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Crystallization of one-dimensional alternating two-component systems

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Abstract

We investigate one-dimensional periodic chains of alternate type of particles interacting through mirror symmetric potentials. The optimality of the equidistant configuration – also called crystallization – is shown in various settings, at any scale and at high density. In particular, we prove the crystallization at any scale for neutral and non-neutral systems with inverse power laws interactions, including the three-dimensional Coulomb potential. We also prove the crystallization at high density for Lennard-Jones type interactions and ionic screened potentials involving inverse power laws and Yukawa potentials. These high density results are derived from a general sufficient condition based on a convexity argument. Furthermore, we derive a necessary condition for crystallization at high density based on the positivity of the Fourier transform of the interaction potentials sum.

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Keywords: Crystallization; Two-component systems; Convexity; Inverse power laws potentials; Lennard-Jones potentials; Optimisation; Ionic crystals.

1 Introduction

In the theory of crystallization which is concerned with large systems of interacting particles, it has been asked using energy minimization principles why many

systems from materials science exhibit the spontaneous formation of ordered structure and in particular periodic structures (see e.g. [9] for a review). Such periodic structures are observed in systems consisting of identical particles (such as e.g. Coulomb gases, Bose-Einstein Condensates and Ginzburg-Landau vortices), but also appear in models composed of different types of particles. For example in ionic compounds (such as NaCl) periodicity is still commonly observed, even though different attractive and repulsive interaction potentials between the ions are present (see e.g. [44]). Motivated by these observations, we consider prototypical one-dimensional models consisting of different types of particles and investigate necessary and sufficient conditions for the optimality of equidistant configurations.

Systems with different types of particles also arise in other models such as e.g. chains of interacting magnetic dipoles (e.g. [40, 5], see also Fig. 2). Also the interaction of stripe type magnetic domains in thin ferromagnetic films can be described in this setting, where the sign of the interaction energy between two interfaces in this model depends on the number of in-between interfaces so that this model can be viewed as a system of alternating particles of two kinds [33, Theorem 2.2.3]. We also note that while one-dimensional model systems do not occur commonly in nature, they can be created by confinement (see e.g. [39]). We also would like to note that the type of models investigated in this paper might also be interesting for biological models related to swarming and flocking between different species (although in a dynamical, higher dimensional setting, see e.g. [12, 11, 28]). The semi-empirical potentials we consider in this paper are also used in social interactions to study group behaviour, see e.g. [29, 37].

For one-dimensional systems of identical particles, Ventevogel and Nijboer [45, 46, 47] have derived several results about the optimality of the equidistant configuration. In their work, interacting potentials are radially symmetric and correspond to semi-empirical potentials used in molecular simulations (see e.g. [34, p. 624]). In particular, they proved the optimality of the equidistant configuration for convex interaction potentials and Lennard-Jones-type potentials (also called “Mie potentials”) among periodic configurations. A similar result by Radin [19] shows the optimality of an equidistant configuration for the classical (12, 6) Lennard-Jones potential, when the number of points – added alternatively to both sides of the configuration – goes to infinity. Another recent result by Bandegi and Shirokoff [4, Sect. 6.1] gives numerical evidences for the global optimality of the equidistant configuration for some values of the density and the parameters of the Morse potential using convex relaxation. The only crystallization result for several kind of particles was proved by Radin in [36]. Using three different radially symmetric short-range interaction potentials, he proved the minimality of a two-dimensional binary quasiperiodic configuration. Furthermore, one-dimensional systems involving power-laws and two kind of species have been numerically studied in [26] in a

different perspective, changing the species ratio and considering interaction only between species of the same kind. We note that similar studies have been made in dimension two for dipolar (inverse power law) interaction [2] and the Yukawa potential [3]. Periodicity of solutions has also been investigated for other one-dimensional systems e.g. in [31, 48, 38, 25].

For higher dimensional systems, partial progress has been made for special potentials or in restricted settings. In dimension two, the optimality of the triangular lattice has been proved for radially symmetric short-range interaction potentials [22, 35, 17, 27] as well as a long-range perturbation of them [43]. In dimension $d \geq 3$, only few crystallization results are known [41, 16]. Quantum models involving nuclei and electrons have also been studied. Blanc and Le Bris [8] proved the periodicity of the ground state for the one-dimensional Thomas-Fermi-von-Weizsäcker energy. Furthermore, for the two-dimensional Thomas-Fermi model, assuming the periodicity of nuclei's positions, the first author and Zhang [7] proved the optimality of the triangular lattice among Bravais lattices at any scale. We note that a different perspective has been taken by Born in [10] where the optimality of the alternate rock-salt charge configuration is proved for a given one-dimensional lattice configuration; we refer to [6] for a generalization of this result to higher dimensions and to more general interaction potentials. Some related results on pattern formation for the Ohta-Kawasaki energy can e.g. be found in [1, 13, 14, 15, 20, 21, 24].

In the present paper, once the charges are fixed, as well as the interaction between species, we show the optimality of the equidistant configuration at any scale or at high density, among one-dimensional periodic configurations of alternating species in different settings. The novelty of the paper consists in the systematic analysis for the ground state energy of alternating two-particle systems. We assume repulsive interaction at short distances between different species in order to avoid a degeneracy of the ground state. We will also show that in the neutral Coulomb case or in the power-law case, the equidistant configuration is the unique maximum of the real energy (i.e. when charges of different (resp. same) signs attract (resp. repel) each other). We note that the model considered is chosen as a simple prototype model. More general, it would be interesting to derive conditions for periodicity in higher-dimensional systems, to consider systems of more than two different particles or to consider the case of different ratio between the involved species.

2 Setting and statement of main results

We consider one-dimensional alternating chains of particles of two types, located at the positions $x_i \in \mathbb{R}$ for $i \in \mathbb{Z}$ (see Fig. 1). Since we are interested in the case when the interaction energy between different types of particles is attractive, we will assume that the different particles are ordered alternatively. For technical reasons, we also assume that the particles positions are $2N$ periodic for a large number N :

Definition 2.1 (Configurations and energy).

- (i) For $N \in 2\mathbb{N}$ and $\rho > 0$, we denote the class of alternating configurations with density ρ and N points per period by

$$\mathcal{A}_N^\rho = \{X = (x_i)_{i \in \mathbb{Z}} : x_0 = 0, x_i < x_{i+1} \text{ and } x_{i+N} = x_i + \rho^{-1}N \text{ for all } i \in \mathbb{Z}\}.$$

The equidistant configuration $e^\rho \in \mathcal{A}_N^\rho$ is given by $e^\rho := (k\rho)_{k \in \mathbb{Z}}$. It is assumed that the particles of type 1 are located on even positions x_{2j} , $j \in \mathbb{Z}$ while the particles of type 2 are located on odd positions.

- (ii) We assume that particles of type i, j interact by the interaction potentials $f_{ij} : \mathbb{R} \rightarrow \mathbb{R}$ for $i, j \in \{0, 1\}$. The functions f_{ij} are assumed to be mirror symmetric, i.e. $f_{ij}(-x) = f_{ij}(x)$. The associated energy is then denoted by

$$E_{\mathcal{F}}(X) := \frac{1}{N} \sum_{n=1}^N \sum_{\substack{k=-\infty \\ k \neq n}}^{\infty} f_{\epsilon_n \epsilon_k}(x_k - x_n),$$

where $\mathcal{F} = (f_{11}, f_{22}, f_{12})$ and where $\epsilon_i = 1$ if $i \in 2\mathbb{Z} + 1$ and $\epsilon_i = 2$ if $i \in 2\mathbb{Z}$.

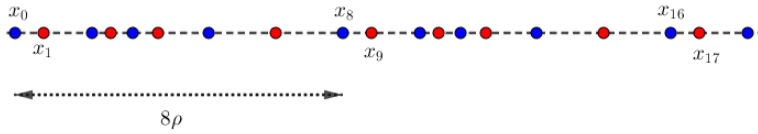


Figure 1: Example of periodic configuration $X \in \mathcal{A}_8^\rho$.

We consider two notions of minimality of the equidistant configuration:

Definition 2.2 (Minimality at any scale or at high density). We say that $X \in \mathcal{A}_N^\rho$ is a minimizer of $E_{\mathcal{F}}$ at any scale if λX is a minimizer on $\mathcal{A}_N^{\rho\lambda}$ for any $\lambda > 0$. We say that $X \in \mathcal{A}_N^\rho$ is a minimizer at high density if there is $\lambda_0 = \lambda_0(\rho, N) > 0$ such that λX is a minimizer on $\mathcal{A}_N^{\rho\lambda}$ for all $\lambda > \lambda_0$.

We start with a necessary condition for the optimality of the equidistant configuration at high density, inspired by Ventevogel and Nijboer's result [47]. We recall that the Fourier transform of a mirror symmetric function $f \in L^1(\mathbb{R})$ in terms of the cosine is given by $\widehat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x) \cos(kx) dx$.

Theorem 2.3 (Necessary condition for high density crystallization). *Suppose that the functions $f_{ij} \in C^2(\mathbb{R}) \cap L^1(\mathbb{R})$ are mirror symmetric and strongly tempered for any $i, j \in \{1, 2\}$, in the sense that there exists $r_0, C, \eta > 0$ such that*

$$|f_{ij}(x)| < C|x|^{-1-\eta} \quad \text{for any } |x| > r_0. \quad (2.1)$$

If e^ρ is a minimizer of $E_{\mathcal{F}}$ at high density for any $N \in 2\mathbb{N}$, then

$$\widehat{f}_{12}(k) + \frac{1}{2}(\widehat{f}_{11}(k) + \widehat{f}_{22}(k)) \geq 0 \quad \text{for all } k \in \mathbb{R}.$$

We notice that the positivity of the Fourier transform of all the potentials is not necessary for the optimality of the equidistant configuration at high density. Note that the notion of strongly tempered potentials has also been used by Sütö [42].

In [45], Ventevogel proved the optimality of e^ρ at any scale when, for any $i \in \{1, 2\}$, $f_{ij} = f$ is a convex function. The following theorem generalizes this result for two kinds of alternating species and three kinds of interactions, and includes also some classes of nonconvex functions:

Theorem 2.4 (Sufficient condition). *Suppose that $f_{ij}(x) = \Phi_{ij}^+(|x|) - \Phi_{ij}^-(|x|)$ where the functions $\Phi_{ij}^\pm : [0, \infty) \rightarrow \mathbb{R}$ are convex and strongly tempered in the sense of (2.1). Moreover, suppose that the function F is convex on $(0, \eta]$ for $\eta \in (0, \infty]$, where*

$$F(r) := 2\Phi_{12}^+(r) - \sum_{k=1}^{\infty} (\Phi_{12}^-((2k-1)r) + \Phi_{22}^-(2kr) + \Phi_{11}^-(2kr)). \quad (2.2)$$

Then the equidistant configuration e^ρ is the unique minimizer of $E_{\mathcal{F}}$ at high density for any $N \in 2\mathbb{N}$, and at any scale for any $N \in 2\mathbb{N}$ if $\eta = \infty$.

As a consequence of Theorem 2.4, the Riesz potentials $f_{11}(x) = f_{22}(x) = -f_{12}(x) = |x|^{-p}$ are minimized by the equidistant configuration for any $p > 1$. The next result improves this result to the case $p \geq p_0$ where $p_0 \approx 0.655$ is the unique solution of

$$\zeta(1 + p_0) + 1 = 2^{1+p_0} \quad \text{in } (0, \infty). \quad (2.3)$$

Theorem 2.5 (Riesz potentials). *Let*

$$f_{12}(x) = -f_{11}(x) = -f_{22}(x) = \frac{1}{|x|^p} \quad \text{for } p \geq p_0,$$

where p_0 is the unique solution of (2.3). Then the equidistant configuration is the unique minimizer of $E_{\mathcal{F}}$ at any scale and for any $N \in 2\mathbb{N}$.

We notice that the alternation of species is the only case where the minimizer is not degenerate. Indeed, if two points of the same kind are adjacent, it is sufficient to merge them in order to get an energy equal to $-\infty$. In order to improve Theorem 2.4 for non-summable potentials, the use of the homogeneity is a key point. In particular, Theorem 2.5 shows the maximality of the alternate equidistant configuration (with charges ± 1), at any scale, for the standard Coulomb energy.

In the following, we present some corollaries of Theorem 2.4 and point to some connections to physical and biological models. The next result is aimed at sums of power type laws (including e.g. the Lennard-Jones potential, but including other situations as well). The results shows how near repulsion at small distance of the interaction potential f_{12} governs the high-density crystallization of binary alternate systems:

Corollary 2.6 (High density crystallization for inverse power laws). *Let $a_2 > 0$, $(a_1, b_1, b_2, c_1, c_2) \in [0, \infty)$, for any $i \in \{1, 2\}$, $p_i, m_i, n_i > 1$, and*

$$f_{12}(x) = \frac{a_2}{|x|^{p_2}} - \frac{a_1}{|x|^{p_1}}, \quad f_{11}(x) = \frac{b_2}{|x|^{m_2}} - \frac{b_1}{|x|^{m_1}}, \quad f_{22}(x) = \frac{c_2}{|x|^{n_2}} - \frac{c_1}{|x|^{n_1}}.$$

Then e^p is the unique minimizer of $E_{\mathcal{F}}$ at high density for any $N \in 2\mathbb{N}$ if one of the following holds:

- (i) $p_2 = \max\{p_1, p_2, m_1, n_1\}$,
- (ii) $p_2 = m_1 = \max\{p_1, p_2, m_1, n_1\}$ and $2a_2p_2(p_2 + 1) > 2^{-m_1}b_1m_1(m_1 + 1)\zeta(m_1)$,
- (iii) $p_2 = n_1 = \max\{p_1, p_2, m_1, n_1\}$ and $2a_2p_2(p_2 + 1) > 2^{-n_1}c_1n_1(n_1 + 1)\zeta(n_1)$.

In the $p_2 = m_1 = n_1 > p_1$ case, the same result can be proved with suitable assumptions on the parameters, as well as for $(a_1, b_1, c_1) \in (-\infty, 0]$. As for Theorem 2.5, we notice that the alternation of species is the only way to have a non-degenerate minimizer, i.e. the minimal energy is not $-\infty$. The same holds if $b_2 = c_2 = 0$. An interesting application of this result is for $f_{12}(x) = \frac{a_2}{|x|^{p_2}} - \frac{a_1}{|x|^{p_1}}$, $p_2 > p_1 > 1$ a Lennard-Jones-type potential (also called ‘‘Mie potentials’’). Then, whatever the interactions between points of the same kind are, the fact that p_2 is the only maximum exponent involved in this system, or a_2 is sufficiently large, ensures the crystallization at high density.

Remark 2.7. The proof of this corollary extends to more general sums of inverse power laws and can also be extended to the case when a convex function g_{ij} is added to each of the interaction potential f_{ij} , as long as g_{ij} is strongly tempered for any $i, j \in \{1, 2\}$ in the sense of (2.1) and $\liminf_{|x| \rightarrow 0} g_{12}(x) > -\infty$ (e.g. for Buckingham potential [34, p. 155]).

We now give a direct application of Theorem 2.4 for systems with alternating charges $1, -\alpha$ and power-law interaction potential, in the integrable case. We can think about two kinds of individuals with “mass” 1 and α interacting via the potentials $x \mapsto \pm|x|^{-p}$. The following result shows that once p is fixed, there exists an interval of α containing $\alpha = 1$ such that the equidistributed configuration is the only minimizer of the energy at any scale. It gives (non-optimal) bounds on α such that this equilibrium is achieved. Another physical motivation are chains of antiparallel dipoles which are common e.g. in the self-assembly of magnetic nanoparticles [40, Fig. 1] and classical models of spin chains [5, Sect. 3] where this regular structure reaches the equilibrium when there is no anisotropy field. Let us consider the following toy model of a chain of dipoles d_n , located at position $(x_n, 0, 0) \in \mathbb{R}^3$ for $n \in \mathbb{Z}$. The dipoles are aligned in direction of the x_2 axis with alternating orientation and with magnitude given by $|d_{2k}| = 1$ and $|d_{2k+1}| = \alpha$ (see Fig. 2). The interaction potentials, up to a positive constant, are then given by $f_{12}(x) = -\alpha|x|^{-3}$, $f_{11}(x) = |x|^{-3}$, $f_{22}(x) = \alpha^2|x|^{-3}$ ([18, Eq. (4.27)]). Hence, the following result gives a condition on α and p such that the equidistant configuration is the only maximum for this system at any scale.

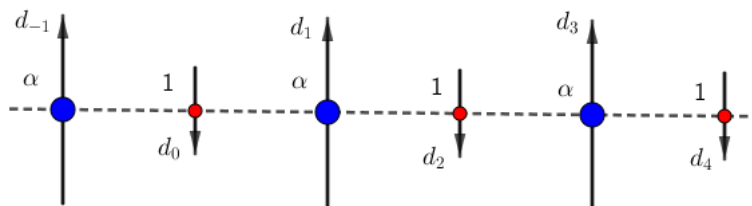


Figure 2: System of alternate oriented dipoles of magnitude 1 and α .

Corollary 2.8 (Crystallization for the inverse power law: the non-neutral case).

Let $f_{12}(x) = \alpha|x|^{-p}$, $f_{11}(x) = -|x|^{-p}$ and $f_{22}(x) = -\alpha^2|x|^{-p}$, for $p > p_1$ where $p_1 \approx 1.46498 > 1$ is the unique solution of $\zeta(p_1) = 2^{p_1}$ and let α be such that

$$\alpha_p < \alpha < \frac{1}{\alpha_p}, \quad \alpha_p := \frac{2^p - \sqrt{4^p - \zeta(p)^2}}{\zeta(p)}. \quad (2.4)$$

Then e^p is the unique minimizer of $E_{\mathcal{F}}$ at any scale and for any $N \in 2\mathbb{N}$.

As in the previous discussed cases, we notice that the alternation of species is the only way to have a non-degenerate minimizer, i.e. the minimal energy is not $-\infty$. We also note that if α is sufficiently large (depending on any fixed p, N) then the equidistributed configuration cannot be a minimizer of $E_{\mathcal{F}}$, the dominant interaction being $f_{22}(x) = -\alpha^2|x|^{-p}$, which forces the particles to be close to each other.

We also note the conceptual connection between this result and recent work by Moser and Seiringer [30] related to the stability, under condition on the mass ratio $m \in [m_2, m_2^{-1}]$, of a systems of two fermions of one species interacting with two fermions of another species via point interactions.

For the interaction of ions, usually it is assumed that the interaction potential is given by $f(x) = ae^{-\alpha|x|} \pm \frac{b}{|x|}$ (see e.g. [34, p. 624] or [23, p. 96]). Obviously, this model is not adapted to the alternate chain of ions of opposite signs because $\lim_{|x| \rightarrow 0} ae^{-\alpha|x|} - \frac{b}{|x|} = -\infty$ (the repulsion at 0 is not strong enough). A good model is to replace the Coulomb potential by the screened Coulomb potential (relevant for ionic crystal, see [34, p. 624]). Then, the following result shows the optimality, at high density, of the equidistant configuration for power-law repulsion at short distance and screened Coulomb tail.

Corollary 2.9 (Ionic interaction). *Let $f_{12}(x) = \frac{a_2}{|x|^p} - \frac{a_1 e^{-\mu|x|}}{|x|}$, $f_{11}(r) = \frac{b_2}{|x|^q} + \frac{b_1 e^{-\mu|x|}}{|x|}$ and $f_{22}(r) = \frac{c_2}{|x|^m} + \frac{c_1 e^{-\mu|x|}}{|x|}$, where for any $i \in \{1, 2\}$ $a_i, b_i, c_i \in (0, +\infty)$, $p > 2$, $(q, m) \in (1, +\infty)^2$ and $\mu > 0$. Then e^ρ is the unique minimizer of $E_{\mathcal{F}}$ at high density for any $N \in 2\mathbb{N}$.*

Remark 2.10. We note that this result can be generalized to sums of Yukawa potentials, i.e. for any $i, j \in \{1, 2\}$ $f_{ij}(x) = \sum_{k=1}^{N_{ij}} a_{ijk} \frac{e^{-\mu_k|x|}}{|x|}$, with suitable assumptions on a_{ijk} and μ_k . Neumann [32] proved that this kind of potential is the most general law under which a set of electric charges can find a stable equilibrium.

3 Proofs

In the following proofs, we use the notation $\ell := \rho^{-1}$.

3.1 Proof of Theorem 2.3

We adapt the proof of [47, Sect. 2] to our case. By assumption, we have, for any N and any $0 < \ell < \ell_0$, $E_{\mathcal{F}}(X) \geq E_{\mathcal{F}}(e^\rho)$ for any $X = (x_i)_{i \in \mathbb{Z}} \in \mathcal{A}_N^\rho$. We choose in particular $x_n := y_n + n\ell - \epsilon$ with $y_n = \epsilon \cos\left(\frac{2\pi mn}{N}\right)$ for some small $\epsilon > 0$ such that $\epsilon < \ell/2$ and for some $m \in \mathbb{Z}$. With this choice, we have $x_0 = 0$ and $x_{i+N} - x_i = N\ell$ and $x_{i+1} - x_i > 0$ for any $i \in \mathbb{Z}$, and hence $X \in \mathcal{A}_N^\rho$. Using Taylor expansion, by minimality of the equidistant configuration we hence get, for ℓ sufficiently small,

$$\sum_{n=1}^N \sum_{j \in \mathbb{Z}}^{\infty} |y_j - y_n|^2 f''_{\epsilon_j \epsilon_n}((j-n)\ell) \geq 0.$$

Hence there is $\ell_1 > 0$ such that for any $\ell \leq \ell_1 \leq \ell_0$ and $g(x) := \frac{1}{2}(f_{11}(x) + f_{22}(x))$,

$$\sum_{j \in \mathbb{Z}} (1 - \cos((2j-1)q)) f_{12}''((2j-1)\ell) + \sum_{j \in \mathbb{Z}} (1 - \cos(2qj)) g''(2j\ell) \geq 0, \quad (3.1)$$

where $q := \frac{2\pi m}{N}$. Since (3.1) holds independently of N , by an approximation argument we also have for any $x \in \mathbb{R}$ and any $0 < \ell \leq \ell_1 \leq \ell_0$,

$$\sum_{j \in \mathbb{Z}} (1 - \cos(2jx - x)) f_{12}''((2j-1)\ell) + \sum_{j \in \mathbb{Z}} (1 - \cos(2jx)) g''(2j\ell) \geq 0. \quad (3.2)$$

Thus, multiplying (3.2) by ℓ , taking $x = \ell k$ and dividing by k^2 , we get

$$\begin{aligned} 0 &\leq \lim_{\ell \rightarrow 0} \left(\ell \sum_{j \in \mathbb{Z}} \frac{(1 - \cos((2j\ell - \ell)k))}{k^2} f_{12}''((2j-1)\ell) + \ell \sum_{j \in \mathbb{Z}} \frac{(1 - \cos(2jk\ell))}{k^2} g''(2j\ell) \right) \\ &= \int_{\mathbb{R}} \frac{1 - \cos((2y-1)k)}{k^2} f_{12}''(2y-1) dy + \int_{\mathbb{R}} \frac{1 - \cos(2yk)}{k^2} g''(2y) dy \\ &= \widehat{f}_{12}(k) + \widehat{g}(k) \quad \text{for all } k \in \mathbb{R} \setminus \{0\}. \end{aligned}$$

3.2 Proof of Theorem 2.4

In this proof, for convenience, we write $\Phi_{ij}^{\pm}(x)$ instead of $\Phi_{ij}(|x|)$. In view of the assumptions of the theorem, for any $X \in \mathcal{A}_N^{\rho}$ we have,

$$\begin{aligned} E_{\mathcal{F}}(X) &= \frac{2}{N} \sum_{n=1}^N \sum_{k=1}^{\infty} \Phi_{12}^+(x_{n+2k-1} - x_n) + \frac{2}{N} \sum_{j=1}^{N/2} \sum_{k=1}^{\infty} \Phi_{22}^+(x_{2j+2k} - x_{2j}) \\ &\quad + \frac{2}{N} \sum_{j=1}^{N/2} \sum_{k=1}^{\infty} \Phi_{11}^+(x_{2j-1+2k} - x_{2j-1}) - \frac{2}{N} \sum_{n=1}^N \sum_{k=1}^{\infty} \Phi_{12}^-(x_{n+2k-1} - x_n) \\ &\quad - \frac{2}{N} \sum_{j=1}^{N/2} \sum_{k=1}^{\infty} \Phi_{22}^-(x_{2j+2k} - x_{2j}) - \frac{2}{N} \sum_{j=1}^{N/2} \sum_{k=1}^{\infty} \Phi_{11}^-(x_{2j-1+2k} - x_{2j-1}) \\ &=: S_1 + S_2 + S_3 - S_4 - S_5 - S_6. \end{aligned}$$

We estimate the six expressions using convexity of the functions and periodicity. By convexity of Φ_{12}^+ and with the notation $d_n := x_{n+1} - x_n$, we have

$$S_1 = \frac{2}{N} \sum_{n=1}^N \Phi_{12}^+(d_n) + 2 \sum_{k=2}^{\infty} \frac{1}{N} \sum_{n=1}^N \Phi_{12}^+(x_{n+2k-1} - x_n)$$

$$\geq \frac{2}{N} \sum_{n=1}^N \Phi_{12}^+(d_n) + 2 \sum_{k=2}^{\infty} \Phi_{12}^+((2k-1)\ell).$$

By convexity of Φ_{22}^+ and Φ_{11}^+ , we furthermore obtain

$$\begin{aligned} S_2 &\geq \sum_{k=1}^{\infty} \Phi_{22}^+ \left(\frac{2}{N} \sum_{j=1}^{N/2} x_{2j+2k} - x_{2j} \right) = \sum_{k=1}^{\infty} \Phi_{22}^+(2k\ell), \\ S_3 &\geq \sum_{k=1}^{\infty} \Phi_{11}^+ \left(\frac{2}{N} \sum_{j=1}^{N/2} x_{2j+2k-1} - x_{2j-1} \right) = \sum_{k=1}^{\infty} \Phi_{11}^+(2k\ell). \end{aligned}$$

For the terms S_4 , S_5 , S_6 with a negative sign, we decompose the distances into nearest-neighbours distances. By convexity of Φ_{12}^- we get

$$S_4 = \frac{2}{N} \sum_{n=1}^N \sum_{k=1}^{\infty} \Phi_{12}^- \left(\sum_{m=1}^{2k+1} d_{n+m-1} \right) \leq \frac{2}{N} \sum_{n=1}^N \sum_{k=1}^{\infty} \Phi_{12}^-((2k-1)d_n).$$

Similarly, by convexity of Φ_{22}^- and Φ_{11}^- , we obtain

$$\begin{aligned} S_5 &= \frac{2}{N} \sum_{j=1}^{N/2} \sum_{k=1}^{\infty} \Phi_{22}^- \left(\sum_{m=1}^{2k} d_{2j+m-1} \right) \leq \frac{2}{N} \sum_{j=1}^{N/2} \sum_{k=1}^{\infty} \frac{1}{2k} \sum_{m=1}^{2k} \Phi_{22}^-(2kd_{2j+m-1}) \\ &\leq \frac{1}{N} \sum_{n=1}^N \sum_{k=1}^{\infty} \Phi_{22}^-(2kd_n), \\ S_6 &= \frac{2}{N} \sum_{j=1}^{N/2} \sum_{k=1}^{\infty} \Phi_{11}^- \left(\sum_{m=1}^{2k} d_{2j+m-2} \right) \leq \frac{1}{N} \sum_{n=1}^N \sum_{k=1}^{\infty} \Phi_{11}^-(2kd_n). \end{aligned}$$

Thus, combining all these inequalities, we have

$$E_{\mathcal{F}}(X) \geq 2 \sum_{k=1}^{\infty} \Phi_{12}^+((2k+1)\ell) + \sum_{k=1}^{\infty} \Phi_{22}^+(2k\ell) + \sum_{k=1}^{\infty} \Phi_{11}^+(2k\ell) + \frac{1}{N} \sum_{n=1}^N F(d_n),$$

where F is given by (2.2). From this formula, it is clear that if F is convex on $(0, \eta]$ with $\eta \in (0, \infty]$, then for any $0 < \ell \leq \ell_0 := \frac{\eta}{N} \in (0, \infty]$, we have $d_n \leq \ell N \leq \eta$ for any $1 \leq n \leq N$. By Jensen's inequality, we hence get

$$E_{\mathcal{F}}(X) \geq 2 \sum_{k=1}^{\infty} \Phi_{12}^+((2k+1)\ell) + \sum_{k=1}^{\infty} \Phi_{22}^+(2k\ell) + \sum_{k=1}^{\infty} \Phi_{11}^+(2k\ell) + F(\ell) = E_{\mathcal{F}}(e^{\rho}),$$

with equality if and only if $X = e^{\rho}$.

3.3 Proof of Theorem 2.5

The main idea is to compare the interaction on distances $|x_i - x_j|$ where $i - j$ is even with interactions of distances where $i - j$ is odd. More precisely, we will use the convex combination

$$x_{n+2k} - x_n = \frac{(2k-j)}{2k} \frac{2k(x_{n+2k} - x_{n+j})}{2k-j} + \frac{j}{2k} \frac{2k(x_{n+j} - x_n)}{j}, \quad (3.3)$$

which holds for all $1 \leq j \leq k$. We set $f(x) := |x|^{-p}$ and use again the notation $d_n := x_{n+1} - x_n$. Inserting (3.3) for $j = 1$ into f and exploiting convexity, we get

$$f(x_{n+2k} - x_n) \leq \frac{2k-1}{2k} f\left(\frac{2k(x_{n+2k} - x_{n+1})}{2k-1}\right) + \frac{1}{2k} f(2kd_n).$$

Since f is homogeneous of degree $-p$, the last line implies

$$f(x_{n+2k} - x_n) \leq \left(\frac{2k-1}{2k}\right)^{1+p} f(x_{n+2k} - x_{n+1}) + \left(\frac{1}{2k}\right)^{1+p} f(d_n). \quad (3.4)$$

Averaging (3.4) over n and using periodicity of X , we get

$$\frac{1}{N} \sum_{n=1}^N f(x_{n+2k} - x_n) \leq \frac{1}{N} \sum_{n=1}^N \left(\left(\frac{2k-1}{2k}\right)^{1+p} f(x_{n+2k-1} - x_n) + \left(\frac{1}{2k}\right)^{1+p} f(d_n) \right),$$

i.e. a bound on the interaction on even distances in terms of the interaction on odd distances. Inserting this estimate into the energy $E_{\mathcal{F}}$ yields the lower bound

$$E_{\mathcal{F}}(X) \geq \frac{2}{N} \sum_{n=1}^N \sum_{k=1}^{\infty} a_k f(x_{n+2k-1} - x_n),$$

where the coefficients a_k are given by

$$a_k := \begin{cases} 1 - \frac{1}{2^{1+p}} - \sum_{j=1}^{\infty} \left(\frac{1}{2j}\right)^{1+p} = 1 - 2^{-(1+p)}(\zeta(1+p) + 1) & \text{for } k = 1, \\ 1 - \left(\frac{2k-1}{2k}\right)^{1+p} & \text{otherwise.} \end{cases}$$

Since $a_1 : p \mapsto 1 - 2^{-(1+p)}(\zeta(1+p) + 1)$ is an increasing function on $(0, \infty)$, p_0 is unique and $p \geq p_0$ implies that $a_k \geq 0$ for all $k \geq 1$. Applying Jensen's inequality and inserting $\frac{1}{N} \sum_{n=1}^N (x_{n+2k-1} - x_n) = (2k-1)\ell$ yields the lower bound

$$E_{\mathcal{F}}(X) \geq 2 \sum_{k=1}^{\infty} a_k f((2k-1)\ell) = E_{\mathcal{F}}(e^\rho),$$

which is strict unless $X = e^\rho$, corresponding to equality in Jensen's inequality.

3.4 Proof of corollaries

Proof of Corollary 2.6. We apply Theorem 2.4. We have

$$F(r) = \frac{2a_2}{r^{p_2}} - \frac{(2^{p_1} - 1)a_1\zeta(p_1)}{2^{p_1}r^{p_1}} - \frac{b_1\zeta(m_1)}{2^{m_1}r^{m_1}} - \frac{c_1\zeta(n_1)}{2^{n_1}r^{n_1}},$$

$$F''(r) = \frac{2a_2p_2(p_2 + 1)}{r^{p_2+2}} - \frac{(2^{p_1} - 1)a_1p_1(p_1 + 1)\zeta(p_1)}{2^{p_1}r^{p_1+2}} - \frac{b_1m_1(m_1 + 1)\zeta(m_1)}{2^{m_1}r^{m_1+2}} - \frac{c_1n_1(n_1 + 1)\zeta(n_1)}{2^{n_1}r^{n_1+2}}.$$

In all three considered cases, $\lim_{r \rightarrow 0} F''(r) > 0$ by direct computation and hence the second point of Theorem 2.4 can be applied. \square

Proof of Corollary 2.8 . We want to apply Theorem 2.4. We have

$$F(r) = \frac{2\alpha}{r^p} - \frac{(\alpha^2 + 1)\zeta(p)}{2^p r^p}, \quad F''(r) = \left(-\frac{\zeta(p)}{2^p} \alpha^2 + 2\alpha - \frac{\zeta(p)}{2^p} \right) \frac{p(p+1)}{r^{p+2}}.$$

The discriminant of the polynomial $P_p(\alpha) := -\frac{\zeta(p)}{2^p} \alpha^2 + 2\alpha - \frac{\zeta(p)}{2^p}$ is $\Delta = 4\left(1 - \frac{\zeta(p)^2}{2^{2p}}\right)$, which is positive if and only if $\zeta(p) < 2^p$, i.e. $p > p_1$, because $p \mapsto 2^p - \zeta(p)$ is an increasing function on $(1, +\infty)$. Then, $P_p(\alpha) > 0$ if and only if α satisfies (2.4), and the proof is completed. \square

Proof of Corollary 2.9. In order to apply Theorem 2.4, we compute

$$F(r) = \frac{2a_2}{r^p} - \frac{a_1}{r} \sum_{k=1}^{\infty} \frac{e^{-\mu(2k-1)r}}{2k-1},$$

$$F''(r) = \frac{2a_2p(p+1)}{r^{p+2}} - a_1 \sum_{k=1}^{\infty} \left(\frac{\mu^2(2k-1)}{r} + \frac{2\mu}{r^2} + \frac{2}{(2k-1)r^3} \right) e^{-\mu(2k-1)r}.$$

Therefore, for the last three terms, using the fact that (respectively), for any $x > 0$, $e^x \geq \frac{x^3}{6}$, $e^x \geq \frac{x^2}{2}$ and $e^x \geq x$, we get

$$F''(r) \geq \frac{2a_2p(p+1)}{r^{p+2}} - \frac{9\zeta(2)a_1}{\mu r^4} = \frac{1}{r^{p+2}} \left(2a_2p(p+1) - \frac{9\zeta(2)a_1}{\mu} r^{p-2} \right),$$

since $\sum_{k=1}^{\infty} \frac{1}{(2k-1)^2} = \zeta(2) - \sum_{k=1}^{\infty} \frac{1}{(2k)^2} = \frac{3}{4}\zeta(2)$. Thus, we have $F''(r) > 0$ for $r^{p-2} < \frac{2a_2p(p+1)\mu}{9\zeta(2)a_1}$. The proof is completed by application of Theorem 2.4. \square

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