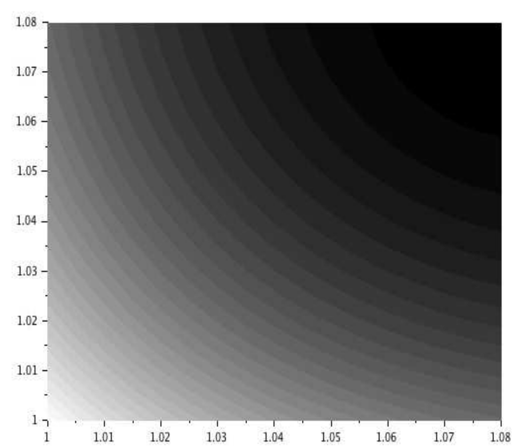


FIGURE 3.4 – Level sets of $(\|u\|, \|v\|) \mapsto E(\sqrt{A_0}L)$. (black = min, white = max)

difficult to prove numerically that Λ_{A_0} is a local minimizer among all lattices. Hence we can write the following conjecture for this problem :

Conjecture : *The triangular lattice Λ_{A_0} is the unique solution of (P).*

3.4.2 Minimum length of the global minimizer

Because our method does not show that the triangular lattice of area A_0 is the global minimizer of the Lennard-Jones energy among lattices, we use Blanc's proof, from [11], in order to find a lower bound for the minimal distance in the globally minimizing lattice. His result was for the Lennard-Jones interaction of N points in $\mathbb{R}^2$ and $\mathbb{R}^3$. Xue in [108] and Schachinger, Addis, Bomze and Schoen in [2] improved this. We use Blanc's method because it is well suited to our problem.

Proposition 3.4.5. *If $L_0 = \mathbb{Z}u \oplus \mathbb{Z}v$ is a solution of (P), then the minimal distance is greater than an explicit constant c. Furthermore, we have $c > 0.74035$.*

Proof. In [11], Blanc proved that

$$E_{LJ}(L_0) \geq V_{LJ}(\|u\|) - 23 + \frac{1}{\|u\|^{12}} \sum_{k\geq 2} \frac{16k+8}{k^{12}} - \frac{1}{\|u\|^6} \sum_{k\geq 2} \frac{32k+16}{k^6}.$$

As we have $E_{LJ}(L_0) \leq E_{LJ}(\Lambda_{A_0}) = -\zeta_{\Lambda_{A_0}}(6)$ we obtain

$$23 - \zeta_{\Lambda_{A_0}}(6) \geq \frac{P+1}{\|u\|^{12}} - \frac{Q+2}{\|u\|^6}.$$

with $P := \displaystyle\sum_{k\geq 2} \frac{16k+8}{k^{12}}$ and $Q := \displaystyle\sum_{k\geq 2} \frac{32k+16}{k^6}$.

Now, setting $t = \|u\|^{-6}$, we have $(P+1)t^2 - (Q+2)t - 23 + \zeta_{\Lambda_{A_0}}(6) \leq 0$ which implies

$$t \leq \frac{Q+2+\sqrt{(Q+2)^2 + 4(23-\zeta_{\Lambda_{A_0}}(6))(P+1)}}{2(P+1)}$$

and we obtain

$$\|u\| \geq \left(\frac{2(P+1)}{Q+2+\sqrt{(Q+2)^2 + 4\left(23-\zeta_{\Lambda_{A_0}}(6)\right)(P+1)}} \right)^{1/6} =: c.$$

Since $P \approx 0.00988$, $Q \approx 1.45918$ and $\zeta_{\Lambda_{A_0}}(6) \approx 6.76425$ we get $c > 0.74035$. □

Remark 3.4.6. As we think that Λ_{A_0} is the unique solution of (P), this lower bound is the best that we can find with this method. Moreover, this bound and the second point of Proposition 3.4.1 imply that $0.47468 < |L_0| < 1$.

3.5 The Thomas-Fermi model in $\mathbb{R}^2$

In Thomas-Fermi's model for interactions in a solid, we consider N nuclei at positions $X_N = (x_1, ..., x_N)$, with for any $1 \leq i \leq N$, $x_i \in \mathbb{R}^2$, associated with N electrons with total density $\rho \geq 0$. Then the **Thomas-Fermi energy** is given by

$$\begin{aligned} E^{TF}(\rho, X_N) = &\int_{\mathbb{R}^2} \rho^2(x)dx - \frac{1}{2}\iint_{\mathbb{R}^2\times\mathbb{R}^2} \log\|x-y\|\rho(x)\rho(y)dxdy \\ &+ \sum_{j=1}^N \int_{\mathbb{R}^2} \log\|x-x_j\|\rho(x)dx - \frac{1}{2}\sum_{j\neq k} \log\|x_j - x_k\|. \end{aligned}$$

To introduce this kind of model property in quantum chemistry, refer to [24]. Because the system is neutral, the number of electrons is exactly N and we study the minimization problem $I_N^{TF} = \inf_{X_N}\{E^{TF}(X_N)\}$ where

$$E^{TF}(X_N) := \inf_{\rho}\left\{E^{TF}(\rho, X_N), \rho \geq 0, \rho \in L^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^2), \int_{\mathbb{R}^2} \rho = N\right\}.$$

By the Euler-Lagrange equations for this minimization problem, we find – as it is explained in Section 2 of [13] and Section 4 of [12] – that the minimizer $\bar{\rho}$ is the solution of

$$-\Delta\bar{\rho} + \pi\bar{\rho} = \pi\sum_{j=1}^N \delta_{x_j}.$$

It is known that the fundamental solution of the modified Helmholtz equation $-\Delta h + h = \delta_0$ – also called "screened Poisson equation" – which goes to 0 at infinity, is the radial modified Bessel function of the second kind, also called the Yukawa potential, defined in [47] and [107], by

$$K_0(\|x\|) = \int_0^{+\infty} e^{-\|x\|\cosh t}dt.$$

Therefore we obtain $\bar{\rho}(x) = \pi\sum_{j=1}^N W_{TF}(\|x-x_j\|)$ where $W_{TF}(\|x\|) = \frac{1}{2}K_0(\sqrt{\pi}\|x\|)$ and finally

$$E^{TF}(X_N) = \sum_{i\neq j} W_{TF}(\|x_i - x_j\|) + NC$$

where C is a constant independent of N and X_N. Now, if we consider that the nuclei are in lattice L, we can study, by taking the mean value of the total energy, the following energy per point

$$E_{TF}(L) = \sum_{p\in L^*} W_{TF}(\|p\|).$$

Theorem 3.5.1. *Λ_A is the unique minimizer of E_{TF} among all lattices of fixed area A.*

Proof. This problem is equivalent to finding the minimizer of $\sum_{p\in L^*} K_0(\|p\|)$ among lattices with a fixed area. We put $y = \frac{1}{2}\|p\|e^t$ for $p \neq 0$ in the integral formula for $K_0(\|p\|)$:

$$\begin{aligned} K_0(\|p\|) = \frac{1}{2}\int_{-\infty}^{+\infty} e^{-\|p\|\cosh t}dt &= \frac{1}{2}\int_0^{+\infty} e^{-\|p\|\cosh(\ln(2y/\|p\|))}\frac{dy}{y} \\ &= \frac{1}{2}\int_0^{+\infty} e^{-y-\frac{\|p\|^2}{4y}}\frac{dy}{y} \\ &= \frac{1}{2}\int_0^{+\infty} e^{-\frac{\|p\|^2}{4y}}e^{-y}\frac{dy}{y}. \end{aligned}$$

Now, for any $y>0$ and any lattice L of area A, we obtain $\sum_{p\in L^*} e^{-\frac{\|p\|^2}{4y}} = \theta_L\left(\frac{1}{8\pi y}\right) - 1.$ Hence, by Montgomery's theorem, the triangular lattice Λ_A minimizes $\theta_L(\alpha)$ for any $\alpha>0$, and it is the unique minimizer of $L\mapsto \theta_L(\alpha)$ among all Bravais lattices with a fixed area A.

Therefore, for any $y>0$, Λ_A is the unique minimizer of the energy $E_y(L) := \sum_{p\in L^*} e^{-\frac{\|p\|^2}{4y}}$ among lattices with a fixed area A. Now it is clear, because $E_y(\Lambda_A)\leq E_y(L)$ for any $y>0$ and for any lattice L with area A, that

$$\frac{1}{2}\int_0^{+\infty} E_y(\Lambda_A)e^{-y}\frac{dy}{y} \leq \frac{1}{2}\int_0^{+\infty} E_y(L)e^{-y}\frac{dy}{y}.$$

Hence, for any L of a fixed area A, we get

$$E_{TF}(\Lambda_A) = \sum_{p\in\Lambda_A^*} W_{TF}(\|p\|) \leq \sum_{p\in L^*} W_{TF}(\|p\|) = E_{TF}(L).$$

□

Remark 3.5.2. The Yukawa potential appears in many vortex interaction models, as the α-model in fluid mechanics and in superconductivity (see for example [1] and [93]). Indeed, the second author recently studied, in [110], Ginzburg-Landau's model for the interactions between vortices in superconductors. He proved, by using a more general method – that it can certainly be used for other potentials – the same result was obtained for minimality of the triangular lattice among all lattices with fixed density. The use of results from Number Theory in Ginzburg-Landau's models for vortices can also be seen in [86].

Chapitre 4

Asymptotics of Optimal Logarithmic Energy on the Sphere

Ce chapitre fait référence à la prépublication [9], écrite en collaboration avec Etienne Sandier.

Sommaire

4.1 Introduction

Let $(x_1, ..., x_n) \in (\mathbb{R}^2)^n$ be a configuration of n points interacting through a logarithmic potential and confined by an external field V. The Hamiltonian of this system, also known as a Coulomb gas, is defined as

$$w_n(x_1, ..., x_n) := -\sum_{i\neq j}^{n} \log|x_i - x_j| + n\sum_{i=1}^{n} V(x_i)$$

where $|\cdot|$ is the Euclidean norm in $\mathbb{R}^2$. The minimization of w_n is linked to the following classical problem of logarithmic potential theory : find a probability measure μ_V on $\mathbb{R}^2$ which minimizes

$$I_V(\mu) := \iint_{\mathbb{R}^2\times\mathbb{R}^2} \left(\frac{V(x)}{2} + \frac{V(y)}{2} - \log|x-y|\right) d\mu(x)d\mu(y) \tag{4.1.1}$$

amongst all probability measures μ on $\mathbb{R}^2$. This type of problem dates back to Gauss. More recent references are the thesis of Frostman [42] and the monography of E.Saff and V.Totik [85]. The usual assumptions on $V : \mathbb{R}^2 \to \mathbb{R} \cup \{+\infty\}$ are that it is lower semicontinuous, that it is finite on a set of nonzero capacity, and that it satisfies the growth assumption

$$\lim_{|x|\to+\infty} \{V(x) - 2\log|x|\} = +\infty. \tag{4.1.2}$$

These assumptions ensure that a unique minimizer μ_V of I_V exists and that it has compact support.

Recently, Hardy and Kuijlaars [53] (see also [52]) proved that if one replaces (4.1.2) by the so-called weak growth assumption

$$\liminf_{|x|\to+\infty} \left\{V(x) - \log(1+|x|^2)\right\} > -\infty, \tag{4.1.3}$$

then I_V still admits a unique minimizer, which may no longer have compact support. Moreover Bloom, Levenberg and Wielonsky [15] proved that the classical Frostman type inequalities still hold in this case.

Coming back to the minimum of the discrete energy w_n, its relation to the minimum of I_V is that as $n \to +\infty$, the minimum of w_n is equivalent to $n^2 \min I_V$. The next term in the asymptotic expansion of w_n was derived by Sandier and Serfaty [87] in the classical case (4.1.2), it reads

$$\min w_n = n^2 \min I_V - \frac{n}{2}\log n + \alpha_V n + o(n),$$

where α_V is related to the minimum of a Coulombian renormalized energy studied in [86] which quantifies the discrete energy of infinitely many positive charges in the plane screened by a uniform negative background. Note that rather strict assumptions in addition to (4.1.2) need to be made on V for this expansion to hold, but they are satisfied in particular if V is smooth and strictly convex.

Here, we show that such an asymptotic formula still holds when the classical growth assumption (4.1.2) is replaced with the weak growth assumption (4.1.3). However it is no longer obvious that the minimum of w_n is achieved in this case, as the weak growth assumption could allows one point to go to infinity.

THEOREM 4.1.1. *Let V be an admissible potential*[1]*. Then the following asymptotic expansion holds.*

$$\inf_{(\mathbb{R}^2)^n} w_n = I_V(\mu_V)n^2 - \frac{n}{2}\log n + \left(\frac{1}{\pi}\min_{\mathcal{A}_1} W - \frac{1}{2}\int_{\mathbb{R}^2} m_V(x)\log m_V(x)dx\right) n + o(n), \tag{4.1.4}$$

where $\mu_V = m_V(x)\,dx$ is the unique minimizer of I_V (see Section 4.2 for precise definitions of W and $\mathcal{A}_1$.)

This result is proved using the methods in [86, 87] suitably adapted to equilibrium measures with possibly non-compact support together with the compactification approach in [53, 52, 15]. This compactification allows also to connect the discrete energy problem for log gases in the plane with the discrete logarithmic energy problem for finitely many points on the unit sphere $\mathbb{S}^2$ in the Euclidean space $\mathbb{R}^3$.

The logarithmic energy of a configuration $(y_1, ..., y_n) \in (\mathbb{S}^2)^n$ is given by

$$\mathrm{E}_{\log}(y_1, ..., y_n) := -\sum_{i\neq j}^{n} \log \|y_i - y_j\|,$$

where $\|\cdot\|$ is the Euclidean norm in $\mathbb{R}^3$. Finding a minimizer of such an energy functional is a problem with many links and ramifications as discussed in the fundamental paper of Saff and Kuijlaars [59] (see also [21]). For instance Smale's 7^{th} problem [92] is to find, for any $n \geq 2$, a universal constant $c \in \mathbb{R}$ and a nearly optimal configuration $(y_1, ..., y_n) \in (\mathbb{S}^2)^n$ such that, letting $\mathcal{E}_{\log}(n)$ denote the minimum of $\mathrm{E}_{\log}$ on $(\mathbb{S}^2)^n$,

$$\mathrm{E}_{\log}(y_1, ..., y_n) - \mathcal{E}_{\log}(n) \leq c\log n.$$

1. See Section 4.3.1 for the precise definition

Identifying the term of order n in the expansion of $\mathcal{E}_{\log}(n)$ can be seen as a modest step towards a better understanding of this problem.

It was known (lower bound by Wagner [106] and upper bound by Kuijlaars and Saff [60]), that

$$\left(\frac{1}{2} - \log 2\right) n^2 - \frac{1}{2} n \log n + c_1 n \leq \mathcal{E}_{\log}(n) \leq \left(\frac{1}{2} - \log 2\right) n^2 - \frac{1}{2} n \log n + c_2 n$$

for some fixed constant c_1 and c_2. Thus one can naturally ask for the existence of the limit

$$\lim_{n \to +\infty} \frac{1}{n} \left[\mathcal{E}_{\log}(n) - \left(\frac{1}{2} - \log 2\right) n^2 + \frac{n}{2} \log n \right].$$

CONJECTURE 1 (Rakhmanov, Saff and Zhou, [81]) : There exists a constant C not depending on n such that

$$\mathcal{E}_{\log}(n) = \left(\frac{1}{2} - \log 2\right) n^2 - \frac{n}{2} \log n + Cn + o(n) \quad \text{as } n \to +\infty.$$

CONJECTURE 2 (Brauchart, Hardin and Saff, [22]) : The constant C in Conjecture 1 is equal to C_{BHS}, where

$$C_{BHS} := 2 \log 2 + \frac{1}{2} \log \frac{2}{3} + 3 \log \frac{\sqrt{\pi}}{\Gamma(1/3)}. \tag{4.1.5}$$

As we will see, our results imply that the last conjecture is equivalent to one concerning the global optimizer of the renormalized energy W.

CONJECTURE 3 (Sandier and Serfaty, [86], or see the review by Serfaty [90]) : The triangular lattice is a global minimizer of W among discrete subsets of $\mathbb{R}^2$ with asymptotic density one.

The expansion (4.1.4) in the particular case $V(x) = \log(1 + |x|^2)$ transported to $\mathbb{S}^2$ using an inverse stereographic projection and appropriate rescaling gives an expansion for $\mathcal{E}_{\log}(n)$ and thus proves Conjecture 1. The constant C in Conjecture 1 can moreover be expressed in terms of the minimum of the renormalized energy W. The value of W for the triangular lattice obviously provides an upper bound for this minimum, and by using the Chowla-Selberg formula to compute the expression given in [86] for this quantity, we show that this upper bound is precisely C_{BHS}. This bound is of course sharp if and only if Conjecture 3 is true. Thus we deduce from (4.1.4) the following.

THEOREM 4.1.2. *There exists $C \neq 0$ independent of n such that, as $n \to +\infty$,*

$$\mathcal{E}_{\log}(n) = \left(\frac{1}{2} - \log 2\right) n^2 - \frac{n}{2} \log n + Cn + o(n), \quad C = \frac{1}{\pi} \min_{\mathcal{A}_1} W + \frac{\log \pi}{2} + \log 2.$$

Moreover $C \leq C_{BHS}$ where C_{BHS} is given in (4.1.5)*, and equality holds iff $\min_{\mathcal{A}_1} W$ is achieved for the triangular lattice of density one.*

The plan of the paper is as follows. In Section 4.2 we recall the definition of W and some of its properties from [86]. In Section 4.3 we recall results about existence, uniqueness and variational Frostman inequalities for μ_V. Moreover, we give the precise definition of an admissible potential V. In Sections 4.4 and 4.5 we adapt the method of [86] to the case of equilibrium measures with noncompact support. The expansion (4.1.4) is proved in Section 4.6. Finally in Section 4.7 we prove Conjecture 1 about the existence of C, the upper bound $C \leq C_{BHS}$ and the equivalence between Conjectures 2 and 3.

4.2 Renormalized Energy

Here we recall the definition of the renormalized energy W (see [87] for more details). For any $R > 0$, B_R denotes the ball centered at the origin with radius R.

Definition 4.2.1. *Let m be a nonnegative number and E be a vector-field in $\mathbb{R}^2$. We say E belongs to the* ***admissible class*** *$\mathcal{A}_m$ if*

$$\operatorname{div} E = 2\pi(\nu - m) \text{ and } \operatorname{curl} E = 0 \tag{4.2.1}$$

where ν has the form

$$\nu = \sum_{p \in \Lambda} \delta_p \text{ , for some discrete set } \Lambda \subset \mathbb{R}^2, \tag{4.2.2}$$

and if

$$\frac{\nu(B_R)}{|B_R|} \text{ is bounded by a constant independent of } R > 1.$$

Remark 4.2.1. The real m is the average density of the points of Λ when $E \in \mathcal{A}_m$.

Definition 4.2.2. *Let m be a nonnegative number. For any continuous function χ and any vector-field E in $\mathbb{R}^2$ satisfying* (4.2.1) *where ν has the form* (4.2.2) *we let*

$$W(E, \chi) = \lim_{\eta \to 0} \left(\frac{1}{2} \int_{\mathbb{R}^2 \setminus \cup_{p \in \Lambda} B(p,\eta)} \chi(x) |E(x)|^2 dx + \pi \log \eta \sum_{p \in \Lambda} \chi(p) \right). \tag{4.2.3}$$

We use the notation χ_{B_R} for positive cutoff functions satisfying, for some constant C independent of R

$$|\nabla \chi_{B_R}| \leq C, \quad \mathrm{Supp}(\chi_{B_R}) \subset B_R, \quad \chi_{B_R}(x) = 1 \text{ if } d(x, B_R^c) \geq 1. \tag{4.2.4}$$

where $d(x, A)$ is the Euclidean distance between x and set A.

Definition 4.2.3. *The* ***renormalized energy*** W *is defined, for* $E \in \mathcal{A}_m$ *and* $\{\chi_{B_R}\}_R$ *satisfying* (4.2.4)*, by*

$$W(E) = \limsup_{R \to +\infty} \frac{W(E, \chi_{B_R})}{|B_R|}.$$

Remark 4.2.2. It is shown in [86, Theorem 1] that the value of W does not depend on the choice of cutoff functions satisfying (4.2.4), and that W is bounded below and *admits a minimizer over* $\mathcal{A}_1$.

Moreover (see [86, Eq. (1.9),(1.12)]), if $E \in \mathcal{A}_m$, $m > 0$, then

$$E' = \frac{1}{\sqrt{m}} E(./\sqrt{m}) \in \mathcal{A}_1 \quad \text{and} \quad W(E) = m\left(W(E') - \frac{\pi}{2} \log m\right).$$

In particular

$$\min_{\mathcal{A}_m} W = m\left(\min_{\mathcal{A}_1} W - \frac{\pi}{2} \log m\right), \tag{4.2.5}$$

and E is a minimizer of W over $\mathcal{A}_m$ if and only if E' minimizes W over $\mathcal{A}_1$.

In the periodic case, we have the following result [86, Theorem 2], which supports Conjecture 3 above :

Theorem 4.2.3. *The unique minimizer, up to rotation, of* W *over Bravais lattices*[2] *of fixed density* m *is the triangular lattice*

$$\Lambda_m = \sqrt{\frac{2}{m\sqrt{3}}}\left(\mathbb{Z}(1,0) \oplus \mathbb{Z}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)\right).$$

This is proved in [86] using the result of Montgomery on minimal theta function [74], we provide below an alternative proof.

Proof. For any Bravais lattice Λ

$$W(\Lambda) = ah(\Lambda) + b,$$

2. A Bravais lattice of $\mathbb{R}^2$, also called "simple lattice" is $L = \mathbb{Z}\vec{u} \oplus \mathbb{Z}\vec{v}$ where $(\vec{u}, \vec{v})$ is a basis of $\mathbb{R}^2$.

where $a > 0$, $b \in \mathbb{R}$ and $h(\Lambda)$ is the height of the flat torus $\mathbb{C}/\Lambda$ (see [78, 27, 32] for more details).

Indeed, Osgood, Phillips and Sarnak [78, Section 4, page 205] proved, for $\Lambda = \mathbb{Z}\oplus\tau\mathbb{Z}$, $\tau = a + ib$, that

$$h(\Lambda) = -\log(b|\eta(\tau)|^4) + C, \quad C \in \mathbb{R},$$

where η is the Dedekind eta function [3]. But from [86] we have

$$W(\Lambda) = -\frac{1}{2}\log\left(\sqrt{2\pi b}|\eta(\tau)|^2\right) + C,$$

therefore $W(\Lambda) = ah(\Lambda) + b$.

Then from [78, Corollary 1(b)], the triangular lattice minimizes h among Bravais lattices with fixed density, hence the same is true for W. $\square$

4.3 Equilibrium Problem in the Whole Plane

In this section we recall results on existence, uniqueness and characterization of the equilibrium measure μ_V and we give the definition of the admissible potentials.

4.3.1 Equilibrium measure, Frostman inequalities and differentiation of U^{μ_V}

Definition 4.3.1. ([15]) *Let $K \subset \mathbb{R}^2$ be a compact set and let $\mathcal{M}_1(K)$ be the family of probability measures supported on K. Then the* ***logarithmic potential*** *and the* ***logarithmic energy*** *of $\mu \in \mathcal{M}_1(K)$ are defined as*

$$U^\mu(x) := -\int_K \log|x-y|d\mu(y) \quad \text{and} \quad I_0(\mu) := -\iint_{K\times K} \log|x-y|d\mu(x)d\mu(y).$$

We say that K is ***log-polar*** *if $I_0(\mu) = +\infty$ for any $\mu \in \mathcal{M}_1(K)$ and we say that a Borel set E is log-polar if every compact subset of E is log-polar. Moreover, we say that an assertion holds* ***quasi-everywhere*** *(q.e.) on $A \subset \mathbb{R}^2$ if it holds on $A\backslash P$ where P is log-polar.*

Remark 4.3.1. We recall that the Lebesgue measure of a log-polar set is zero.

Now we recall results about the existence, the uniqueness and the characterization of the equilibrium measure μ_V proved in [42, 85] for the classical growth assumption

3. See Section 4.7.3

(4.1.2), and by Hardy and Kuijlaars [52, 53] (for existence and uniqueness) and Bloom, Levenberg and Wielonsky [15] (for Frostman type variational inequalities) for weak growth assumption (4.1.3).

Theorem 4.3.2. ([42, 85, 52, 53, 15]) *Let V be a lower semicontinuous function on $\mathbb{R}^2$ such that $\{x \in \mathbb{R}^2; V(x) < +\infty\}$ is a non log-polar subset of $\mathbb{R}^2$ satisfying*

$$\liminf_{|x|\to+\infty}\{V(x) - \log(1+|x|^2)\} > -\infty.$$

Then we have :

1. $\inf\limits_{\mu\in\mathcal{M}_1(\mathbb{R}^2)} I_V(\mu)$ *is finite, where I_V is given by* (4.1.1).
2. *There exists a unique equilibrium measure $\mu_V \in \mathcal{M}_1(\mathbb{R}^2)$ with*

$$I_V(\mu_V) = \inf_{\mu\in\mathcal{M}_1(\mathbb{R}^2)} I_V(\mu)$$

   and the logarithmic energy $I_0(\mu_V)$ is finite.
3. *The support Σ_V of μ_V is contained in $\{x \in \mathbb{R}^2; V(x) < +\infty\}$ and Σ_V is not log-polar.*
4. *Let*

$$c_V := I_V(\mu_V) - \int_{\mathbb{R}^2} \frac{V(x)}{2} d\mu_V(x) \tag{4.3.1}$$

   denote the Robin constant. Then we have the following Frostman variational inequalities :

$$U^{\mu_V}(x) + \frac{V(x)}{2} \geq c_V \quad \text{q.e. on } \mathbb{R}^2, \tag{4.3.2}$$

$$U^{\mu_V}(x) + \frac{V(x)}{2} \leq c_V \quad \text{for all } x \in \Sigma_V. \tag{4.3.3}$$

Remark 4.3.3. In particular we have $U^{\mu_V}(x) + \dfrac{V(x)}{2} = c_V$ q.e. on Σ_V.

As explained in [52], the hypothesis of Theorem 4.3.2 can be usefully transported to the sphere $\mathcal{S}$ in $\mathbb{R}^3$ centred at $(0,0,1/2)$ with radius $1/2$, by the inverse stereographic projection $T : \mathbb{R}^2 \to \mathcal{S}$ defined by

$$T(x_1,x_2) = \left(\frac{x_1}{1+|x|^2}, \frac{x_2}{1+|x|^2}, \frac{|x|^2}{1+|x|^2}\right), \text{for any } x = (x_1,x_2) \in \mathbb{R}^2.$$

We know that T is a conformal homeomorphism from $\mathbb{R}^2$ to $\mathcal{S}\backslash\{N\}$ where $N := (0,0,1)$ is the North pole of $\mathcal{S}$.

The procedure is as follows : Given $V : \mathbb{R}^2 \to \mathbb{R}$, we may define (see [52]) $\mathcal{V} : \mathcal{S} \to \mathbb{R}$ by letting

$$\mathcal{V}(T(x)) = V(x) - \log(1 + |x|^2), \quad \mathcal{V}(N) = \liminf_{|x|\to+\infty} \{V(x) - \log(1 + |x|^2)\}. \tag{4.3.4}$$

Then (see [52]), V satisfies the hypothesis of Theorem 4.3.2 if and only if $\mathcal{V}$ is a lower-semicontinuous function on $\mathcal{S}$ which is finite on a nonpolar set. Therefore, in this case, the minimum of

$$I_{\mathcal{V}}(\mu) := \iint_{\mathcal{S}\times\mathcal{S}} \left(-\log \|x - y\| + \frac{\mathcal{V}(x)}{2} + \frac{\mathcal{V}(y)}{2} \right) d\mu(x)\, d\mu(y)$$

among probability measures on $\mathcal{S}$ is achieved. Here $\|x - y\|$ denotes the euclidean norm in $\mathbb{R}^3$. Moreover, still from [52], the minimizer $\mu_{\mathcal{V}}$ is related to μ_V by the following relation

$$\mu_{\mathcal{V}} = T\sharp\mu_V, \tag{4.3.5}$$

where $T\sharp\mu$ denotes the push-forward of the measure μ by the map T.

Definition 4.3.2. *We say that $V : \mathbb{R}^2 \to \mathbb{R}$ is* ***admissible*** *if it is of class C^3 and if, defining $\mathcal{V}$ as above,*

1. **(H1)** *: The set $\{x \in \mathbb{R}^2; V(x) < +\infty\}$ is not log-polar and $\liminf_{|x|\to+\infty}\{V(x) - \log(1 + |x|^2)\} > -\infty$.*
2. **(H2)** *: The equilibrium measure $\mu_{\mathcal{V}}$ is of the form $m_{\mathcal{V}}(x)\mathbf{1}_{\Sigma_{\mathcal{V}}}(x)\, dx$, where $m_{\mathcal{V}}$ is a C^1 function on $\mathcal{S}$ and dx denotes the surface element on $\mathcal{S}$, where the function $m_{\mathcal{V}}$ is bounded above and below by positive constants $\bar{m}$ and $\underline{m}$, and where $\Sigma_{\mathcal{V}}$ is a compact subset of $\mathcal{S}$ with C^1 boundary.*

Remark 4.3.4. Using (H2) and (4.3.5), we find that

$$d\mu_V(x) = m_V(x)\mathbf{1}_{\Sigma_V}\, dx,$$

where $\Sigma_V = T^{-1}(\Sigma_{\mathcal{V}})$ and

$$m_V(x) = \frac{m_{\mathcal{V}}(T(x))}{(1 + |x|^2)^2}. \tag{4.3.6}$$

Note that $(1 + |x|^2)^{-2}$ is the jacobian of the transformation T.

4.4 Splitting Formula

Assume V is admissible. We define as in [87] the blown-up quantities :

$$x' = \sqrt{n}x, \qquad m'_V(x') = m_V(x), \qquad d\mu'_V(x') = m'_V(x')dx'$$

and we define

$$\zeta(x) := U^{\mu_V}(x) + \frac{V(x)}{2} - c_V, \tag{4.4.1}$$

where c_V is the Robin constant given in (4.3.1). Then by (4.3.2) and (4.3.3), $\zeta(x) = 0$ q.e. in Σ_V and $\zeta(x) \geq 0$ q.e. in $\mathbb{R}^2 \backslash \Sigma_V$.

For $(x_1, ..., x_n) \in (\mathbb{R}^2)^n$, we define $\nu_n = \sum_{i=1}^n \delta_{x_i}$ and

$$H_n := -2\pi\Delta^{-1}(\nu_n - n\mu_V) = -\int_{\mathbb{R}^2} \log|.-y| d(\nu_n - n\mu_V)(y) = -\sum_{i=1}^n \log|.-x_i| - nU^{\mu_V}$$

where Δ^{-1} is the convolution operator with $\frac{1}{2\pi}\log|\cdot|$, hence such that $\Delta \circ \Delta^{-1} = I_2$ where Δ denotes the usual laplacian. Moreover we set

$$H'_n := -2\pi\Delta^{-1}(\nu'_n - \mu'_V) \tag{4.4.2}$$

where $\nu'_n = \sum_{i=1}^n \delta_{x'_i}$.

Lemma 4.4.1. *Let V be an admissible potential. Then we have*

$$\lim_{R\to+\infty} \int_{B_R} H_n(x) d\mu_V(x) = \int_{\mathbb{R}^2} H_n(x) d\mu_V(x) \quad \textit{and} \quad \lim_{R\to+\infty} W(\nabla H_n, \mathbf{1}_{B_R}) = W(\nabla H_n, \mathbf{1}_{\mathbb{R}^2}). \tag{4.4.3}$$

Proof. From (4.3.6) and the bounds on $m_{\mathcal{V}}$ we get [4]

$$\int_{\mathbb{R}^2} \log(1+|y|) d\mu_V(y) < +\infty. \tag{4.4.4}$$

Therefore by the dominated convergence argument given in [71, Theorem 9.1, Chapter 5] (used for the continuity of U^{μ_V}), we have

$$H_n(x) = \sum_{i=1}^n \int_{\mathbb{R}^2} \log\left(\frac{|x-y|}{|x-x_i|}\right) d\mu_V(y). \tag{4.4.5}$$

4. We note that μ_V is an equilibrium measure is sufficient to obtain (4.4.4), as explained by Mizuta in [71, Theorem 6.1, Chapter 2] or by Bloom, Levenberg and Wielonsky in [15, Lemma 3.2]

It follows that $H_n(x) = O\left(|x|^{-1}\right)$ as $|x| \to +\infty$ which implies the first equality using (4.3.6).

The second equality follows from the dominated convergence argument of Mizuta in [70, Theorem 1], because from (4.4.5) we have $\nabla H_n(x) = O(|x|^{-2})$ as $|x| \to +\infty$ and thus $|\nabla H_n|^2$ in in $L^1(\mathbb{R}^2)$. $\square$

Lemma 4.4.2. *Let V be admissible. Then, for every configuration $(x_1, ...x_n) \in (\mathbb{R}^2)^n$, $n \geq 2$, we have*

$$w_n(x_1, ..., x_n) = n^2 I_V(\mu_V) - \frac{n}{2}\log n + \frac{1}{\pi} W(\nabla H_n', \mathbf{1}_{\mathbb{R}^2}) + 2n\sum_{i=1}^{n} \zeta(x_i). \tag{4.4.6}$$

Proof. We may proceed as in the proof of [87, Lemma 3.1] and make use of the Frostman type inequalities (4.3.2) and (4.3.3) and Lemma 4.4.1. The important point is that, as shown in the proof of the previous lemma, we have $H_n(x) = O(|x|^{-1})$ and $\nabla H_n(x) = O(|x|^{-2})$ as $|x| \to +\infty$ which implies, exactly like in the compact support case, that

$$\lim_{R \to +\infty} \int_{\partial B_R} H_n(x) \nabla H_n(x).\vec{\nu}(x) dx = 0$$

where $\vec{\nu}(x)$ is the outer unit normal vector at $x \in \partial B_R$. $\square$

4.5 Lower bound

Here we follow the strategy of [87], pointing out the required modifications in the noncompact case.

4.5.1 Mass spreading result and modified density g

We have the following result from [87, Proposition 3.4] :

Lemma 4.5.1. *Let V be admissible and assume (ν, E) are such that $\nu = \sum_{p\in\Lambda} \delta_p$ for some finite subset $\Lambda \subset \mathbb{R}^2$ and $\operatorname{div} E = 2\pi(\nu - m_V)$, $\operatorname{curl} E = 0$ in $\mathbb{R}^2$. Then, given any $\rho > 0$ there exists a signed measure g supported on $\mathbb{R}^2$ and such that :*

- *there exists a family $\mathcal{B}_\rho$ of disjoint closed balls covering $Supp(\nu)$, with the sum of the radii of the balls in $\mathcal{B}_\rho$ intersecting with any ball of radius 1 bounded by ρ, and such that*

$$g(A) \geq -C(\|m_V\|_\infty + 1) + \frac{1}{4}\int_A |E(x)|^2 \mathbf{1}_{\Omega \setminus \mathcal{B}_\rho}(x) dx, \quad \textit{for any } A \subset \mathbb{R}^2,$$

where C depends only on ρ;

— *we have*

$$dg(x) = \frac{1}{2}|E(x)|^2 dx \quad \text{outside } \bigcup_{p\in\Lambda} B(p,\lambda)$$

where λ depends only on ρ;

— *for any function χ compactly supported in $\mathbb{R}^2$ we have*

$$\left| W(E,\chi) - \int \chi dg \right| \leq CN(\log N + \|m_V\|_\infty)\|\nabla\chi\|_\infty \tag{4.5.1}$$

where $N = \#\{p \in \Lambda; B(p,\lambda) \cap Supp(\nabla\chi) \neq \emptyset\}$ for some λ and C depending only on ρ;

— *for any $U \subset \Omega$*

$$\#(\Lambda \cap U) \leq C(1 + \|m_V\|_\infty^2 |\hat{U}| + g(\hat{U})) \tag{4.5.2}$$

where $\hat{U} := \{x \in \mathbb{R}^2; d(x,U) < 1\}$.

Definition 4.5.1. *Assume $\nu_n = \sum_{i=1}^n \delta_{x_i}$. Letting $\nu_n' = \sum_{i=1}^n \delta_{x_i'}$ be the measure in blown-up coordinates and $E_{\nu_n} = \nabla H_n'$, we denote by g_{ν_n} the result of applying the previous proposition to (ν_n', E_{ν_n}).*

The following result [87, Lemma 3.7] connects g and the renormalized energy.

Lemma 4.5.2. ([87]) *For any $\nu_n = \sum_{i=1}^n \delta_{x_i}$, we have*

$$W(\nabla H_n', \mathbf{1}_{\mathbb{R}^2}) = \int_{\mathbb{R}^2} dg_{\nu_n}. \tag{4.5.3}$$

4.5.2 Ergodic Theorem

We adapt the abstract setting in [87, Section 4.1]. We are given a Polish space X, which is a space of functions, on which $\mathbb{R}^2$ acts continuously. We denote this action $(\lambda, u) \to \theta_\lambda u := u(.+\lambda)$, for any $\lambda \in \mathbb{R}^2$ and $u \in X$. We assume it is continuous with respect to both λ and u.

We also define $T^{\varepsilon}_{\lambda}$ and T_{λ} acting on $\mathbb{R}^2 \times X$, by $T^{\varepsilon}_{\lambda}(x,u) := (x+\varepsilon\lambda, \theta_{\lambda}u)$ and $T_{\lambda}(x,u) := (x, \theta_{\lambda}u)$.

For a probability measure P on $\mathbb{R}^2 \times X$ we say that P is $T_{\lambda(x)}$-invariant if for every function λ of class C^1, it is invariant under the mapping $(x,u) \mapsto (x, \theta_{\lambda(x)}u)$.

We let $\{f_\varepsilon\}_\varepsilon$, and f be measurable functions defined on $\mathbb{R}^2 \times X$ which satisfy the following properties. For any sequence $\{x_\varepsilon, u_\varepsilon\}_\varepsilon$ such that $x_\varepsilon \to x$ as $\varepsilon \to 0$ and such that for any $R > 0$,

$$\limsup_{\varepsilon \to 0} \int_{B_R} f_\varepsilon(x_\varepsilon + \varepsilon\lambda, \theta_\lambda u_\varepsilon) d\lambda < +\infty,$$

we have

1. (Coercivity) $\{u_\varepsilon\}_\varepsilon$ has a convergent subsequence ;
2. (Γ-liminf) If $\{u_\varepsilon\}_\varepsilon$ converge to u, then $\liminf_{\varepsilon \to 0} f_\varepsilon(x_\varepsilon, u_\varepsilon) \geq f(x,u)$.

Remark 4.5.3. In contrast with the compact case we do not have the convergence of $\{x_\varepsilon\}$.

Now let V be an admissible potential on $\mathbb{R}^2$ and μ_V its associated equilibrium measure. We have

Theorem 4.5.4. *Let V, X, $(f_\varepsilon)_\varepsilon$ and f be as above. We define*

$$F_\varepsilon(u) := \int_{\mathbb{R}^2} f_\varepsilon(x, \theta_{\frac{x}{\varepsilon}} u) d\mu_V(x)$$

Assume $(u_\varepsilon)_\varepsilon \in X$ is a sequence such that $F_\varepsilon(u_\varepsilon) \leq C$ for any $\varepsilon > 0$. Let P_ε be the image of μ_V by $x \mapsto (x, \theta_{\frac{x}{\varepsilon}} u_\varepsilon)$, then :

1. *$(P_\varepsilon)_\varepsilon$ admits a convergent subsequence to a probability measure P,*
2. *the first marginal of P is μ_V,*
3. *P is $T_{\lambda(x)}$-invariant,*
4. *for $P-a.e.$ (x,u), (x,u) is of the form $\lim_{\varepsilon \to 0}(x_\varepsilon, \theta_{\frac{x_\varepsilon}{\varepsilon}} u_\varepsilon)$,*
5. $\liminf_{\varepsilon \to 0} F_\varepsilon(u_\varepsilon) \geq \int_{\mathbb{R}^2 \times X} f(x,u) dP(x,u)$.
6. *Moreover we have*

$$\int_{\mathbb{R}^2 \times X} f(x,u) dP(x,u) = \int_{\mathbb{R}^2 \times X} \left(\lim_{R \to +\infty} \fint_{B_R} f(x, \theta_\lambda u) d\lambda \right) dP(x,u). \tag{4.5.4}$$

where $\fint_{B_R}$ denote the integral average over B_R.

Proof. The proof follows [86, 87] but with μ_V replacing the normalized Lebesgue measure on a compact set Σ_V. We sketch it and detail the parts where modifications are needed. For any $R > 0$ we let μ_V^R denote the restriction of μ_V to B_R, and P_ε^R denote the image of μ_V^R by the map $x \mapsto (x, \theta_{\frac{x}{\varepsilon}} u_\varepsilon)$.

STEP 1 : Convergence of a subsequence of (P_ε) to a probability measure P. It suffices to prove that the sequence $\{P_\varepsilon\}_\varepsilon$ is tight. From [86, 87], which deals with the compact case, $\{P_\varepsilon^R\}_\varepsilon$ is tight, for any $R > 0$.

Now take any $\delta > 0$, we need to prove that there exists a compact subset K_δ of $\mathbb{R}^2 \times X$ such that $P_\varepsilon(K_\delta) > 1 - \delta$ for any $\varepsilon > 0$. For this we choose first $R > 0$ large enough so that $(\mu_V - \mu_V^R)(\mathbb{R}^2) < \delta/2$. This implies that P_ε^R has total measure at least $1 - \delta/2$ and then we may use the tightness of $\{P_\varepsilon^R\}_\varepsilon$ to find that there exists a compact set K_δ such that $P_\varepsilon^R(K_\delta) > 1 - \delta$. It follows that $P_\varepsilon(K_\delta) > 1 - \delta$, and then that $\{P_\varepsilon\}_\varepsilon$ is tight.

STEP 2 : P is $T_{\lambda(x)}$-invariant. Let λ be a function of class C^1 on $\mathbb{R}^2$, Φ be a bounded continuous function on $\mathbb{R}^2 \times X$ and P_λ be the image of P by $(x, u) \mapsto (x, \theta_{\lambda(x)} u)$. By the change of variables $y = \varepsilon\lambda(x) + x = (\varepsilon\lambda + I_2)(x)$, we obtain

$$\begin{aligned}
\int_{\mathbb{R}^2 \times X} \Phi(x, u) dP_\lambda(x, u) &= \int_{\mathbb{R}^2 \times X} \Phi(x, \theta_{\lambda(x)} u) dP(x, u) \\
&= \lim_{\varepsilon \to 0} \int_{\mathbb{R}^2 \times X} \Phi(x, \theta_{\lambda(x)} u) dP_\varepsilon(x, u) \\
&= \lim_{\varepsilon \to 0} \int_{\mathbb{R}^2} \Phi(x, \theta_{\lambda(x) + \frac{x}{\varepsilon}} u_\varepsilon) d\mu_V(x) \\
&= \lim_{\varepsilon \to 0} \int_{\mathbb{R}^2} \Phi(x, \theta_{\frac{\varepsilon\lambda(x) + x}{\varepsilon}} u_\varepsilon) d\mu_V(x) \\
&= \lim_{\varepsilon \to 0} \int_{\mathbb{R}^2} \frac{\Phi\left((\varepsilon\lambda + I_2)^{-1}(y), \theta_{\frac{y}{\varepsilon}} u_\varepsilon\right) m_V((\varepsilon\lambda + I_2)^{-1}(y)) dy}{|\det(I_2 + \varepsilon D\lambda((I_2 + \varepsilon\lambda)^{-1}(y)))|},
\end{aligned}$$

where $D\lambda$ is the differential of λ.

From the boundedness of Φ and the decay properties of m_V (see (4.3.6)) it is straightforward to show that

$$\begin{aligned}
&\lim_{\varepsilon \to 0} \int_{\mathbb{R}^2} \frac{\Phi\left((\varepsilon\lambda + I_2)^{-1}(y), \theta_{\frac{y}{\varepsilon}} u_\varepsilon\right) m_V((\varepsilon\lambda + I_2)^{-1}(y)) dy}{|\det(I_2 + \varepsilon D\lambda((I_2 + \varepsilon\lambda)^{-1}(y)))|} \\
&= \lim_{\varepsilon \to 0} \int_{\mathbb{R}^2} \Phi\left((\varepsilon\lambda + I_2)^{-1}(y), \theta_{\frac{y}{\varepsilon}} u_\varepsilon\right) m_V(y)\, dy \\
&= \lim_{\varepsilon \to 0} \int_{\mathbb{R}^2 \times X} \Phi\left((\varepsilon\lambda + I_2)^{-1}(y), u\right) dP_\varepsilon(y, u).
\end{aligned}$$

Then, arguing as in [87] using the tightness of $(P_\varepsilon)_\varepsilon$ we obtain

$$\lim_{\varepsilon\to 0}\int_{\mathbb{R}^2\times X}\Phi\left((\varepsilon\lambda+I_2)^{-1}(y),u\right)dP_\varepsilon(y,u)=\lim_{\varepsilon\to 0}\int_{\mathbb{R}^2\times X}\Phi(y,u)dP_\varepsilon(y,u)$$
$$=\int_{\mathbb{R}^2\times X}\Phi(x,u)dP(x,u),$$

Which concludes the proof that $\displaystyle\int_{\mathbb{R}^2\times X}\Phi(x,u)dP_\lambda(x,u)=\int_{\mathbb{R}^2\times X}\Phi(x,u)dP(x,u)$, i.e. that P is $T_{\lambda(x)}$-invariant.

Items 2 and 4 in the theorem are obvious consequences of the definition of P and items 5 and 6. require no modification from [87]. We have proved above items 1 and 3. $\square$

4.6 Asymptotic Expansion of the Hamiltonian

We define

$$\alpha_V:=\frac{1}{\pi}\int_{\mathbb{R}^2}\min_{\mathcal{A}_{m_V(x)}}W\,dx=\frac{1}{\pi}\min_{\mathcal{A}_1}W-\frac{1}{2}\int_{\mathbb{R}^2}m_V(x)\log m_V(x)dx, \qquad (4.6.1)$$

where the equality is a consequence of (4.2.5). The fact that α_V is finite follows from (4.3.6), which ensures that the integral converges.

We also let

$$F_n(\nu)=\begin{cases}\dfrac{1}{n}\left(\dfrac{1}{\pi}W(\nabla H_n',\mathbf{1}_{\mathbb{R}^2})+2n\displaystyle\int\zeta d\nu\right) & \text{if } \nu \text{ is of the form } \dfrac{1}{n}\displaystyle\sum_{i=1}^n\delta_{x_i},\\ +\infty & \text{otherwise.}\end{cases}$$

For $\nu_n'=\displaystyle\sum_{i=1}^n\delta_{x_i'}$, let E_{ν_n} be a solution of $\operatorname{div}E_{\nu_n}=2\pi(\nu_n'-m_V')$, $\operatorname{curl}E_{\nu_n}=0$ and we set

$$P_{\nu_n}:=\int_{\mathbb{R}^2}\delta_{(x,E_{\nu_n}(x\sqrt{n}+.))}d\mu_V(x).$$

The following result extends [87, Theorem 2] to a class of equilibrium measures with possibly unbounded support, which requires a restatement which makes it slightly different from its counterpart in [87]. It is essentially a Gamma-Convergence (see [18]) statement, consisting of a lower bound and an upper bound, the two implying the convergence of $\dfrac{1}{n}\left[w_n(x_1,...,x_n)-n^2I_V(\mu_V)+\dfrac{n}{2}\log n\right]$ to α_V for a minimizer $(x_1,...,x_n)$ of w_n.

4.6.1 Main result

Theorem 4.6.1. *Let $1 < p < 2$ and $X = \mathbb{R}^2 \times L^p_{loc}(\mathbb{R}^2, \mathbb{R}^2)$. Let V be an admissible function.*

A. Lower bound : *Let $(\nu_n)_n$ such that $F_n(\nu_n) \leq C$, then :*

1. *P_{ν_n} is a probability measure on X and admits a subsequence which converges to a probability measure P on X,*
2. *the first marginal of P is μ_V,*
3. *P is $T_{\lambda(x)}$-invariant,*
4. *$E \in \mathcal{A}_{m_V(x)}$ P-a.e.,*
5. *we have the lower bound*

$$\liminf_{n\to+\infty} \frac{1}{n\pi} W(\nabla H_n', \mathbf{1}_{\mathbb{R}^2}) \geq \frac{1}{\pi} \int_{\mathbb{R}^2} \frac{W(E)}{m_V(x)} dP(x,E) \geq \alpha_V. \tag{4.6.2}$$

B. Upper bound. *Conversely, assume P is a $T_{\lambda(x)}$-invariant probability measure on X whose first marginal is μ_V and such that for P-almost every (x,E) we have $E \in \mathcal{A}_{m_V(x)}$. Then there exist a sequence $\{\nu_n = \sum_{i=1}^n \delta_{x_i}\}_n$ of measures on $\mathbb{R}^2$ and a sequence $\{E_n\}_n$ in $L^p_{loc}(\mathbb{R}^2, \mathbb{R}^2)$ such that $\operatorname{div} E_n = 2\pi(\nu_n' - m_V')$ and such that, defining $P_n = \int_{\mathbb{R}^2} \delta_{(x, E_n(x\sqrt{n}+.))} d\mu_V(x)$, we have $P_n \to P$ as $n \to +\infty$ and*

$$\limsup_{n\to+\infty} F_n(\nu_n) \leq \frac{1}{\pi} \int_{\mathbb{R}^2} \frac{W(E)}{m_V(x)} dP(x,E). \tag{4.6.3}$$

C. Consequences for minimizers. *If $(x_1, ..., x_n)$ minimizes w_n for every n and measure $\nu_n = \sum_{i=1}^n \delta_{x_i}$, then :*

1. *for P-almost every (x,E), E minimizes W over $\mathcal{A}_{m_V(x)}$;*
2. *we have*

$$\lim_{n\to+\infty} F_n(\nu_n) = \lim_{n\to+\infty} \frac{1}{n\pi} W(\nabla H_n', \mathbf{1}_{\mathbb{R}^2}) = \frac{1}{\pi} \int_{\mathbb{R}^2} \frac{W(E)}{m_V(x)} dP(x,E) = \alpha_V, \tag{4.6.4}$$

hence we obtain the following asymptotic expansion, as $n \to +\infty$:

$$\min_{(\mathbb{R}^2)^n} w_n = I_V(\mu_V) n^2 - \frac{n}{2} \log n + \alpha_V n + o(n). \tag{4.6.5}$$

4.6.2 Proof of the lower bound

We follow the same lines as in [87, Section 4.2]. Because $F_n(\nu_n) \le C$ and (4.4.6), we have that

$$\frac{1}{n^2} w_n(x_1, \dots x_n) \to I_V(\mu_V),$$

therefore ν_n converges to μ_V (this follows from the results in [52]).

We let $\nu_n' = \sum_i \delta_{x_i'}$, and E_n, H_n', g_n be as in Definition 4.5.1.

Let χ be a C^∞ cutoff function with support the unit ball B_1 and integral equal to 1. We define

$$\mathbf{f}_n(x, \nu, E, g) := \begin{cases} \dfrac{1}{\pi} \displaystyle\int_{\mathbb{R}^2} \frac{\chi(y)}{m_V(x)} dg(y) & \text{if } (\nu, E, g) = \theta_{\sqrt{n}x}(\nu_n', E_n, g_n), \\ +\infty & \text{otherwise.} \end{cases}$$

As in [87, Section 4.2, Step 1], if we let

$$\mathbf{F}_n(\nu, E, g) := \int_{\mathbb{R}^2} \mathbf{f}_n \left(x, \theta_{x\sqrt{n}}(\nu, E, g) \right) d\mu_V(x), \tag{4.6.6}$$

then

$$\begin{aligned} \mathbf{F}_n(\nu_n', E_n, g_n) = \int_{\mathbb{R}^2} \frac{1}{\pi} \int_{\mathbb{R}^2} \frac{\chi(y)}{m_V(x)} d(\theta_{x\sqrt{n}} \sharp g) d\mu_V(x) &= \frac{1}{\pi} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \chi(y - x\sqrt{n}) dx dg_n(y) \\ &\le \frac{1}{n\pi} W(\nabla H_n', \mathbf{1}_{\mathbb{R}^2}) + \frac{g_n^-(U^c)}{n\pi}, \end{aligned}$$

by (4.5.3), where $U = \{x' : d(x', \mathbb{R}^2 \backslash \Sigma) \ge 1\}$. As in [87], we have $g_n^-(U^c) = o(n)$. Hence, if $(\nu, E, g) = (\nu_n', E_n, g_n)$, as $n \to +\infty$:

$$\mathbf{F}_n(\nu, E, g) \le \frac{1}{n\pi} W(\nabla H_n', \mathbf{1}_{\mathbb{R}^2}) + o(1),$$

and $\mathbf{F}_n(\nu, E, g) = +\infty$ otherwise.

Now, as in [87], we want to use Theorem 4.5.4 with $\varepsilon = \frac{1}{\sqrt{n}}$ and $X = \mathcal{M}_+ \times L^p_{loc}(\mathbb{R}^2, \mathbb{R}^2) \times \mathcal{M}$ where $p \in]1, 2[$, $\mathcal{M}_+$ is the set of nonnegative Radon measures on $\mathbb{R}^2$ and $\mathcal{M}$ the set of Radon measures bounded below by $-C_V := -C(\|m_V\|_\infty^2 + 1)$. Let Q_n be the image of μ_V by $x \mapsto (x, \theta_{x\sqrt{n}}(\bar{\nu}_n', E_n, g_n))$. We have :

1) The fact that $\mathbf{f}_n$ is coercive is proved as in [87, Lemma 4.4]. Indeed, if $(x_n, \nu(n), E(n), g(n))_n$ is such that $x_n \to x$ and, for any $R > 0$,

$$\limsup_{n \to +\infty} \int_{B_R} \mathbf{f}_n \left(x_n + \frac{\lambda}{\sqrt{n}}, \theta_\lambda(\nu(n), E(n), g(n)) \right) d\lambda < +\infty,$$

then the integrand is bounded for a.e. λ. By assumption on $\mathbf{f}_n$, for any n,

$$\theta_\lambda(\nu(n), E(n), g(n)) = \theta_{x_n\sqrt{n}+\lambda}(\nu'_n, E_n, g_n),$$

hence it follows that

$$(\nu(n), E(n), g(n)) = \theta_{x_n\sqrt{n}}(\nu'_n, E_n, g_n).$$

For any $R > 0$, there exists $C_R > 0$ such that for any $n > 0$, noting $B_R(x)$ the closed ball of radius R centred at a point x,

$$\begin{aligned}
\int_{B_R} \mathbf{f}_n\left(x_n + \frac{\lambda}{\sqrt{n}}, \theta_\lambda(\nu_n, E_n, g_n)\right) d\lambda &= \int_{B_R} \frac{1}{\pi} \int_{\mathbb{R}^2} \frac{\chi(y)}{m_V\left(x_n + \frac{\lambda}{\sqrt{n}}\right)} d(\theta_{\lambda+x_n\sqrt{n}}\sharp g_n(y)) d\lambda \\
&= \frac{1}{\pi} \int_{B_R} \int_{\mathbb{R}^2} \frac{\chi(y - x_n\sqrt{n} - \lambda)}{m_V\left(x_n + \frac{\lambda}{\sqrt{n}}\right)} dg_n(y) d\lambda \\
&= \frac{1}{\pi} \int_{\mathbb{R}^2} \chi * \left(\mathbf{1}_{B_R(x_n\sqrt{n})} \frac{1}{m_V(./\sqrt{n})}\right)(y) dg_n(y) < C_R.
\end{aligned}$$

This, inequalities (4.3.6) and the fact that g_n is bounded below imply that $g_n(B_R(x_n\sqrt{n}))$ is bounded independently of n. Hence by the same argument as in [87, Lemma 4.4], we have the convergence of a subsequence of (ν_n, E_n, g_n).

2) We have the Γ-liminf property : if $(x_n, \nu_n, E_n, g_n) \to (x, \nu, E, g)$ as $n \to +\infty$, then, by Fatou's Lemma,

$$\liminf_{n\to+\infty} \mathbf{f}_n(x_n, \nu_n, E_n, g_n) \geq f(x, \nu, E, g) := \frac{1}{\pi} \int \frac{\chi(y)}{m_V(x)} dg(y),$$

obviously if the left-hand side is finite. Therefore, Theorem 4.5.4 applies and implies that :

1. The measure Q_n admits a subsequence which converges to a measure Q which has μ_V as first marginal.
2. It holds that Q-almost every (x, ν, E, g) is of the form $\lim\limits_{n\to+\infty} (x_n, \theta_{x_n\sqrt{n}}(\nu'_n, E_n, g_n))$.
3. The measure Q is $T_{\lambda(x)}$-invariant.
4. We have $\liminf\limits_{n\to+\infty} \mathbf{F}_n(\nu'_n, E_n, g_n) \geq \frac{1}{\pi} \int_{\mathbb{R}^2} \left(\int_{\mathbb{R}^2} \frac{\chi(y)}{m_V(x)} dg(y)\right) dQ(x, \nu, E, g)$.
5. $\frac{1}{\pi} \int \int \frac{\chi(y)}{m_V(x)} dg(y) dQ(x, \nu, E, g) = \int \left(\lim\limits_{R\to+\infty} \fint_{B_R} \int \frac{\chi(y-\lambda)}{m_V(x)} dg(y) d\lambda\right) dQ(x, \nu, E, g)$.

Now we can follow exactly the lines of [87, Section 4.2, Step 3] to deduce from 4), after noticing that P_n is the marginal of Q_n corresponding to the variables (x, E) which converge to a $T_{\lambda(x)}$-invariant probability measure. Moreover

$$\begin{aligned}\liminf_{n\to+\infty} \frac{1}{n\pi} W(\nabla H'_n, \mathbf{1}_{\mathbb{R}^2}) &\geq \int \left(\int \chi dg \right) \frac{dQ(x,\nu,E,g)}{m_V(x)} \\ &= \int \lim_{R\to+\infty} \left(\frac{1}{\pi R^2} \int \chi * \mathbf{1}_{B_R} dg \right) \frac{dQ(x,\nu,E,g)}{m_V(x)} \\ &\geq \frac{1}{\pi} \int W(E) \frac{dQ(x,\nu,E,g)}{m_V(x)} = \frac{1}{\pi} \int \frac{W(E)}{m_V(x)} dP(x,E).\end{aligned}$$

Thus the lower bound (4.6.2) is proved. The fact that the right-hand side is larger than α_V is obvious because the first marginal of $\dfrac{dP}{m_V}$ is the Lebesgue measure.

4.6.3 Proof of the upper bound, the case $\mathrm{Supp}(\mu_V) \neq \mathbb{R}^2$

The discussion following Theorem 4.3.2 permits to immediately reduce the case of V's such that $\mathrm{Supp}(\mu_V) \neq \mathbb{R}^2$ to the case of a compact support. Indeed in this case there exists $y \in \mathcal{S}$ which does not belong to the support of $\mu_{\mathcal{V}}$. Let R be a rotation such that $R(N) = y$, then the minimum of $I_{\mathcal{V}\circ R}$ is $\mu_{\mathcal{V}\circ R} = R^{-1}\sharp\mu_{\mathcal{V}}$ hence N does not belong to its support.

Letting $\varphi = T^{-1}RT$, we have that φ is of the form $z \to \dfrac{az+b}{cz+d}$ with $ad - bc = 1$, and applying (4.3.4), (4.3.5) to $\mathcal{V} \circ R$ we have that

$$\mu_{V_\varphi} = T^{-1}\sharp\mu_{\mathcal{V}\circ R},$$

where

$$\mathcal{V} \circ R(T(x)) = V_\varphi(x) - \log(1 + |x|^2).$$

This implies that μ_{V_φ} has compact support since N does not belong to the support of $\mu_{\mathcal{V}\circ R}$. Moreover, using (4.3.4) again to evaluate $\mathcal{V}(RT(x))$ we find for any x such that $RT(x) \neq N$, i.e. $x \neq -d/c$,

$$\begin{aligned}&V_\varphi(x) = V(T^{-1}RT(x)) - \log(1 + |T^{-1}RT(x)|^2) + \log(1 + |x|^2),\\ &V_\varphi(-d/c) = \mathcal{V}(N) + \log(1 + |d/c|^2) = \log(1 + |d/c|^2) + \liminf_{|x|\to+\infty}\{V(x) - \log(1 + |x|^2)\}.\end{aligned}$$

Finally we find that

$$V_\varphi(x) = V(\varphi(x)) - \log(1 + |\varphi(x)|^2) + \log(1 + |x|^2), \quad V_\varphi(-d/c) = \liminf_{y\to-d/c} V_\varphi(y). \quad (4.6.7)$$

Now we rewrite the discrete energy by changing variables, to find that, writing $w_{n,V}$ instead of w_n to clarify the dependence on V,

$$w_{n,V}(x_1,\dots,x_n) = -\sum_{i\neq j}^{n} \log|\varphi(y_i)-\varphi(y_j)| + n\sum_{i=1}^{n} V(\varphi(y_i)), \tag{4.6.8}$$

where $x_i = \varphi(y_i)$. Now we use the identity (see [52])

$$\|T(x)-T(y)\| = \frac{|x-y|}{\sqrt{1+|x|^2}\sqrt{1+|y|^2}}$$

applied to $\varphi(x)$, $\varphi(y)$ together with the fact that $\varphi = T^{-1}RT$ and that R is a rotation to get

$$\|T(x)-T(y)\| = \frac{|\varphi(x)-\varphi(y)|}{\sqrt{1+|\varphi(x)|^2}\sqrt{1+|\varphi(y)|^2}}.$$

The two together imply that

$$\log|\varphi(x)-\varphi(y)| = \log|x-y| + \frac{1}{2}\log(1+|\varphi(x)|^2) + \frac{1}{2}\log(1+|\varphi(y)|^2) - \frac{1}{2}\log(1+|x|^2) - \frac{1}{2}\log(1+|y|^2).$$

Replacing in (4.6.8) shows that

$$w_{n,V}(x_1,\dots,x_n) = w_{n,V_\varphi}(y_1,\dots,y_n) + \sum_i \log(1+|\varphi(y_i)|^2) - \sum_i \log(1+|y_i|^2), \quad x_i = \varphi(y_i). \tag{4.6.9}$$

It follows from (4.6.9) that an upper bound for $\min w_{n,V}$ can be computed by using a minimizer for w_{n,V_φ} as a test function. But now we recall that μ_{V_φ} has compact support, hence the results of [87] apply and we find, using the fact that for such a minimizer $\frac{1}{n}\sum_i \delta_{y_i}$ converges to μ_{V_φ},

$$\min w_{n,V} \le n^2 I_{V_\varphi}(\mu_{V_\varphi}) - \frac{1}{2}n\log n + \left(\alpha_{V_\varphi} + \int \log\left(\frac{1+|\varphi(x)|^2}{1+|x|^2}\right) d\mu_{V_\varphi}(x)\right) n + o(n), \tag{4.6.10}$$

where

$$\alpha_{V_\varphi} = \frac{\alpha_1}{\pi} - \frac{1}{2}\int_{\Sigma_{V_\varphi}} m_{V_\varphi}(x)\log m_{V_\varphi}(x)\,dx, \quad \alpha_1 := \min_{\mathcal{A}_1} W.$$

We remark that $I_{V_\varphi}(\mu_{V_\varphi}) = I_V(\mu_V)$ because $\mu_{V_\varphi} = \varphi^{-1}\sharp\mu_V$. Moreover, it follows from (4.3.6) that

$$m_{V_\varphi}(x) = m_V(\varphi(x))\left(\frac{1+|\varphi(x)|^2}{1+|x|^2}\right)^2,$$

which plugged in the expression for α_{V_φ} and then in (4.6.10) yields,

$$\min w_{n,V} \le n^2 I_V(\mu_V) - \frac{1}{2}n\log n + \alpha_V n + o(n),$$

which matches the lower-bound we already obtained and thus proves Theorem 4.1.1 in the case where the support of μ_V is not the full plane.

4.6.4 Proof of the upper bound by compactification and conclusion

Here we assume that $\Sigma_V = \mathbb{R}^2$. Let

$$\varphi(z) := -\frac{1}{z} = \varphi^{-1}(z).$$

Then, using the notations of the previous section, we deduce from (4.6.7) that

$$V_\varphi(z) = V(\varphi(z)) + 2\log|z|.$$

To simplify exposition and notation, we assume that $\mu_V(B_1) = \mu_V(B_1^c) = 1/2$, otherwise there would exist R such that $\mu_V(B_R) = \mu_V(B_R^c) = 1/2$ and we should use the transformation $\varphi_R(z) = \varphi_R^{-1}(z) = -Rz^{-1}$ instead.

Our idea is to cut $\Sigma_V = \mathbb{R}^2$ into two parts in order to construct a sequence of $2n$ points associated to a sequence of vector-fields. We will only construct test configurations with an even number of points, again to simplify exposition and avoid unessential technicalities.

STEP 1 : Reminder of the compact case and notations. We need [87, Corollary 4.6] when K is a compact set of $\mathbb{R}^2$:

Theorem 4.6.2. ([87]) *Let P be a $T_{\lambda(x)}$-invariant probability measure on $X = K \times L^p_{loc}(\mathbb{R}^2, \mathbb{R}^2)$, where K is a compact subset of $\mathbb{R}^2$ with C^1 boundary.*

We assume that P has first marginal $dx_{|K}/|K|$ and that for P-almost every (x, E) we have $E \in \mathcal{A}_{m(x)}$, where m is a smooth function on K bounded above and below by positive constants. Then there exists a sequence $\{\nu_n = \sum_{i=1}^n \delta_{x_i}\}_n$ of empirical measures on K and a sequence $\{E_n\}_n$ in $L^p_{loc}(\mathbb{R}^2, \mathbb{R}^2)$ such that $\operatorname{div} E_n = 2\pi(\nu_n' - m')$, *such that $E_n = 0$ outside K and such that $P_n := \fint_K \delta_{(x, E_n(\sqrt{n}x + .))} dx \to P$ as $n \to +\infty$. Moreover*

$$\limsup_{n\to+\infty} \frac{1}{n\pi} W(E_n, \mathbf{1}_{\mathbb{R}^2}) \le \frac{|K|}{\pi} \int W(E) dP(x, E).$$

We write $\mu_V = \mu_V^1 + \mu_V^2$ where $\mu_V^1 := \mu_{V|B_1}$ and $\mu_V^2 := \mu_{V|\bar{B}_1^c}$, where $\bar{A}$ denotes the closure of set A in $\mathbb{R}^2$. Let $\tilde{\mu}_V^2 := \varphi\sharp\mu_V^2$, then we have

$$d\mu_V^1(x) = m_V(x)\mathbf{1}_{B_1}(x)dx =: m_V^1(x)dx \quad \text{and} \quad d\tilde{\mu}_V^2(x) = m_{V_\varphi}(x)\mathbf{1}_{B_1}(x)dx =: m_{V_\varphi}^2(x)dx,$$

where $m_{V_\varphi}(x) = m_V(\varphi^{-1}(x))|\det(D\varphi_x^{-1})|$.

Note that, by assumption **(H2)** and (4.3.6) we have that there exists positive constants $\bar{m}$ and $\underline{\mathrm{m}}$ such that, for any $x \in B_1$,

$$0 < \underline{\mathrm{m}} \le m_V(x) \le \bar{m} \quad \text{and} \quad 0 < \underline{\mathrm{m}} \le m_{V_\varphi}(x) \le \bar{m}.$$

Moreover the boundary ∂B_1 is C^1.

Now let P be a $T_{\lambda(x)}$-invariant probability measure on X whose first marginal is μ_V and be such that for P-almost very (x, E), we have $E \in \mathcal{A}_{m_V(x)}$. We can write

$$P = P^1 + P^2,$$

where P^1 is the restriction of P to $B_1 \times L^p_{loc}(B_1, \mathbb{R}^2)$ with first marginal μ_V^1, and P^2 is the restriction of P to $B_1^c \times L^p_{loc}(B_1^c, \mathbb{R}^2)$ with first marginal μ_V^2. We define $\tilde{P}^1$ by the relation

$$dP^1(x, u) = m_V(x)|B_1|d\tilde{P}^1(x, u),$$

and then $\tilde{P}^1$ is a $T_{\lambda(x)}$-invariant probability measure on $B_1 \times L^p_{loc}(B_1, \mathbb{R}^2)$ with first marginal $dx_{|B_1}/|B_1|$ and such that, for $\tilde{P}^1$-a.e. (x, E), $E \in \mathcal{A}_{m^1_V(x)}$. We denote by $\varphi\sharp P^2$ the pushforward of P^2 by

$$(x, E) \mapsto \left(y, \tilde{E}\right), \quad \text{where} \quad y := \varphi(x) \text{ and } \tilde{E} := (D\varphi_y)^T E(D\varphi_y \cdot), \tag{4.6.11}$$

where $D\varphi_x = \lambda(x)I_2$ is the differential of φ at point x. Then if $\operatorname{div} E = 2\pi(\nu - m_V(x)dx)$ then $\operatorname{div} \tilde{E} = 2\pi(\varphi\sharp\nu - \lambda^2(y)m_V(\varphi(y)))$ so that for $\varphi\sharp P^2$-a.e. $(y, \tilde{E})$ the vector field $\tilde{E}$ belongs to $\mathcal{A}_{m_{V_\varphi}(y)}$, since

$$m_{V_\varphi}(y)\, dy = m_V(\varphi(y))\, d(\varphi(y)) = m_V(\varphi(y))\lambda(y)^2\, dy.$$

We define $\tilde{P}^2$ by the relation

$$d(\varphi\sharp P^2)(y, \tilde{E}) = m_{V_\varphi}(y)|B_1|d\tilde{P}^2(y, \tilde{E}),$$

and then $\tilde{P}^2$ is a $T_{\lambda(x)}$-invariant probability measure on $B_1 \times L^p_{loc}(B_1, \mathbb{R}^2)$ with first marginal $dy_{|B_1}/|B_1|$ and such that, for $\tilde{P}^2$ a.e. $(y, \tilde{E})$, $\tilde{E} \in \mathcal{A}_{m_{V_\varphi}(y)}$.

STEP 2 : Application of Theorem 4.6.2. We may now apply Theorem 4.6.2 to $\tilde{P}^1$ and $\tilde{P}^2$. We thus construct a sequence $\{\nu_n^1 := \sum_{i=1}^n \delta_{x_i^1}\}$ of empirical measures on B_1 and a sequence $\{E_n^1\}_n$ in $L^p_{loc}(B_1, \mathbb{R}^2)$ such that

$$\operatorname{div} E_n^1 = 2\pi((\nu_n^1)' - (m_V^1)') \quad \text{and} \quad \tilde{P}_n^1 := \fint_{B_1} \delta_{(x, E_n^1(\sqrt{n}x + .))} dx \to \tilde{P}^1,$$

as $n \to +\infty$. Moreover, we have

$$\limsup_{n \to +\infty} \frac{1}{n\pi} W(E_n^1, \mathbf{1}_{\mathbb{R}^2}) \leq \frac{|B_1|}{\pi} \int W(E) d\tilde{P}^1(x, E). \tag{4.6.12}$$

Applying now the same Theorem to $\tilde{P}^2$, we construct a sequence $\{\tilde{\nu}_n^2 := \sum_{i=1}^n \delta_{\tilde{x}_i^2}\}$ of empirical measures on B_1 and a sequence $\{\tilde{E}_n^2\}_n$ in $L^p_{loc}(B_1, \mathbb{R}^2)$ such that

$$\operatorname{div} \tilde{E}_n^2 = 2\pi((\tilde{\nu}_n^2)' - (m_{V_\varphi}^2)') \quad \text{ and } \tilde{P}_n^2 := \fint_{B_1} \delta_{(x, \tilde{E}_n^2(\sqrt{n}x+.))} dx \to \tilde{P}^2,$$

as $n \to +\infty$. Moreover, we have

$$\limsup_{n\to+\infty} \frac{1}{n\pi} W(\tilde{E}_n^2, \mathbf{1}_{\mathbb{R}^2}) \leq \frac{|B_1|}{\pi} \int W(\tilde{E}) d\tilde{P}^2(y, \tilde{E}). \tag{4.6.13}$$

STEP 3 : Construction of sequences and conclusion. It is not difficult to see that we can assume $\tilde{x}_j^2 \neq 0$ for any j and any $n \geq 2$ (otherwise we translate a little bit the point). Now we set $x_j^2 := \varphi(\tilde{x}_j^2)$ and in view of (4.6.11), for each n we define

$$\nu_n^2 := \varphi\sharp\tilde{\nu}_n^2 = \sum_{j=1}^n \delta_{x_j^2} \quad \text{ and } \quad E_n^2(x) := (D\varphi_{n^{-1/2}x})^T \tilde{E}_n^2(n^{1/2}\varphi(n^{-1/2}x)).$$

Hence, we have a sequence of vector-fields E_n^2 of $L^p_{loc}(B_1^c, \mathbb{R}^2)$ such that

$$\operatorname{div} E_n^2 = 2\pi((\nu_n^2)' - (m_V^2)')$$

where $m_V^2(x) = m_V(x)\mathbf{1}_{\bar{B}_1^c}(x)$ is the density of μ_V^2.

We have, for sufficiently small η such that $0 \notin B(\tilde{x}_i^2, \eta)$ for every i,

$$\begin{aligned}
&W(E_n^2, \mathbf{1}_{\mathbb{R}^2})\\
&= \lim_{\eta\to 0} \left(\frac{1}{2} \int_{\mathbb{R}^2 \setminus \bigcup_{i=1}^n B(x_i^2, \eta)} |E_n^2(x')|^2 dx' + \pi n \log \eta \right)\\
&= \lim_{\eta\to 0} \left(\frac{1}{2} \int_{\mathbb{R}^2 \setminus \bigcup_{i=1}^n B(x_i^2, \eta)} |(D\varphi_{n^{-1/2}x'})^T \tilde{E}_n^2(n^{1/2}\varphi(n^{-1/2}x'))|^2 dx' + \pi n \log \eta \right)\\
&= \lim_{\eta\to 0} \left(\frac{1}{2} \int_{\mathbb{R}^2 \setminus \bigcup_{i=1}^n B(y_i^2, |\varphi'(x_i^2)|\eta)} |\tilde{E}_n^2(y')|^2 dy' + \pi n \log \eta \right)\\
&= \lim_{\eta\to 0} \left(\frac{1}{2} \int_{\mathbb{R}^2 \setminus \bigcup_{i=1}^n B(y_i^2, |\varphi'(x_i^2)|\eta)} |\tilde{E}_n^2(y')|^2 dy' + \pi \sum_{i=1}^n \log |\varphi'(x_i)|\eta - \pi \sum_{i=1}^n \log |\varphi'(x_i)| \right)\\
&= W(\tilde{E}_n^2, \mathbf{1}_{\mathbb{R}^2}) - \pi \sum_{i=1}^n \log |\varphi'(x_i)|,
\end{aligned}$$

where the change of variable is $y' = n^{1/2}\varphi(n^{-1/2}x')$.
Furthermore, we have

$$\int W(\tilde{E}) d\tilde{P}^2(y, \tilde{E}) = \frac{1}{|B_1|} \int W(\tilde{E}) \frac{d(\varphi\sharp P^2)(y, \tilde{E})}{m_{V_\varphi}(y)} = \frac{1}{|B_1|} \int W\left(D\varphi_y^T E(D\varphi_y .)\right) \frac{dP^2(x, E)}{m_{V_\varphi}(y)}$$

by change of variable $y=\varphi(x)$ and $\tilde{E}=D\varphi_y^T E(D\varphi_y\cdot)$.
Now we remark that, for $\lambda>0$ and $E\in\mathcal{A}_m$,

$$W(\lambda E(\lambda.))=\lim_{R\to+\infty}\frac{1}{\pi R^2}\lim_{\eta\to 0}\left(\frac{1}{2}\int_{\mathbb{R}^2\setminus\bigcup_i B(y_i,\eta)}\chi_R(y)\lambda^2|E(\lambda y)|^2dy+\pi\sum_i\chi_R(y_i)\log\eta\right)$$
$$=\lim_{R\to+\infty}\frac{1}{\pi R^2}\lim_{\eta\to 0}\left(\frac{1}{2}\int_{\mathbb{R}^2\setminus\bigcup_i B(x_i,\lambda\eta)}\chi_R(x/\lambda)|E(x)|^2dx+\pi\sum_i\chi_R(x_i/\lambda)\log\eta\right)$$

where $x=\lambda y$. Thus, setting $R'=R\lambda$ and $\eta'=\eta\lambda$, we get

$$\begin{aligned}&W(\lambda E(\lambda.))\\&=\lim_{R'\to+\infty}\frac{\lambda^2}{\pi R'^2}\lim_{\eta'\to 0}\left(\frac{1}{2}\int_{\mathbb{R}^2\setminus\bigcup_i B(x_i,\eta')}\chi_{R'}(x)|E(x)|^2dx+\pi\sum_i\chi_{R'}(x_i)\left(\log\eta'-\log\eta\right)\right)\\&=\lambda^2\left(W(E)-m\log\lambda\right).\end{aligned}$$

Applying this equality with $\lambda=|\varphi'(x)|^{-1}=|\varphi'^{-1}(y)|$, we obtain

$$\begin{aligned}&\limsup_{n\to+\infty}\frac{1}{n\pi}\left(W(E_n^2,\mathbf{1}_{\mathbb{R}^2})+\pi\sum_{i=1}^n\log|\varphi'(x_i)|\right)\\&\le\frac{1}{\pi}\int\frac{1}{|\varphi'(x)|^2}\left(W(E)+\log|\varphi'(x)|m_V^2(x)\right)\frac{dP^2(x,E)}{m_{V_\varphi}(y)},\end{aligned}$$

that is to say, because m_V^2 is the density of points $\{x_i\}$ as $n\to+\infty$,

$$\begin{aligned}&\limsup_{n\to+\infty}\frac{1}{n\pi}W(E_n^2,\mathbf{1}_{\mathbb{R}^2})+\int_{B_1^c}\log|\varphi'(x)|d\mu_V^2(x)\\&\le\frac{1}{\pi}\int W(E)\frac{dP^2(x,E)}{m_V(x)}+\int_{B_1^c}\log|\varphi'(x)|dP^2(x).\end{aligned}$$

As $\int_{B_1^c}\log|\varphi'(x)|dP^2(x)=\int_{B_1^c}\log|\varphi'(x)|d\mu_V^2(x)$, it follows that

$$\limsup_{n\to+\infty}\frac{1}{n\pi}W(E_n^2,\mathbf{1}_{\mathbb{R}^2})\le\frac{1}{\pi}\int W(E)\frac{dP^2(x,E)}{m_V(x)}.\tag{4.6.14}$$

Finally, we set

$$\nu_{2n}:=\nu_n^1+\nu_n^2\quad\text{ and }\quad E_{2n}:=E_n^1+E_n^2,$$

and by (4.6.12) and (4.6.14), we have, since E_n^1 and E_n^2 have disjoint supports,

$$\limsup_{n\to+\infty}\frac{1}{n\pi}W(E_n,\mathbf{1}_{\mathbb{R}^2})\le\frac{1}{\pi}\int\frac{W(E)}{m_V(x)}dP^1(x,E)+\frac{1}{\pi}\int\frac{W(E)}{m_V(x)}dP^2(x,E)$$

$$= \frac{1}{\pi} \int \frac{W(E)}{m_V(x)} dP(x,E)$$

which proves (4.6.3). Furthermore, by changes of variable,

$$P_n^1 := \int_{B_1} \delta_{(x, E_n^1(x\sqrt{n}+.))} d\mu_V(x) \to P^1 \quad \text{and} \quad P_n^2 := \int_{B_1^c} \delta_{(x, E_n^2(x\sqrt{n}+.))} d\mu_V(x) \to P^2$$

in the weak sense of measure, and it follows that

$$P_n = P_n^1 + P_n^2 \to P^1 + P^2 = P.$$

Part **C** follows from **A** and **B** as in [87].

4.7 Consequence : the Logarithmic Energy on the Sphere

As we have an asymptotic expansion of the minimum of the Hamiltonian w_n where minimizers can be in the whole plane – not only in a compact set as in the classical case – we will use the inverse stereographic projection from $\mathbb{R}^2$ to a sphere in order to determine the asymptotic expansion of optimal logarithmic energy on sphere.

4.7.1 Inverse stereographic projection

Here we recall properties of the inverse stereographic projection used by Hardy and Kuijlaars [52, 53] and by Bloom, Levenberg and Wielonsky [15] in order to prove Theorem 4.3.2.
Let $\mathcal{S}$ be the sphere of $\mathbb{R}^3$ centred at $(0,0,1/2)$ of radius $1/2$, Σ be an unbounded closed set of $\mathbb{R}^2$ and $T : \mathbb{R}^2 \to \mathcal{S}$ be the associated inverse stereographic projection defined by

$$T(x_1, x_2) = \left(\frac{x_1}{1+|x|^2}, \frac{x_2}{1+|x|^2}, \frac{|x|^2}{1+|x|^2} \right), \quad \text{for any } x = (x_1, x_2) \in \mathbb{R}^2,$$

where $\mathbb{R}^2 := \{(x_1, x_2, 0); x_1, x_2 \in \mathbb{R}\}$. We know that T is a conformal homeomorphism from $\mathbb{C}$ to $\mathcal{S}\backslash\{N\}$ where $N := (0,0,1)$ is the North pole of $\mathcal{S}$.

We have the following identity :

$$\|T(x) - T(y)\| = \frac{|x-y|}{\sqrt{1+|x|^2}\sqrt{1+|y|^2}}, \text{ for any } x, y \in \mathbb{R}^2.$$

Furthermore, if $|y| \to +\infty$, we obtain, for any $x \in \mathbb{R}^2$:

$$\|T(x) - N\| = \frac{1}{\sqrt{1 + |x|^2}}. \tag{4.7.1}$$

We note $\Sigma_{\mathcal{S}} = T(\Sigma) \cup \{N\}$ the closure of $T(\Sigma)$ in $\mathcal{S}$. Let $\mathcal{M}_1(\Sigma)$ be the set of probability measures on Σ. For $\mu \in \mathcal{M}_1(\Sigma)$, we denote by $T\sharp\mu$ its push-forward measure by T characterized by

$$\int_{\Sigma_{\mathcal{S}}} f(z) dT\sharp\mu(z) = \int_{\Sigma} f(T(x)) d\mu(x),$$

for every Borel function $f : \Sigma_{\mathcal{S}} \to \mathbb{R}$. The following result is proved in [52] :

Lemma 4.7.1. *The correspondance $\mu \to T\sharp\mu$ is a homeomorphism from the space $\mathcal{M}_1(\Sigma)$ to the set of $\mu \in \mathcal{M}_1(\Sigma_S)$ such that $\mu(\{N\}) = 0$.*

4.7.2 Asymptotic expansion of the optimal logarithmic energy on the unit sphere

An important case is the equilibrium measure associated to the potential

$$V(x) = \log(1 + |x|^2)$$

corresponding to the external field $\mathcal{V} \equiv 0$ on $\mathcal{S}$ and where $T\sharp\mu_V$ is the uniform probability measure on $\mathcal{S}$ (see [52]). Hence V is an admissible potential and from (4.3.6) we find

$$d\mu_V(x) = \frac{dx}{\pi(1 + |x|^2)^2} \quad \text{and} \quad \Sigma_V = \mathbb{R}^2.$$

We define

$$\overline{w}_n(x_1, ..., x_n) := -\sum_{i \neq j}^{n} \log|x_i - x_j| + (n-1) \sum_{i=1}^{n} \log(1 + |x_i|^2),$$

and we recall that the logarithmic energy of a configuration $(y_1, ..., y_n) \in \mathcal{S}^n$ is given by

$$\mathrm{E}_{\log}(y_1, ..., y_n) := -\sum_{i \neq j}^{n} \log\|y_i - y_j\|.$$

Furthermore, we recall that $\mathcal{E}_{\log}(n)$ denotes the minimal logarithmic energy of n points on $\mathbb{S}^2$.

Lemma 4.7.2. *For any* $(x_1, ..., x_n) \in (\mathbb{R}^2)^n$*, we have the following equalities :*

$$\overline{w}_n(x_1, ..., x_n) = \mathrm{E}_{\log}(T(x_1), ..., T(x_n)) \quad \textit{and} \quad w_n(x_1, ..., x_n) = \mathrm{E}_{\log}(T(x_1), ..., T(x_n), N),$$

which imply that

$$\begin{aligned}
(x_1, ..., x_n) \textit{ minimizes } \overline{w}_n &\iff (T(x_1), ..., T(x_n)) \textit{ minimizes } \mathrm{E}_{\log} \\
(x_1, ..., x_n) \textit{ minimizes } w_n &\iff (T(x_1), ..., T(x_n), N) \textit{ minimizes } \mathrm{E}_{\log}.
\end{aligned}$$

Proof. For any $1 \le i \le n$, we set $y_i := T(x_i)$, hence we get, by (4.7.1),

$$\begin{aligned}
\mathrm{E}_{\log}(y_1, ..., y_n) &:= -\sum_{i \neq j}^{n} \log \|y_i - y_j\| \\
&= -\sum_{i \neq j}^{n} \log \|T(x_i) - T(x_j)\| \\
&= -\sum_{i \neq j}^{n} \log \left(\frac{|x_i - x_j|}{\sqrt{1 + |x_i|^2}\sqrt{1 + |x_j|^2}} \right) \\
&= -\sum_{i \neq j}^{n} \log |x_i - x_j| + (n-1) \sum_{i=1}^{n} \log(1 + |x_i|^2) \\
&= \overline{w}_n(x_1, ..., x_n).
\end{aligned}$$

Furthermore, by (4.7.1), we obtain

$$\begin{aligned}
w_n(x_1, ..., x_n) &= \overline{w}_n(x_1, ..., x_n) + \sum_{i=1}^{n} \log(1 + |x_i|^2) \\
&= -\sum_{i \neq j} \log \|y_i - y_j\| - 2 \sum_{i=1}^{n} \log \|y_i - N\| = \mathrm{E}_{\log}(y_1, ..., y_n, N).
\end{aligned}$$

□

Lemma 4.7.3. *If* $(x_1, ..., x_n)$ *minimizes* w_n *or* $\overline{w}_n$*, then, for* $\nu_n := \sum_{i=1}^{n} \delta_{x_i}$*, we have*

$$\frac{\nu_n}{n} \to \mu_V, \qquad \textit{as } n \to +\infty,$$

in the weak sense of measures.

Proof. Let $(x_1, ..., x_n)$ be a minimizer of $\bar{w}_n$, then $(T(x_1), ..., T(x_n))$ is a minimizer of $\mathrm{E}_{\log}$. Brauchart, Dragnev and Saff proved in [20, Proposition 11] that

$$\frac{1}{n} \sum_{i=1}^{n} \delta_{T(x_i)} \to T\sharp\mu_V.$$

As $T\sharp\mu_V(N) = 0$, by Lemma 4.7.1 we get the result.
If $(x_1, ..., x_n)$ is a minimizer of w_n, then $(T(x_1), ..., T(x_n), N)$ minimizes $\mathrm{E}_{\log}$ and we can use our previous argument because

$$\frac{1}{n+1}\left(\sum_{i=1}^{n} \delta_{T(x_i)} + \delta_N\right) = \frac{1}{n}\sum_{i=1}^{n} \delta_{T(x_i)} \left(\frac{n}{n+1}\right) + \frac{\delta_N}{n+1} \to T\sharp\mu_V,$$

in the weak sense of measures, and we have the same conclusion. $\square$

Lemma 4.7.4. *If $(x_1, ..., x_n)$ is a minimizer of w_n and if $\nu_n := \sum_{i=1}^{n} \delta_{x_i}$ then*

$$\lim_{n\to+\infty} \frac{1}{n}\int_{\mathbb{R}^2} \log(1+|x|^2)d\nu_n(x) = \int_{\mathbb{R}^2} \log(1+|x|^2)d\mu_V(x).$$

There exists minimizers of $\overline{w}_n$ for which the same is true.

Proof. Let $(x_1, ..., x_n)$ be a minimizer of $\overline{w}_n$. We define $y_i := T(x_i)$ for any $1 \le i \le n$ and we notice that

$$\begin{aligned}\frac{1}{n}\int_{\mathbb{R}^2} \log(1+|x|^2)d\nu_n(x) &= -\frac{2}{n}\int_{\mathbb{R}^2} \log\left(\frac{1}{\sqrt{1+|x|^2}}\right) d\nu_n(x)\\ &= -\frac{2}{n}\int_{\mathcal{S}} \log\|y-N\| dT\sharp\nu_n(y),\end{aligned}$$

and by the previous Lemma, $(y_1, ..., y_n)$ is a minimizer of $\mathrm{E}_{\log}$ on $\mathcal{S}$. For any rotation R of $\mathcal{S}$ the rotated configuration of points is still a minimizer, and it is clear that the average over rotations R of

$$-\frac{2}{n}\sum_i \log\|Ry_i - N\|$$

is equal to

$$-2\fint_{\mathcal{S}} \log\|y-N\|\, dy.$$

It follows that there exists a rotated configuration $(\bar{y}_1, ..., \bar{y}_n)$ such that

$$\frac{1}{n}\sum_i \log\|\bar{y}_i - N\| = \fint_{\mathcal{S}} \log\|y-N\|\, dy.$$

Transporting this equality back to $\mathbb{R}^2$ with T^{-1}, we obtain a minimizer $(\bar{x}_1, ..., \bar{x}_n)$ of $\overline{w}_n$ such that

$$\frac{1}{n}\sum_i \log(1+|\bar{x}_i|^2) = \int_{\mathbb{R}^2} \log(1+|x|^2)d\mu_V(x).$$

If $(x_1, \ldots, x_n)$ is a minimizer of w_n we use [20, Theorem 15] about the optimal point separation which yields the existence of constants C and n_0 such that for any $n \geq n_0$ and any minimizer $\{y_1, ..., y_n\} \in \mathcal{S}^n$ of the logarithmic energy on the sphere, we have

$$\min_{i \neq j} \|y_i - y_j\| > \frac{C}{\sqrt{n-1}}.$$

Letting $y_i = T(x_i)$ we have that $(N, y_1, \ldots, y_n)$ is a minimizer of the logarithmic energy, hence for any $1 \leq i \leq n$,

$$\|y_i - N\| > \frac{C}{\sqrt{n-1}}. \tag{4.7.2}$$

For $n \geq n_0$ and $\delta > 0$ sufficiently small, we define, for any $0 < r \leq \delta$,

$$n(r) := \# \{y_i \mid y_i \in B(N, r) \cap \mathcal{S}\},$$

and $r_i = \|y_i - N\|$. From the separation property there exists a constant C such that $n(r) \leq Cr^2 n$ for any r. Hence we have, using integration by parts,

$$\begin{aligned} - \sum_{y_i \in B(N,\delta)} \log r_i &= - \int_{1/\sqrt{n-1}}^{\delta} \log r n'(r) dr \\ &= -n(\delta) \log \delta + \int_{1/\sqrt{n-1}}^{\delta} \frac{n(r)}{r} dr \\ &\leq -Cn\delta^2 \log \delta + Cn \int_{1/\sqrt{n-1}}^{\delta} r dr \leq C\delta^2 n |\log \delta|. \end{aligned}$$

It follows that

$$\lim_{\delta \to 0} \lim_{n \to +\infty} \frac{1}{n} \int_{B(N,\delta) \cap \mathcal{S}} \log \|y - N\| dT \sharp \nu_n(y) = \lim_{\delta \to 0} \lim_{n \to +\infty} - \sum_{i=1}^{n_\delta} \frac{1}{n} \log \|y_i - N\| = 0. \tag{4.7.3}$$

By Lemma 4.7.3, $\dfrac{\nu_n}{n}$ goes weakly to the measure μ_V on B_R for any R, hence we get

$$\begin{aligned} &\lim_{n \to +\infty} \frac{1}{n} \int_{\mathbb{R}^2} \log(1 + |x|^2) d\nu_n(x) \\ &= \lim_{n \to +\infty} \frac{1}{n} \left(\int_{B_R} \log(1 + |x|^2) d\nu_n(x) + \int_{B_R^c} \log(1 + |x|^2) d\nu_n(x) \right) \\ &= \int_{B_R} \log(1 + |x|^2) d\mu_V(x) + \lim_{n \to +\infty} \frac{1}{n} \int_{B_R^c} \log(1 + |x|^2) d\nu_n(x). \end{aligned}$$

Therefore it follows from (4.7.3) that

$$\begin{aligned}
&\lim_{n\to+\infty}\frac{1}{n}\int_{\mathbb{R}^2}\log(1+|x|^2)d\nu_n(x)\\
&=\lim_{R\to+\infty}\left(\int_{B_R}\log(1+|x|^2)d\mu_V(x)+\lim_{n\to+\infty}\frac{1}{n}\int_{B_R^c}\log(1+|x|^2)d\nu_n(x)\right)\\
&=\int_{\mathbb{R}^2}\log(1+|x|^2)d\mu_V(x).
\end{aligned}$$

The convergence is proved. $\square$

The following result proves the existence of the constant C in the Conjecture 1 of Rakhmanov, Saff and Zhou.

Theorem 4.7.5. *We have*

$$\mathcal{E}_{\log}(n)=\left(\frac{1}{2}-\log 2\right)n^2-\frac{n}{2}\log n+\left(\frac{1}{\pi}\min_{\mathcal{A}_1}W+\frac{\log\pi}{2}+\log 2\right)n+o(n),\quad \text{as } n\to+\infty.$$

Proof. As $\mathrm{E}_{\log}$ is invariant by translation of the 2-sphere, we work on the sphere $\tilde{\mathbb{S}}^2$ of radius 1 and centred in $(0,0,1/2)$. Let $(y_1,...,y_n)\in\tilde{\mathbb{S}}^2$ be a minimizer of $\mathrm{E}_{\log}$. Without loss of generality, for any n, we can choose this configuration such that $y_i\neq N$ for any $1\leq i\leq n$. Hence there exists $(x_1,...,x_n)$ such that $\frac{y_i}{2}=T(x_i)$ for any i and we get

$$\begin{aligned}
\mathrm{E}_{\log}(y_1,....,y_n)&=-\sum_{i\neq j}^{n}\log\|y_i-y_j\|\\
&=-\sum_{i\neq j}^{n}\log\|T(x_i)-T(x_j)\|-n(n-1)\log 2\\
&=\overline{w}_n(x_1,...,x_n)-n(n-1)\log 2.
\end{aligned}$$

By Lemma 4.7.2, $(y_1,...,y_n)$ is a minimizer of $\mathrm{E}_{\log}$ if and only if $(x_1,...,x_n)$ is a minimizer of $\overline{w}_n$. By the lower bound (4.6.2) and the convergence of Lemma 4.7.4, we have, for some minimizer $(\bar{x}_1,...,\bar{x}_n)$ of $\overline{w}_n$:

$$\begin{aligned}
&\liminf_{n\to+\infty}\frac{1}{n}\left[\overline{w}_n(\bar{x}_1,...,\bar{x}_n)-n^2I_V(\mu_V)+\frac{n}{2}\log n\right]\\
&=\liminf_{n\to+\infty}\frac{1}{n}\left[w_n(\bar{x}_1,...,\bar{x}_n)-\sum_{i=1}^{n}\log(1+|\bar{x}_i|^2)-n^2I_V(\mu_V)+\frac{n}{2}\log n\right]\\
&\geq\alpha-\int_{\mathbb{R}^2}\log(1+|x|^2)d\mu_V(x).
\end{aligned}$$

The upper bound (4.6.3) and Lemma 4.7.3 yield, $(x_1, ..., x_n)$ being a minimizer of w_n :

$$\begin{aligned}
&\limsup_{n\to+\infty} \frac{1}{n}\left[\overline{w}_n(\bar{x}_1, ..., \bar{x}_n) - n^2 I_V(\mu_V) + \frac{n}{2}\log n\right] \\
&\le \limsup_{n\to+\infty} \frac{1}{n}\left[\overline{w}_n(x_1, ..., x_n) - n^2 I_V(\mu_V) + \frac{n}{2}\log n\right] \\
&= \limsup_{n\to+\infty} \frac{1}{n}\left[w_n(x_1, ..., x_n) - \sum_{i=1}^n \log(1+|x_i|^2) - n^2 I_V(\mu_V) + \frac{n}{2}\log n\right] \\
&= \alpha_V - \int_{\mathbb{R}^2} \log(1+|x|^2) d\mu_V(x).
\end{aligned}$$

Thus, we get

$$\lim_{n\to+\infty} \frac{1}{n}\left[\overline{w}_n(\bar{x}_1, ..., \bar{x}_n) - n^2 I_V(\mu_V) + \frac{n}{2}\log n\right] = \alpha_V - \int_{\mathbb{R}^2} \log(1+|x|^2) d\mu_V(x).$$

Therefore, we have the following asymptotic expansion, as $n \to +\infty$, when $(\bar{x}_1, ..., \bar{x}_n)$ is a minimizer of $\overline{w}_n$:

$$\begin{aligned}
&\overline{w}_n(\bar{x}_1, ..., \bar{x}_n) \\
&= n^2 I_V(\mu_V) - \frac{n}{2}\log n + \left(\frac{1}{\pi}\min_{\mathcal{A}_1} W - \frac{1}{2}\int_{\mathbb{R}^2} m_V(x)\log m_V(x) dx - \int_{\mathbb{R}^2} V(x) d\mu_V(x)\right) n + o(n).
\end{aligned}$$

We know that $I_V(\mu_V) = \dfrac{1}{2}$ (see [19, Eq. (2.26)]) and

$$\begin{aligned}
\int_{\mathbb{R}^2} \log(1+|x|^2) d\mu_V(x) &= \frac{1}{\pi}\int_{\mathbb{R}^2} \frac{\log(1+|x|^2)}{(1+|x|^2)^2} \\
&= 2\int_0^{+\infty} \frac{r\log(1+r^2)}{(1+r^2)^2} dr \\
&= -\left[\frac{\log(1+r^2)}{1+r^2}\right]_0^{+\infty} + \int_{\mathbb{R}^2} \frac{2r}{(1+r^2)^2} dr \\
&= -\left[\frac{1}{1+r^2}\right]_0^{+\infty} \\
&= 1.
\end{aligned}$$

Hence we obtain, as $n \to +\infty$,

$$\begin{aligned}
\overline{w}_n(\bar{x}_1, ..., \bar{x}_n) &= \frac{n^2}{2} - \frac{n}{2}\log n + \left(\frac{1}{\pi}\min_{\mathcal{A}_1} W + \frac{1}{2}\int \log(\pi(1+|x|^2)^2) d\mu_V(x) - 1\right) n + o(n) \\
&= \frac{n^2}{2} - \frac{n}{2}\log n + \left(\frac{1}{\pi}\min_{\mathcal{A}_1} W + \frac{\log \pi}{2} + \int \log(1+|x|^2) d\mu_V(x) - 1\right) n + o(n)
\end{aligned}$$

$$= \frac{n^2}{2} - \frac{n}{2}\log n + \left(\frac{1}{\pi}\min_{\mathcal{A}_1} W + \frac{\log \pi}{2}\right) n + o(n),$$

and the asymptotic expansion of $\mathcal{E}_{\log}(n)$ is

$$\mathcal{E}_{\log}(n) = \left(\frac{1}{2} - \log 2\right) n^2 - \frac{n}{2}\log n + \left(\frac{1}{\pi}\min_{\mathcal{A}_1} W + \frac{\log \pi}{2} + \log 2\right) n + o(n).$$

□

Remark 4.7.6. It follows from lower bound proved by Rakhmanov, Saff and Zhou [81, Theorem 3.1], that

$$\frac{1}{\pi}\min_{\mathcal{A}_1} W + \frac{\log \pi}{2} + \log 2 = \lim_{n\to+\infty}\frac{1}{n}\left[\mathrm{E}_{\log}(y_1, ..., y_n) - \left(\frac{1}{2} - \log 2\right) n^2 + \frac{n}{2}\log n\right]$$
$$\geq -\frac{1}{2}\log\left[\frac{\pi}{2}(1-e^{-a})^b\right],$$

where $a := \frac{2\sqrt{2\pi}}{\sqrt{27}}\left(\sqrt{2\pi + \sqrt{27}} + \sqrt{2\pi}\right)$ and $b := \frac{\sqrt{2\pi + \sqrt{27}} - \sqrt{2\pi}}{\sqrt{2\pi + \sqrt{27}} + \sqrt{2\pi}}$, and we get

$$\min_{\mathcal{A}_1} W \geq -\frac{\pi}{2}\log\left[2\pi^2(1-e^{-a})^b\right] \approx -4.6842707.$$

4.7.3 Computation of renormalized energy for the triangular lattice and upper bound for the term of order n

Sandier and Serfaty proved in [86, Lemma 3.3] that

$$W(\Lambda_{1/2\pi}) = -\frac{1}{2}\log\left(\sqrt{2\pi b}|\eta(\tau)|^2\right),$$

where $\Lambda_{1/2\pi}$ is the triangular lattice corresponding to the density $m = 1/2\pi$, $\tau = a + ib = 1/2 + i\frac{\sqrt{3}}{2}$ and η is the Dedekind eta function defined, with $q = e^{2i\pi\tau}$, by

$$\eta(\tau) = q^{1/24}\prod_{n\geq 1}(1-q^n).$$

We recall Chowla-Selberg formula (see [28] or [29, Proposition 10.5.11] for details) :

$$\prod_{m=1}^{|D|}\Gamma\left(\frac{m}{|D|}\right)^{\frac{w}{2}\left(\frac{D}{m}\right)} = 4\pi\sqrt{-D}b|\eta(\tau)|^4,$$

for τ a root of the integral quadratic equation $\alpha z^2 + \beta z + \gamma = 0$ where $D = \beta^2 - 4\alpha\gamma < 0$, $\left(\frac{D}{m}\right)$ is the Kronecker symbol, w the number of roots of unity in $\mathbb{Q}(i\sqrt{-D})$ and when the class number of $\mathbb{Q}(i\sqrt{-D})$ is equal to 1. In our case $b = \sqrt{3}/2$, $w = 6$, $\alpha = \beta = \gamma = 1$ because τ is a root of unity, hence $D = -3$, $\left(\dfrac{-3}{1}\right) = 1$ and $\left(\dfrac{-3}{2}\right) = -1$ by the Gauss Lemma. Therefore we obtain

$$\Gamma(1/3)^3\Gamma(2/3)^{-3} = 4\pi\sqrt{3}\frac{\sqrt{3}}{2}|\eta(\tau)|^4,$$

and by Euler's reflection formula $\Gamma(1-1/3)\Gamma(1/3) = \dfrac{\pi}{\sin(\pi/3)}$, we get

$$\frac{\Gamma(1/3)^6 3\sqrt{3}}{8\pi^3} = \frac{4\pi\sqrt{3}\times\sqrt{3}|\eta(\tau)|^4}{2}.$$

Finally we obtain

$$|\eta(\tau)|^4 = \frac{\Gamma(1/3)^6\sqrt{3}}{16\pi^4}.$$

Now it is possible to find the exact value of the renormalized energy of the triangular lattice Λ_1 of density $m = 1$:

$$\begin{aligned}
W(\Lambda_1) &= 2\pi W(\Lambda_{1/2\pi}) - \pi\frac{\log(2\pi)}{2}\\
&= -\pi\log\left(\sqrt{2\pi b}|\eta(\tau)|^2\right) - \pi\frac{\log(2\pi)}{2}\\
&= \pi\log\pi - \frac{\pi}{2}\log 3 - 3\pi\log(\Gamma(1/3)) + \frac{3}{2}\pi\log 2\\
&= \pi\log\left(\frac{2\sqrt{2}\pi}{\sqrt{3}\Gamma(1/3)^3}\right)\\
&\approx -4.1504128.
\end{aligned}$$

Thus, we get

$$\begin{aligned}
&\frac{1}{\pi}W(\Lambda_1) + \frac{\log\pi}{2} + \log 2\\
&= \frac{1}{\pi}\left(\pi\log\pi - \frac{\pi}{2}\log 3 - 3\pi\log(\Gamma(1/3)) + \frac{3}{2}\pi\log 2\right) + \frac{\log\pi}{2} + \log 2\\
&= 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)} = C_{BHS} \approx -0.0556053,
\end{aligned}$$

and we find exactly the value C_{BHS} conjectured by Brauchart, Hardin and Saff in [22, Conjecture 4]. Therefore Conjecture 2 is true if and only if the triangular lattice Λ_1 is a global minimizer of W among vector-fields in $\mathcal{A}_1$, i.e.

$$\min_{\mathcal{A}_1} W = W(\Lambda_1) = \pi\log\left(\frac{2\sqrt{2}\pi}{\sqrt{3}\Gamma(1/3)^3}\right).$$

Thus we obtain the following result

Theorem 4.7.7. *We have :*

1. *It holds*

$$\lim_{n\to+\infty} \frac{1}{n}\left[\mathcal{E}_{\log}(n) - \left(\frac{1}{2} - \log 2\right) n^2 + \frac{n}{2}\log n\right] \leq 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)}.$$

2. *Conjectures 2 and 3 are equivalent, i.e.* $\min_{\mathcal{A}_1} W = W(\Lambda_1) \iff C = C_{BHS}$.

Annexe A

Proof of Montgomery Theorem

In this annex, we give the proof of Montgomery theorem from [74] :

Theorem A.0.8. *For any real number $\alpha > 0$ and a Bravais lattice L, let*

$$\theta_L(\alpha) := \Theta_L(i\alpha) = \sum_{p\in L} e^{-2\pi\alpha\|p\|^2}, \tag{A.0.1}$$

where Θ_L is the Jacobi theta function of the lattice L defined for $Im(z) > 0$. Then, for any $\alpha > 0$, Λ_A is the unique minimizer of $L \to \theta_L(\alpha)$, up to rotation, among Bravais lattices of area A.

We reproduce this proof with all details and references.

A.1 Preliminaries

This problem of minimization among lattices can be viewed as a minimization among positive definite binary quadratic forms with real coefficients. For

$$f(m,n) = am^2 + bmn + cn^2$$

such that its discriminant is $b^2 - 4ac = -1$, we define the theta function associated to f by

$$\theta_f(\alpha) = \sum_{m,n} e^{-2\pi\alpha f(m,n)}.$$

Let

$$h(m,n) = \frac{1}{\sqrt{3}}(m^2 + mn + n^2)$$

be a positive definite binary quadratic form with discriminant 1 corresponding to the triangular lattice. Our goal is to prove the following result : for any $\alpha > 0$ and any positive definite binary quadratic form f with real coefficients,

$$\theta_f(\alpha) \geq \theta_h(\alpha).$$

Moreover, if there is an $\alpha > 0$ for which $\theta_f(\alpha) = \theta_h(\alpha)$, then f and h are equivalent forms, i.e. there is a $C \in SL_2(\mathbb{Z})$ such that $f(x,y) = h(C(x,y))$, and $\theta_f \equiv \theta_h$.

Firstly, if we let $b = 2ax$ and $c = a(x^2 + y^2)$, we may factorize f as

$$f(m,n) = a(m + zn)(m + \bar{z}n)$$

where $z = x + iy$, and, without loss of generality, $y > 0$. Moreover, $b^2 - 4ac = -1$, we deduce that $4a^2x^2 - 4a^2(x^2 + y^2) = -1$, therefore

$$a = \frac{1}{2y}.$$

Hence, we can write

$$f(m,n) = \frac{1}{2y}(m + zn)(m + \bar{z}n) = \frac{1}{2y}(m + xn)^2 + \frac{1}{2}yn^2$$

and it follows that we define

$$\theta(\alpha; x, y) := \theta_f(\alpha) = \sum_{n \in \mathbb{Z}} e^{-\pi\alpha y n^2} \sum_{m \in \mathbb{Z}} e^{-\pi\alpha(m+nx)^2/y}. \tag{A.1.1}$$

Definition A.1.1. *A positive definite binary quadratic form $f(m,n) = am^2 + bmn + cn^2$ is reduced if*

$$-a < b \leq a < c \quad \text{or} \quad 0 \leq b \leq a = c.$$

Hence f is reduced if and only if

$$-\frac{1}{2y} < \frac{x}{y} \leq \frac{1}{2y} < \frac{x^2 + y^2}{2y} \quad \text{or} \quad 0 \leq \frac{2x}{2y} \leq \frac{1}{2y} = \frac{x^2 + y^2}{2y},$$

that is to say $z \in \mathcal{D}$ where

$$\mathcal{D} := \left\{ z; -\frac{1}{2} < x \leq \frac{1}{2}, |z| > 1, y > 0 \right\} \cup \left\{ z; 0 \leq x \leq \frac{1}{2}, |z| = 1, y > 0 \right\}$$

is the fundamental domain of the modular group. As we know that each positive definite binary quadratic form is equivalent to a unique reduced form (see for example [73, Theorem 3.1] for a proof), we may confine our attention to reduced forms. Furthermore, for any $x \in \mathbb{R}$ we have

$$\theta(\alpha; -x, y) = \theta(\alpha; x, y),$$

hence throughout this annex,

$$z \in \left\{ z; 0 \le x \le \frac{1}{2}, |z| \ge 1, y > 0 \right\}.$$

The strategy of Montgomery is to prove the following two lemmas which give automatically Theorem A.0.8 :

Lemma A.1.1. *If $\alpha > 0$, $0 < x < \frac{1}{2}$ and $y \ge \frac{1}{2}$, then*

$$\frac{\partial}{\partial x} \theta(\alpha; x, y) < 0.$$

Lemma A.1.2. *If $\alpha > 0$, $0 \le x \le \frac{1}{2}$ and $x^2 + y^2 \ge 1$, then*

$$\frac{\partial}{\partial y} \theta(\alpha; x, y) \ge 0,$$

with equality if and only if (x, y) is one of the points $(0, 1)$, $(1/2, \sqrt{3}/2)$.

A.2 Properties of 1D and 2D theta functions

Definition A.2.1. *The classical one-dimensional theta function is defined by*

$$\theta(t; \beta) := \sum_{k \in \mathbb{Z}} e^{-\pi k^2 t + 2i\pi k\beta} \tag{A.2.1}$$

for $\beta \in \mathbb{C}$ and $Re(t) > 0$.

Lemma A.2.1. *The one-dimensional theta function satisfies the functional equation*

$$\theta(t; \beta) = t^{-1/2} \sum_{m \in \mathbb{Z}} e^{-\pi(m-\beta)^2/t}. \tag{A.2.2}$$

Proof. Firstly we remark that

$$\theta(t; \beta) = \vartheta(\beta; it)$$

where

$$\vartheta(z; \tau) := \sum_{n \in \mathbb{Z}} e^{i\pi n^2 \tau + 2i\pi nz} \tag{A.2.3}$$

is the Jacobi theta function defined for $z \in \mathbb{C}$ and τ in the upper half-plane. We have (see for example [94, Theorem 1.6, Chapter 10]),

$$\vartheta(z; -\tau^{-1}) = \sqrt{\frac{\tau}{i}} e^{i\pi\tau z^2} \vartheta(z\tau; \tau),$$

that is to say, for $\tau = -u^{-1}$,

$$\vartheta(z; u) = \sqrt{-\frac{1}{ui}} e^{-i\pi z^2/u} \vartheta\left(-\frac{z}{u}; -\frac{1}{u}\right). \tag{A.2.4}$$

Hence, applying (A.2.4) with $z = \beta$ and $u = it$, we get

$$\begin{aligned}
\theta(t; \beta) = \vartheta(\beta; it) &= \frac{1}{\sqrt{t}} e^{-\pi\beta^2/t} \vartheta\left(-\frac{\beta}{it}; -\frac{1}{it}\right) \\
&= \frac{1}{\sqrt{t}} e^{-\pi\beta^2/t} \sum_{n\in\mathbb{Z}} e^{-\pi n^2/t - 2\pi n\beta/t} \\
&= \frac{1}{\sqrt{t}} \sum_{n\in\mathbb{Z}} e^{-\pi(\beta+n)^2/t} \\
&= \frac{1}{\sqrt{t}} \sum_{m\in\mathbb{Z}} e^{-\pi(m-\beta)^2/t}.
\end{aligned}$$

□

Now we can prove the classical functional equation for θ_f.

Proposition A.2.2. *For any $\alpha > 0$ and any positive definite binary quadratic form f of discriminant 1, we have*

$$\theta_f\left(\frac{1}{\alpha}\right) = \alpha\theta_f(\alpha). \tag{A.2.5}$$

Proof. By (A.1.1) and (A.2.2), we have, for any $\alpha > 0$, any $y > 0$ and any $0 \le x \le 1/2$,

$$\theta(\alpha; x, y) = \sum_{n\in\mathbb{Z}} e^{-\pi\alpha y n^2} \theta\left(\frac{y}{\alpha}; nx\right) \sqrt{\frac{y}{\alpha}}. \tag{A.2.6}$$

Now, using (A.2.2) we obtain

$$\begin{aligned}
\theta(\alpha; x, y) &= \sqrt{\frac{y}{\alpha}} \sum_{n\in\mathbb{Z}} e^{-\pi\alpha y n^2} \sum_{k\in\mathbb{Z}} e^{-\pi k^2 y/\alpha + 2i\pi knx} \\
&= \sqrt{\frac{y}{\alpha}} \sum_{k\in\mathbb{Z}} e^{-\pi k^2 y/\alpha} \sum_{n\in\mathbb{Z}} e^{-\pi\alpha y n^2 + 2i\pi knx}
\end{aligned}$$

$$
\begin{aligned}
&= \sqrt{\frac{y}{\alpha}} \sum_{k\in\mathbb{Z}} e^{-\pi k^2 y/\alpha} \theta(\alpha y; nx) \\
&= \sqrt{\frac{y}{\alpha}} \sum_{k\in\mathbb{Z}} e^{-\pi k^2 y/\alpha} \frac{1}{\sqrt{\alpha y}} \sum_{m\in\mathbb{Z}} e^{-\pi(m-nx)^2/\alpha y} \\
&= \frac{1}{\alpha}\theta\left(\frac{1}{\alpha}; x, y\right).
\end{aligned}
$$

$\square$

Lemma A.2.3. *It holds, for any t such that $Re(t) > 0$ and $\beta \in \mathbb{C}$,*

$$
\theta(t;\beta) = \prod_{r=1}^{+\infty} \left(1 - e^{-2\pi r t}\right) \left(1 + 2e^{-(2r-1)\pi t}\cos(2\pi\beta) + e^{-2(2r-1)\pi t}\right). \tag{A.2.7}
$$

Proof. We use the Jacobi triple product formula (see [94, Theorem 1.3, Chapter 10]) for the Jacobi theta function (A.2.3) given, for $z \in \mathbb{C}$ and τ in the upper half-plane, by

$$
\vartheta(z;\tau) = \prod_{r=1}^{+\infty} (1 - q^{2r})(1 + q^{2r-1}e^{2i\pi z})(1 + q^{2r-1}e^{-2i\pi z})
$$

where $q = e^{i\pi z}$. Therefore we obtain

$$
\begin{aligned}
\theta(t;\beta) = \vartheta(\beta; it) &= \prod_{r=1}^{+\infty} \left(1 - e^{-2\pi n t}\right)\left(1 + e^{-(2r-1)\pi t + 2i\pi\beta}\right)\left(1 + e^{-(2r-1)\pi t - 2i\pi\beta}\right) \\
&= \prod_{r=1}^{+\infty} \left(1 - e^{-2\pi r t}\right)\left(1 + 2e^{-(2r-1)\pi t}\cos(2\pi\beta) + e^{-2(2r-1)\pi t}\right).
\end{aligned}
$$

$\square$

Lemma A.2.4. *Let*

$$
Q(t;\beta) := -\frac{\partial_\beta \theta(t;\beta)}{\sin(2\pi\beta)},
$$

and suppose that $t > 0$ is fixed. Then

- *$Q(t;\beta)$ is an even function of β with period* 1*,*
- *$Q(t;\beta) \geq 0$ for any β,*
- *$\beta \mapsto Q(t;\beta)$ is a decreasing function in the interval* $[0, 1/2]$.

Proof. We have, by differentiating (A.2.7),

$$
Q(t;\beta) = 4\pi \sum_{s=1}^{+\infty} (1 - e^{-2\pi s t}) e^{-(2s-1)\pi t} \prod_{\substack{r=1 \\ r\neq s}}^{+\infty} (1 - e^{-2\pi r t}) \left(1 + 2e^{-(2r-1)\pi t}\cos(2\pi\beta) + e^{-2(2r-1)\pi t}\right).
$$

Hence $\beta \mapsto Q(t;\beta)$ is obviously even and with period 1 because $\cos(2\pi(-\beta)) = \cos(2\pi\beta)$ and $\cos(2\pi(\beta+1)) = \cos(2\pi\beta)$. Moreover, in this product, each term is positive and the function $\beta \mapsto \left(1 + 2e^{-(2r-1)\pi t}\cos(2\pi\beta) + e^{-2(2r-1)\pi t}\right)$ is decreasing in $[0, 1/2]$ for any $s \geq 1$ and any $r \geq 1$. $\square$

Lemma A.2.5. *Let*

$$A(t) = \begin{cases} t^{-3/2} e^{-\pi/4t} & \textit{if } 0 < t < 1 \\ \left(1 - \frac{1}{3000}\right) 4\pi e^{-\pi t} & \textit{if } t \geq 1, \end{cases}$$

and

$$B(t) = \begin{cases} t^{-3/2} & \textit{if } 0 < t < 1 \\ \left(1 + \frac{1}{3000}\right) 4\pi e^{-\pi t} & \textit{if } t \geq 1. \end{cases}$$

Then, for any β and any $t > 0$, we have

$$A(t) \leq Q(t;\beta) \leq B(t). \tag{A.2.8}$$

Proof. By the previous Lemma, $\beta \mapsto Q(t;\beta)$ is a decreasing function in $[0, 1/2]$. Thus, it suffices to show that

$$Q(t; 1/2) \geq A(t) \tag{A.2.9}$$

and that

$$Q(t; 0) \leq B(t). \tag{A.2.10}$$

Let us prove inequality (A.2.9). By L'Hôpital's rule, we get

$$Q(t; 1/2) = \lim_{\beta_0 \to 1/2} \frac{-\partial_\beta \theta(t;\beta)_{|\beta=\beta_0}}{\sin(2\pi\beta_0)} = \frac{1}{2\pi} \partial_\beta^2 \theta(t;\beta)_{|\beta=1/2}.$$

For $t \geq 1$, by differentiating (A.2.1), we get

$$\partial_\beta \theta(t;\beta) = \sum_{k\in\mathbb{Z}} 2i\pi k e^{-\pi k^2 t + 2i\pi\beta k}$$

and we obtain

$$\partial_\beta^2 \theta(t;\beta) = 4\pi^2 \sum_{k\in\mathbb{Z}} -k^2 e^{2i\pi\beta k} e^{-\pi k^2 t}. \tag{A.2.11}$$

Hence we have

$$Q(t; 1/2) = \frac{1}{2\pi} \partial_\beta^2 \theta(t;\beta)_{|\beta=1/2} = 2\pi \sum_{k\in\mathbb{Z}} -k^2 e^{i\pi k} e^{-\pi k^2 t}$$

$$
\begin{aligned}
&= 2\pi \sum_{k\in\mathbb{Z}} (-1)^{k-1} k^2 e^{-\pi k^2 t} \\
&= 4\pi \sum_{k=1}^{+\infty} (-1)^{k-1} k^2 e^{-\pi k^2 t} \\
&= 4\pi e^{-\pi t} \sum_{k=1}^{+\infty} (-1)^{k-1} k^2 e^{-\pi k^2 t + \pi t} \\
&= 4\pi e^{-\pi t} \left[e^{-\pi t + \pi t} + \sum_{k=2}^{+\infty} (-1)^{k-1} k^2 e^{-\pi (k^2-1) t} \right] \\
&\geq 4\pi e^{-\pi t} \left[1 - \sum_{k=2}^{+\infty} k^2 e^{-\pi (k^2-1) t} \right].
\end{aligned}
$$

Now we remark that $t \mapsto \sum_{k=2}^{+\infty} k^2 e^{-\pi(k^2-1)t}$ is a decreasing function of t, therefore, for any $t \geq 1$,

$$
\sum_{k=2}^{+\infty} k^2 e^{-\pi(k^2-1)t} < \sum_{k=2}^{+\infty} k^2 e^{-\pi(k^2-1)} < 0.0003228 < \frac{1}{3000} \tag{A.2.12}
$$

and we get

$$
Q(t; 1/2) \geq 4\pi e^{-\pi t} \left(1 - \frac{1}{3000} \right) = A(t),
$$

i.e. we have (A.2.9) for $t \geq 1$. When $0 < t < 1$, by differentiating (A.2.2), we obtain

$$
\partial_\beta \theta(t; \beta) = \frac{1}{t^{3/2}} \sum_{m\in\mathbb{Z}} 2\pi (m - \beta) e^{-\pi (m-\beta)^2/t}
$$

and it follows that

$$
\partial_\beta^2 \theta(t; \beta) = 2\pi t^{-3/2} \sum_{m\in\mathbb{Z}} \left(\frac{2\pi (m-\beta)^2}{t} - 1 \right) e^{-\pi (m-\beta)^2/t}. \tag{A.2.13}
$$

Therefore, we get

$$
\begin{aligned}
Q(t; 1/2) &= \frac{1}{2\pi} \partial_\beta^2 \theta(t; \beta)_{|\beta = 1/2} = t^{-3/2} \sum_{m\in\mathbb{Z}} \left(\frac{2\pi (m-1/2)^2}{t} - 1 \right) e^{-\pi (m-1/2)^2/t} \\
&= 2t^{-3/2} \sum_{m=1}^{+\infty} \left(\frac{2\pi (m-1/2)^2}{t} - 1 \right) e^{-\pi (m-1/2)^2/t} + t^{-3/2} e^{-\pi/4t} \left(\frac{\pi}{2t} - 1 \right).
\end{aligned}
$$

Here all terms are non-negative and the term $m = 1$ is equal to

$$
2t^{-3/2} \left(\frac{2\pi (1-1/2)^2}{t} - 1 \right) e^{-\pi/4t} = t^{-3/2} \left(\frac{\pi}{t} - 2 \right) e^{-\pi/4t} > t^{-3/2} e^{-\pi/4t} = A(t)
$$

because $t < 1 < \frac{\pi}{3}$. Hence we have $Q(t;1/2) > A(t)$ when $0 < t < 1$ and we obtain inequality (A.2.9) for $t < 1$.

Let us prove inequality (A.2.10). By L'Hôpital's rule, we find that

$$Q(t;0) = -\frac{1}{2\pi}\partial_\beta^2\theta(t;\beta)_{|\beta=0}.$$

Thus, by (A.2.11), we have

$$Q(t;0) = 4\pi\sum_{k=1}^{+\infty} k^2 e^{-\pi k^2 t} = 4\pi e^{-\pi t}\left(1 + \sum_{k=2}^{+\infty} k^2 e^{-\pi(k^2-1)t}\right).$$

By (A.2.12), we obtain, for $t \geq 1$,

$$Q(t;0) < 4\pi e^{-\pi t}\left(1 + \frac{1}{3000}\right) = B(t),$$

i.e. we have inequality (A.2.10) for $t \geq 1$. Now suppose that $0 < t < 1$, by (A.2.13) we get

$$\begin{aligned} Q(t;0) = t^{-3/2}\sum_{m\in\mathbb{Z}}\left(1 - \frac{2\pi m^2}{t}\right)e^{-\pi m^2/t} &= t^{-3/2} + 2\sum_{m=1}^{+\infty}\left(1 - \frac{2\pi m^2}{t}\right)e^{-\pi m^2/t} \\ &= B(t) + 2\sum_{m=1}^{+\infty}\left(1 - \frac{2\pi m^2}{t}\right)e^{-\pi m^2/t} \\ &\leq B(t) \end{aligned}$$

because $t < 1 < 2\pi m^2$ for any $m \geq 1$. Hence we have (A.2.10) and the proof is complete. □

A.3 Proof of Lemma A.1.1

Let $\alpha > 0$, $x \in (0, 1/2)$ and $y \geq 1/2$ be real numbers. We want to prove that

$$\partial_x\theta(\alpha; x, y) < 0.$$

In view of (A.2.5), we may suppose that $\alpha \geq 1$. Moreover, by (A.2.6) and symmetry of summation, we have

$$\partial_x\theta(\alpha; x, y) = 2\sqrt{\frac{y}{\alpha}}\sum_{n=1}^{+\infty} n e^{-\pi\alpha y n^2}\partial_\beta\theta\left(\frac{y}{\alpha}, \beta\right)_{|\beta=nx}$$

$$= 2\sqrt{\frac{y}{\alpha}}\left[e^{-\pi\alpha y}\partial_\beta\theta\left(\frac{y}{\alpha},\beta\right)_{|\beta=x} + \sum_{n=2}^{+\infty} ne^{-\pi\alpha y n^2}\partial_\beta\theta\left(\frac{y}{\alpha},\beta\right)_{|\beta=nx}\right]$$
$$\leq 2\sqrt{\frac{y}{\alpha}}\left[-A(y/\alpha)\sin(2\pi x)e^{-\pi\alpha y} + \sum_{n=2} ne^{-\pi\alpha y n^2}B(y/\alpha)|\sin(2\pi nx)|\right],$$

because by (A.2.8), for any $n \geq 1$, $y > 0$, $\alpha > 0$ and $0 < x < 1/2$,

$$-B(y/\alpha) \leq \frac{\partial_\beta\theta(y/\alpha;\beta)_{|\beta=nx}}{\sin(2\pi nx)} \leq -A(y/\alpha).$$

Since $\left|\frac{\sin(2\pi nx)}{\sin(2\pi x)}\right| \leq n$ for any $0 < x < 1/2$ and any $n \geq 1$, we have

$$-A(y/\alpha)\sin(2\pi x)e^{-\pi\alpha y} + \sum_{n=2} ne^{-\pi\alpha y n^2}B(y/\alpha)|\sin(2\pi nx)|$$
$$\leq -A(y/\alpha)\sin(2\pi x)e^{-\pi\alpha y} + \sum_{n=2}^{+\infty} n^2 e^{-\pi\alpha y n^2}B(y/\alpha)\sin(2\pi x)$$
$$= \sin(2\pi x)\left(-A(y/\alpha)e^{-\pi\alpha y} + B(y/\alpha)\sum_{n=2}^{+\infty} n^2 e^{-\pi\alpha y n^2}\right).$$

We remark that, if

$$\sum_{n=2}^{+\infty} n^2 e^{-\pi\alpha y(n^2-1)} < \frac{A(y/\alpha)}{B(y/\alpha)} \tag{A.3.1}$$

then

$$\sin(2\pi x)\left(-A(y/\alpha)e^{-\pi\alpha y} + B(y/\alpha)\sum_{n=2}^{+\infty} n^2 e^{-\pi\alpha y n^2}\right) < 0.$$

i.e. $\partial_x\theta(\alpha;x,y) < 0$. Since $y \geq 1/2$, then we have

$$\alpha y = \frac{\alpha}{y}y^2 \geq \frac{\alpha}{4y}$$

and it follows that

$$\sum_{n=2}^{+\infty} n^2 e^{-\pi\alpha y(n^2-1)} \leq \sum_{n=2}^{+\infty} n^2 e^{-\pi(n^2-1)\alpha/4y}$$
$$= e^{-\pi\alpha/4y}\sum_{n=2}^{+\infty} e^{-\pi(n^2-2)\alpha/4y}.$$

Suppose that $\alpha > y$, then $\frac{y}{\alpha} < 1$ and by definition of $A(t)$ and $B(t)$ with $0 < t < 1$, we have

$$\frac{A(y/\alpha)}{B(y/\alpha)} = e^{-\pi\alpha/4y}.$$

Since $\frac{\alpha}{4y} > \frac{1}{4}$, then

$$\sum_{n=2}^{+\infty} e^{-\pi(n^2-2)\alpha/4y} < \sum_{n=2}^{+\infty} n^2 e^{-\pi(n^2-2)/4} < 1$$

therefore we have

$$\sum_{n=2}^{+\infty} n^2 e^{-\pi\alpha y(n^2-1)} < e^{-\pi\alpha/4y}$$

i.e. (A.3.1) holds.
If $\alpha \le y$, then

$$\frac{B(y/\alpha)}{A(y/\alpha)} = \frac{1+\frac{1}{3000}}{1-\frac{1}{3000}}$$

and $\alpha y \ge \alpha^2 \ge 1$, therefore, by (A.2.12), we obtain

$$\sum_{n=2}^{+\infty} n^2 e^{-\pi(n^2-1)\alpha y} \le \sum_{n=2}^{+\infty} n^2 e^{-\pi(n^2-1)} < \frac{1}{3000}$$

and it follows that

$$\frac{B(y/\alpha)}{A(y/\alpha)} \sum_{n=2}^{+\infty} n^2 e^{-\pi(n^2-1)\alpha y} < \frac{1}{3000} \times \frac{1+\frac{1}{3000}}{1-\frac{1}{3000}} < 1$$

and (A.3.1) holds and Lemma A.1.1 is proved.

A.4 Proof of Lemma A.1.2

Lemma A.4.1. *If* $\alpha > 0$, $0 \le x \le 1/2$ *and* $x^2 + y^2 \ge 1$*, then*

$$\partial_y^2 \theta(\alpha; x, y) + \frac{2}{y} \partial_y \theta(\alpha; x, y) > 0$$

Proof. In view of (A.2.5), we may assume that $\alpha \ge 1$. By differentiating (A.1.1), we get

$$\partial_y \theta(\alpha; x, y) = -\pi\alpha \sum_{m,n} n^2 e^{-2\pi\alpha f(m,n)} + \pi\alpha \sum_{m,n} \frac{(m+nx)^2}{y^2} e^{-2\pi\alpha f(m,n)}$$

and, for the second derivative,

$$\partial_y^2 \theta(\alpha; x, y) = -\frac{2\pi\alpha}{y^3} \sum_{m,n} (m+nx)^2 e^{-2\pi\alpha f(m,n)} + \sum_{m,n} \left(-\pi\alpha n^2 + \frac{\pi\alpha}{y^2}(m+nx)^2\right)^2 e^{-2\pi\alpha f(m,n)}$$

Hence, we obtain

$$\partial_y^2\theta(\alpha;x,y)+\frac{2}{y}\partial_y\theta(\alpha;x,y)=(\pi\alpha)^2\sum_{m,n}\left(n^2-\frac{(m-nx)^2}{y^2}\right)^2 e^{-2\pi\alpha f(m,n)} - \frac{2\pi\alpha}{y}\sum_{m,n}n^2e^{-2\pi\alpha f(m,n)} \tag{A.4.1}$$

In the first sum, the terms $(m,n)=(\pm 1,0)$ contribute an amount

$$2(\pi\alpha)^2y^{-4}e^{-\pi\alpha/y}=KP_1$$

with

$$K=2\pi\alpha e^{-\pi\alpha(x^2+y^2)/y} \quad \text{and} \quad P_1=\pi\alpha y^{-4}e^{\pi\alpha(x^2+y^2-1)/y}.$$

Moreover, the terms $(m,n)=(0,\pm 1)$ contribute an amount

$$2(\pi\alpha)^2\left(1-\frac{x^2}{y^2}\right)^2 e^{-\pi\alpha(x^2+y^2)/y}=KP_2$$

with

$$P_2=\pi\alpha\left(1-\frac{x^2}{y^2}\right)^2.$$

Since each term in this first sum is positive, we have

$$(\pi\alpha)^2\sum_{m,n}\left(n^2-\frac{(m-nx)^2}{y^2}\right)^2 e^{-2\pi\alpha f(m,n)}\geq K(P_1+P_2).$$

On the other hand, the second sum in (A.4.1) is equal, by symmetry and splitting into two parts ($n=1$ and $n\geq 2$), to

$$K\left(\frac{2}{y}\sum_{m\in\mathbb{Z}}e^{\pi\alpha(x^2-(x-m)^2)/y}+\frac{2}{y}e^{\pi\alpha(x^2+y^2)/y}\sum_{n=2}^{+\infty}n^2e^{-\pi\alpha n^2y}\sum_{m\in\mathbb{Z}}e^{-\pi\alpha(m-nx)^2/y}\right).$$

By pairing m and $-m$ terms, we see that

$$\begin{aligned}\sum_{m\in\mathbb{Z}}e^{\pi\alpha(x^2-(x-m)^2)/y}&=1+\sum_{m=1}^{+\infty}\left[e^{\pi\alpha(x^2-(x-m)^2)/y}+e^{\pi\alpha(x^2-(x+m)^2)/y}\right]\\&=1+\sum_{m=1}^{+\infty}e^{-\pi\alpha m^2/y}\left(e^{2\pi\alpha xm/y}+e^{-2\pi\alpha xm/y}\right)\\&=1+2\sum_{m=1}^{+\infty}e^{-\pi\alpha m^2/y}\cosh(2\pi\alpha mx/y),\end{aligned}$$

which is an increasing function of x. Hence we get,

$$\begin{aligned}1+2\sum_{m=1}^{+\infty} e^{-\pi\alpha m^2/y}\cosh(2\pi\alpha m x/y) &\leq 1+2\sum_{m=1}^{+\infty} e^{-\pi\alpha m^2/y}\cosh(\pi\alpha m/y)\\ &= 1+\sum_{m=1}^{+\infty}\left[e^{-\pi\alpha m(m-1)/y}+e^{-\pi\alpha m(m+1)/y}\right]\\ &\leq 1+2\sum_{m=1}^{+\infty} e^{-\pi\alpha m(m-1)/y}\\ &\leq 1+2\sum_{m=1}^{+\infty} e^{-\pi\alpha (m-1)^2/y}\\ &= 1+\sum_{m\in\mathbb{Z}} e^{-\pi\alpha m^2/y}.\end{aligned}$$

Now it is clear by (A.2.1) that

$$\max_{\beta}\theta(t;\beta)=\theta(t;0)$$

and it follows, by (A.2.2), that, for any $t>0$ and any β,

$$t^{-1/2}\sum_{m\in\mathbb{Z}} e^{-\pi(m-\beta)^2/t}\leq t^{-1/2}\sum_{m\in\mathbb{Z}} e^{-\pi m^2/t}.$$

Therefore, we have

$$\sum_{m\in\mathbb{Z}} e^{-\pi\alpha(m-nx)^2/y}\leq\sum_{m\in\mathbb{Z}} e^{-\pi\alpha m^2/y}.$$

Since $0\leq x\leq\frac{y}{\sqrt{3}}$ in the domain under consideration, we remark that

$$e^{\pi\alpha(x^2+y^2)/y}\leq e^{4\pi\alpha y/3},$$

and we finally get

$$\frac{2\pi\alpha}{y}\sum_{m,n} n^2 e^{-2\pi\alpha f(m,n)}\leq KR$$

where

$$R=\frac{2}{y}+\frac{2}{y}\left(\sum_{m\in\mathbb{Z}} e^{-\pi\alpha m^2/y}\right)\left(1+\sum_{n=2}^{+\infty} n^2 e^{-\pi\alpha(n^2-4/3)y}\right).$$

Hence we obtain

$$\partial_y^2\theta(\alpha;x,y)+\frac{2}{y}\partial_y\theta(\alpha;x,y)>K(P_1+P_2-R).$$

The sums in R are decreasing functions of α, while P_1 and P_2 are increasing, therefore it is sufficient to prove that $R < P_1 + P_2$ when $\alpha = 1$ in order to have $P_1 + P_2 - R > 0$ for any $\alpha \geq 1$.
Since $y \geq \sqrt{3}/2$ by definition of our domain, we have

$$\sum_{n=2}^{+\infty} n^2 e^{-\pi\alpha(n^2-4/3)y} \leq \sum_{n=2}^{+\infty} n^2 e^{-\pi(n^2-4/3)\sqrt{3}/2} < 0.002826$$

and by (A.2.2), we have

$$\sum_{m\in\mathbb{Z}} e^{-\pi\alpha m^2/y} = \sqrt{y}\sum_{k\in\mathbb{Z}} e^{-\pi k^2 y} \leq \sqrt{y}\sum_{k\in\mathbb{Z}} e^{-\pi k^2\sqrt{3}/2} < 1.1317\sqrt{y}.$$

Thus, we get

$$R \leq \frac{2}{y} + 2.27\sqrt{y} =: S.$$

Now we show that $S < P_1 + P_2$. Since

$$\log P_1 = \log\pi - 4\log y + \frac{\pi x^2}{y} + \pi y - \frac{\pi}{y}$$

and $x^2 \leq 1/4$, we remark that

$$\partial_y \log P_1 = \frac{\partial_y P_1}{P_1} = \frac{-4y - \pi x^2 + \pi y^2 + \pi}{y^2} \geq \frac{\pi y^2 - 4y + 3\pi/4}{y^2} > 0$$

and P_1 is an increasing function of y. Moreover, P_2 is also an increasing function of y, while S is decreasing. Therefore, it is sufficient to consider x and y such that $x^2+y^2 = 1$, that is to say $y = \sqrt{1-x^2}$ because $0 \leq x \leq 1/2$. We remark that, for any $0 \leq x \leq 1/2$,

$$S(x) := \frac{2}{\sqrt{1-x^2}} + \frac{2.27}{(1-x^2)^{1/4}} < \frac{\pi}{(1-x^2)^2} + \pi\left(1 - \frac{x^2}{1-x^2}\right)^2 =: T(x)$$

because, in $[0, 1/2]$, S is an increasing function of x and

$$T(x) = 2\pi\left(1 + \frac{x^4}{(1-x^2)^2}\right)$$

is also increasing such that $S(1/2) \approx 4.75$ and $T(0) = 2\pi$. Furthermore, we have

$$T(x) \leq P_1 + P_2$$

therefore

$$R \leq S < P_1 + P_2$$

for $\alpha = 1$ and the proof is complete. □

Lemma A.4.2. *Suppose that*

$$f'(y) + \frac{2}{y} f(y) > 0$$

for all $y \geq y_0 > 0$ *and that* $f(y_0) \geq 0$. *Then* $f(y) > 0$ *for all* $y > y_0$.

Proof. We remark that, for any $y \geq y_0 > 0$,

$$f'(y) + \frac{2}{y} f(y) > 0 \iff y^2 f'(y) + 2y f(y) > 0 \iff (y^2 f(y))' > 0.$$

Thus $y \mapsto y^2 f(y)$ is strictly increasing on $[y_0, +\infty)$, therefore

$$y^2 f(y) \geq y_0^2 f(y_0)$$

and it follows that

$$f(y) \geq f(y_0) \left(\frac{y_0}{y}\right)^2 \geq 0$$

when $y > y_0$. □

Proof of Lemma A.1.2. By the previous two lemmas, it is sufficient to prove that

$$\partial_y \theta(\alpha; x, y) \geq 0$$

when $x^2 + y^2 = 1$ and $0 \leq x \leq 1/2$ with equality is and only if $x \in \{0, 1/2\}$. Indeed, for $\alpha > 0$ and $0 \leq x \leq 1/2$ fixed, let $f(y) = \partial_y \theta(\alpha; x, y)$, then by Lemma A.4.1, for $y \geq \sqrt{1 - x^2}$,

$$f'(y) + \frac{2}{y} f(y) > 0.$$

Thus, by Lemma A.4.2, if $f(\sqrt{1 - x^2}) \geq 0$ then $f(y) > 0$ for any $y > \sqrt{1 - x^2}$.

Let

$$g(r) = \theta(\alpha; r\cos\phi, r\sin\phi)$$

where $\phi \in (0, \pi)$ is fixed. We remark that

$$g(1/r) = g(r)$$

and it follows that

$$g'(1) = -g'(1) = 0.$$

Thus, we get

$$g'(1) = \partial_x \theta(\alpha; \cos\phi, \sin\phi) \cos\phi + \partial_y \theta(\alpha; \cos\phi, \sin\phi) \sin\phi = 0,$$

therefore

$$\partial_x \theta(\alpha; \cos\phi, \sin\phi)\cos\phi = -\partial_y \theta(\alpha; \cos\phi, \sin\phi)\sin\phi.$$

By Lemma A.1.1, we see that $\partial_x \theta(\alpha; \cos\phi, \sin\phi) \le 0$ when $\pi/3 \le \phi \le \pi/2$ with equality only at endpoints and it follows that $\partial_y \theta(\alpha; \cos\phi, \sin\phi) \ge 0$.

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Résumé

Dans cette thèse, nous étudions des problèmes de minimisation d'énergies discrètes et nous cherchons à comprendre pourquoi une structure périodique peut être un minimiseur pour une énergie d'interaction, c'est ce que l'on appelle un problème de cristallisation. Après avoir montré qu'un réseau de $\mathbb{R}^d$ soumis à un certain potentiel paramétré peut être vu comme un minimum local, nous démontrons des résultats d'optimalité du réseau triangulaire parmi les réseaux de Bravais du plan pour certaines énergies par point, avec ou sans densité fixée. Finalement, nous démontrons, à partir des travaux de Sandier et Serfaty sur les gaz de Coulomb bidimensionnels, la conjecture de Rakhmanov-Saff-Zhou, c'est-à-dire l'existence d'un terme d'ordre n dans le développement asymptotique de l'énergie logarithmique optimale pour n points sur la sphère unité de $\mathbb{R}^3$. De plus, nous montrons l'équivalence entre la conjecture de Brauchart-Hardin-Saff portant sur la valeur de ce terme d'ordre n et celle de Sandier-Serfaty sur l'optimalité du réseau triangulaire pour une énergie coulombienne renormalisée.

Mots clés : Réseaux ; Energies ; Interaction ; Potentiels ; Gaz de Coulomb ; 7ème Problème de Smale.

Abstract

In this thesis, we study minimization problems for discrete energies and we search to understand why a periodic structure can be a minimizer for an interaction energy, that is called a crystallization problem. After showing that a given Bravais lattice of $\mathbb{R}^d$ submitted to some parametrized potential can be viewed as a local minimum, we prove that the triangular lattice is optimal, among Bravais lattices of $\mathbb{R}^2$, for some energies per point, with or without a fixed density. Finally, we prove, from Sandier and Serfaty works about 2D Coulomb gases, Rakhmanov-Saff-Zhou conjecture, that is to say the existence of a term of order n in the asymptotic expansion of the optimal logarithmic energy for n points on the 2-sphere. Furthermore, we show the equivalence between Brauchart-Hardin-Saff conjecture about the value of this term of order n and Sandier-Serfaty conjecture about the optimality of triangular lattice for a coulombian renormalized energy.

Keywords : Lattices ; Energies ; Interaction ; Potentials ; Coulomb gases ; 7th Smale's Problem.