CAUCHY–BORN STRAIN ENERGY DENSITY FOR COUPLED INCOMMENSURATE ELASTIC CHAINS

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Abstract. The recent fabrication of weakly interacting incommensurate two-dimensional layer stacks (A. Geim and I. Grigorieva, *Nature* **499** (2013) 419–425) requires an extension of the classical notion of the Cauchy–Born strain energy density since these atomistic systems are typically not periodic. In this paper, we rigorously formulate and analyze a Cauchy–Born strain energy density for weakly interacting incommensurate one-dimensional lattices (chains) as a large body limit and we give error estimates for its approximation by finite samples as well as the popular supercell method.

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INTRODUCTION

Graphene has recently been isolated as a free-standing two-dimensional hexagonal lattice [6]. Its continuum mechanical deformation can be modeled by the classical Cauchy–Born strain energy density [2, 3, 27], which is defined as the atomistic potential energy density of the unit cell for a homogeneously deformed lattice or multilattice [11, 21, 26, 30].

Even more recently, weakly interacting incommensurate two-dimensional lattices such as single layer molybdenum disulfide (MoS_2) on graphene have been fabricated with the potential for improved design of electronic properties [13]. The classical Cauchy–Born rule can be used to link the macroscopic mechanical deformations to atomic displacements in independent monolayers such as graphene since they are multilattices, see *e.g.* [1], but an extension of the classical Cauchy–Born energy density is needed to accurately model the deformation of few layers stackings of weakly interacting incommensurate two-dimensional lattices since these atomistic systems have no periodicity, either due to differences in lattice constants or to a rotation angle between the respective lattices.

The Cauchy–Born strain energy density has been used to coarse-grain the deformation of a lattice away from defects in hybrid atomistic-to-continuum methods [10, 20, 21, 23]. The extension of these hybrid atomistic-to-continuum methods to incommensurate systems introduces the additional errors analyzed in this paper since the incommensurate Cauchy–Born strain energy density must be approximated on supercells.

In this work, we consider some simple one-dimensional toy models as a setting in which to rigorously formulate and analyze a Cauchy–Born strain energy density for weakly interacting incommensurate two-dimensional lattices as a large body limit. In particular, we provide a closed-form expression of the Cauchy–Born strain energy density, as well as a detailed study of the convergence with respect to system size of the energy density of incommensurate system.

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FIGURE 1. Sketch of a system of weakly coupled incommensurate atomic chains.

Our motivation also stems from the study of more realistic problems, where one may not have available an explicit form of the elastic energy components, e.g., when atomic forces are computed using density functional theory [5]. In such cases, the thermodynamic limit can only be numerically investigated, by a sequence of computations on systems with increasing but finite sizes. Due to the high computational cost of increasing the system size, it is then crucial to understand the convergence behavior of such sequences to ensure that such computations provide meaningful results.

We believe some insights can be gained from the study of our simple toy model: we observe that convergence is typically slow (sublinear) and very nonuniform, but a quadratic order of convergence can be obtained when the system size is carefully chosen. We show that optimal choices are the denominators of rational approximations of the irrational (incommensurate) ratio of the lattice spacing of the two weakly interacting chains, obtained by the continued fraction algorithm. We also give error estimates for the popular supercell approximation which is based on approximating an incommensurate multi-layer system by a sequence of periodic configurations [7, 17, 29].

Finally, let us remark that our expression for the Cauchy–Born strain energy density (1.14) could easily be generalized to the case of incommensurate two-dimensional lattices, thanks to their ergodic averaging properties [4]. However, it is highly non-trivial to extend the convergence analysis provided here to two dimensions. Indeed, there is no equivalent to the continued fraction algorithm for matrices. However, a similar role is played by the Moiré pattern which provides a first "good" choice for a periodic approximation, and a possible avenue for further studies.

1. An elementary model

1.1. Finite system

We will study the simple one-dimensional problem presented in Figure 1. We consider two parallel one-dimensional chains of atoms of approximate length $L \ge 1$, characterized by their isolated ground state lattice constants, respectively 1 for chain C^1 and α for chain C^{α} , where α is an irrational real number in (0, 1). The chains are separated by a fixed distance. In each chain, atoms interact *via* a smooth nearest-neighbor atomic potential, respectively, $\psi_1(\Delta s)$ and $\psi_{\alpha}(\Delta s)$ where Δs is the distance between the atoms.

The two chains are also interacting through a long-range smooth pairwise atomic potential, such as the Lennard-Jones or Morse potentials. This potential can be rewritten as $V_{int}(\Delta s)$ where Δs is the abscissa difference between two atoms of each chain along the direction of the chains, not their respective distance.

In general, a displacement of the finite chains is a pair of maps u_1, u_α defined for $0 \le i \le [L]$ and $0 \le j \le [L/\alpha]$, where [·] denotes the closest integer to the real argument. The corresponding deformation of the atomistic chains is given by the real mappings y_1, y_α with $y_1(i) = i + u_1(i)$ and $y_\alpha(j) = \alpha j + u_\alpha(j)$. The energy of a displacement $u = (u_1, u_\alpha)$ can be then written as

$$\mathcal{E}^{a}(u) = \sum_{i=1}^{[L]} \psi_{1} \left(y_{1}(i) - y_{1}(i-1) \right) + \sum_{j=1}^{[L/\alpha]} \psi_{\alpha} \left(y_{\alpha}(j) - y_{\alpha}(j-1) \right) + \sum_{i=0}^{[L]} \sum_{j=0}^{[L/\alpha]} V_{\text{int}} \left(y_{1}(i) - y_{\alpha}(j) \right).$$
(1.1)

For simplicity, we consider a dead load external force applied to the system. Let f_1 and f_{α} be two real mappings defined respectively for $0 \le i \le [L]$ and $0 \le j \le [L/\alpha]$. Then we seek a solution of

$$u \in \operatorname{argmin}\{\mathcal{E}^{a}(u) - \langle f, u \rangle\},\tag{1.2}$$

where $\langle f, u \rangle = \sum_{i=0}^{[L]} f_1(i) u_1(i) - \sum_{i=0}^{[L/\alpha]} f_\alpha(j) u_\alpha(j).$

1.2. Cauchy–Born approximation

Now, we are interested in a coarse-grained model of this system of chains in the thermodynamic limit (at zero temperature) as $L \to \infty$, removing the dependency on the boundary conditions. To approximate the atomistic description, a common strategy is to model the chains using a continuum elasticity model with an energy functional of the form

$$\mathcal{E}^{c}(u) = \int_{\mathbb{R}} W(\nabla u) \mathrm{d}x, \qquad (1.3)$$

where $W: (-1, \infty) \to \mathbb{R}$ is a suitable strain energy function and the displacement u is now defined for $x \in \mathbb{R}$. The problem of elastostatics corresponding to (1.2) for a given load $f: \mathbb{R} \to \mathbb{R}$ would then be given as

$$u \in \operatorname{argmin} \{ \mathcal{E}^c(u) - \langle f, u \rangle \}.$$
(1.4)

The gradient ∇u is usually interpreted as a homogeneous strain applied to the system, and $W(\nabla u)$ is the resulting energy per unit volume corresponding to the atomistic model (1.1) under uniform strain. In the periodic crystal case, a closed-form expression for this averaged energy is usually readily available [3] and the errors introduced by this coarse-graining scheme are well understood [21, 24]. However, in the incommensurate case, it is not clear what this *Cauchy–Born strain energy density function* should be since no unit volume is the same.

Following the Cauchy–Born approach, we now suppose that the atoms in each chain are always equally spaced and the chains deform with a common uniform strain ε , while the left end of the chains is fixed at 0. Atomic positions are then given by:

$$\begin{cases} y_1(i) = (1+\varepsilon)i & \text{for } 0 \le i \le [L] \text{ for atoms in the first chain,} \\ y_\alpha(j) = (1+\varepsilon)\alpha j & \text{for } 0 \le j \le [L/\alpha] \text{ for atoms in the second chain.} \end{cases}$$
(1.5)

A central assumption of this model is that the chains remain pinned together, and hence the ratio of lattice constants remains α . Modeling the strain as uniform is further justified by the fact that intra-chain interactions (modeling covalent bonds) are much stronger than the inter-chain interaction (modeling Van-der-Waals forces), minimizing microstructural relaxation effects driven by discommensuration between the chains. The coupled system can thus be considered as a perturbation of the periodic crystal case, where the Cauchy–Born model is well grounded in rigorous analysis [8, 12, 21]. Thanks to this rigidity assumption, the rescaled potential energy of the coupled system per unit length is given exactly by:

$$\mathcal{E}(\varepsilon;L) = \frac{1}{L} \left([L]\psi_1(1+\varepsilon) + [L/\alpha]\psi_\alpha(\alpha+\varepsilon\alpha) \right) + \frac{1}{L} \sum_{i=0}^{[L]} \sum_{j=0}^{[L/\alpha]} V_{\text{int}} \left((\alpha j - i)(1+\varepsilon) \right).$$
(1.6)

Note that the elastic constant per unit length of the system in the Cauchy–Born approximation can be deduced from (1.6) as

$$\mathcal{K}(\varepsilon_{\rm eq}; L) = \frac{\partial^2 \mathcal{E}}{\partial \varepsilon^2}(\varepsilon_{\rm eq}(L); L), \qquad (1.7)$$

where $\varepsilon_{eq}(L)$ corresponds to a minimum of the function $\mathcal{E}(\varepsilon; L)$, *i.e.*, characterizes a ground state of the coupled system.

1.3. Limit behavior

Let us now study the elastic behavior of the system in the thermodynamic limit $L \to \infty$, and in particular the definition of a length-independent elastic constant as the limit of (1.7). We will assume that the intra-chain potentials $\psi_1(s)$ and $\psi_{\alpha}(s)$ are at least twice continuously differentiable on $\mathbb{R} \setminus \{0\}$ and are bounded as well as their derivatives when s goes to $+\infty$. We will also assume that the long-range potential V_{int} is at least twice continuously differentiable and decays fast enough at infinity: for a given $\eta > 0$,

$$V_{\rm int}(s) = \mathcal{O}\left(\frac{1}{|s|^{1+\eta}}\right), \quad V_{\rm int}'(s) = \mathcal{O}\left(\frac{1}{|s|^{2+\eta}}\right)$$
$$V_{\rm int}''(s) = \mathcal{O}\left(\frac{1}{|s|^{3+\eta}}\right) \text{ as } s \to \pm\infty.$$
(1.8)

Remark 1.1. Note that this forbids us to consider electrostatic interactions.

We will further assume that our potentials include a short-range repulsion component, that is $\psi_1(s)$ and $\psi_{\alpha}(s)$ blow up as $s \to 0$, *i.e.*, for some $s_0 > 0$,

$$\forall s \in (-s_0, s_0), \quad \psi_1(s), \psi_\alpha(\alpha s) \ge \frac{2}{|s|} \int_{\mathbb{R}} |V_{\text{int}}(t)| \mathrm{d}t.$$

$$(1.9)$$

Note that in most practical cases the repulsion is in fact much stronger at short distances. For example, in the commonly used Lennard-Jones potential the repulsive part grows as $(\sigma/s)^{12}$ when $s \to 0$, where σ is a typical distance and s the distance between atoms.

This technical assumption allows us to avoid situations where $\varepsilon_{eq}(L) \to -1$, *i.e.*, the chains collapse. This is shown by the following result which we prove in Appendix A.

Lemma 1.2. If (1.8) and (1.9) are satisfied, there exists $\varepsilon_{\min} > -1$ such that:

$$\forall L \ge 2, \quad \varepsilon_{\min} \le \varepsilon_{eq}(L),$$
(1.10)

where $\varepsilon_{eq}(L)$ is any minimizer of $\mathcal{E}(\varepsilon, L)$ defined by (1.6).

Remark 1.3. We could also easily study, *e.g.*, convex intra-chain potentials that blow up as s goes to $+\infty$. In this case, the minima $\varepsilon_{eq}(L)$ would remain bounded in some interval $[\varepsilon_{\min}, \varepsilon_{\max}]$. The estimates and convergence analysis that follow would then apply in this compact interval.

Now, due to Lemma 1.2, we can restrict our attention to those values of ε which belong to $[\varepsilon_{\min}, \infty)$. Thanks to (1.8), the absolutely convergent series

$$V_{\text{per}}: (s,\varepsilon) \mapsto \sum_{i=-\infty}^{\infty} V_{\text{int}} \left((s-i)(1+\varepsilon) \right), \tag{1.11}$$

defines a smooth function $V_{\text{per}} \in C^2(\mathbb{R} \times [\varepsilon_{\min}, \infty))$ which is 1-periodic in the *s* variable. We then consider the approximate periodized energy per unit length

$$\widetilde{\mathcal{E}}(\varepsilon;L) = \psi_1(1+\varepsilon) + \alpha^{-1}\psi_\alpha(\alpha+\varepsilon\alpha) + \alpha^{-1}\frac{1}{[L/\alpha]+1}\sum_{j=0}^{[L/\alpha]} V_{\text{per}}\left(\{\alpha j\},\varepsilon\right),\tag{1.12}$$

where $\{\cdot\}$ denotes the fractional part of a real number. The following lemma, which we also prove in Appendix A, shows that (1.12) defines a good approximation to the exact energy, with an error essentially due to the boundary.

Lemma 1.4. If (1.8) holds, there exists C > 0 independent of L and ε such that for $\varepsilon > \varepsilon_{\min}$ and $n \in \{0, 1, 2\}$:

$$\left| \frac{\partial^{n} \widetilde{\mathcal{E}}}{\partial \varepsilon^{n}}(\varepsilon; L) - \frac{\partial^{n} \mathcal{E}}{\partial \varepsilon^{n}}(\varepsilon; L) \right| < \begin{cases} C/L^{\eta} & \text{if } 0 < \eta < 1, \\ C \ln(L)/L & \text{if } \eta = 1, \\ C/L & \text{if } \eta > 1. \end{cases}$$
(1.13)

As a consequence, the difference between the two energies $\widetilde{\mathcal{E}} - \mathcal{E}$ converges to zero in $C^2([\varepsilon_{\min}, \infty))$ as $L \to \infty$. Therefore, it suffices to study the limit behavior of $\widetilde{\mathcal{E}}$ to determine the averaged elastic properties of the coupled system of chains in the limit $L \to \infty$. It is well-known [19] that the sequence $\{\alpha j\}_{j \in \mathbb{N}}$ is equidistributed in [0, 1) for irrational α . This suffices to proves the following proposition.

Proposition 1.5 (Pointwise convergence of elastic energies). Let

$$\mathcal{E}^{\infty}(\varepsilon) = \psi_1(1+\varepsilon) + \alpha^{-1}\psi_{\alpha}(\alpha+\varepsilon\alpha) + \alpha^{-1}\int_0^1 V_{\text{per}}(s,\varepsilon)\,\mathrm{d}s.$$
(1.14)

Then, for all $\varepsilon \geq \varepsilon_{\min}$, $n \in \{0, 1, 2\}$,

$$\lim_{L \to \infty} \frac{\partial^n \mathcal{E}}{\partial \varepsilon^n}(\varepsilon; L) = \lim_{L \to \infty} \frac{\partial^n \widetilde{\mathcal{E}}}{\partial \varepsilon^n}(\varepsilon; L) = \frac{\partial^n \mathcal{E}^\infty}{\partial \varepsilon^n}(\varepsilon).$$
(1.15)

The energy functional $\mathcal{E}^{\infty}(\varepsilon)$ can thus be considered as the Cauchy–Born elastic energy density of the coupled system of chains, relating the strain ε to the potential energy of the system.

2. Convergence analysis

The pointwise convergence result obtained in Proposition 1.5 is not enough to ensure neither the uniform convergence of the energy functionals \mathcal{E} and $\tilde{\mathcal{E}}$, nor the convergence of their minimizers (Γ -convergence). To prove these statements, and to obtain more precise error estimates useful, *e.g.*, for the numerical computation of the quantities of interest at the macroscopic level, we wish to understand in particular the convergence behavior of the Birkhoff sum appearing in (1.12):

$$\frac{1}{N}\sum_{j=0}^{N-1} V_{\text{per}}\left(\{\alpha j\},\varepsilon\right).$$

To do so, we need some results from discrepancy theory which we recall in the following.

2.1. Notations

We will denote by \mathbb{Z} , \mathbb{Q} , and \mathbb{R} respectively the sets of integers, rational, and real numbers. The unit circle \mathbb{T} is defined as the quotient \mathbb{R}/\mathbb{Z} , which can be identified with the interval [0, 1] with periodic boundary conditions. For r a positive integer, we introduce the set C^r of r-times continuously differentiable functions on \mathbb{T} , and we denote the associated norm $\|\cdot\|_{C^r}$ with

$$\|\phi\|_{C^r} = \sum_{k=0}^r \sup_{x \in \mathbb{T}} |\phi^{(k)}(x)| \text{ for } \phi \in C^r.$$

For $s \ge 0$, we denote by H^s the Sobolev space of periodic functions on \mathbb{T} equipped with the norm

$$\|\phi\|^2_{H^s} = |\widehat{\phi}(0)|^2 + \sum_{k \in \mathbb{Z} \setminus \{0\}} |k|^{2s} |\widehat{\phi}(k)|^2 \quad \text{for } \phi \in H^s,$$

where $\widehat{\phi}$ is the Fourier coefficients series of ϕ , with the special case of square-integrable functions $L^2 = H^0$. Finally, the total variation of a function $\phi : \mathbb{T} \to \mathbb{R}$ is the (possibly infinite) positive number

$$\|\phi\|_{\mathrm{TV}} = \sup_{p \ge 1, \ 0 < x_1 < \dots < x_p < 1} \left(|\phi(x_1) - \phi(0)| + \sum_{j=2}^p |\phi(x_j) - \phi(x_{j-1})| + |\phi(1) - \phi(x_p)| \right)$$

The function ϕ is said to be of *bounded variation* if $\|\phi\|_{TV} < \infty$.

2.2. A primer on discrepancy and Birkhoff sums

Let $\omega = (x_n)_{n \ge 1}$ be a given sequence of real numbers in the interval [0, 1]. For a positive integer N and a subset E of [0, 1], let the counting function $A(E; N; \omega)$ be defined as the number of terms x_n for $1 \le n \le N$ for which $\{x_n\} \in E$. Where no confusion is possible, we write A(E; N) instead of $A(E; N; \omega)$.

Definition 2.1 (Discrepancy). Let x_1, \ldots, x_N be a finite sequence of real numbers in the interval [0, 1]. The number

$$D_N = D_N(x_1, \dots, x_N) = \sup_{0 \le \alpha < \beta \le 1} \left| \frac{A([\alpha, \beta); N)}{N} - (\beta - \alpha) \right|,$$
(2.1)

is called the discrepancy of the given sequence. For an infinite sequence ω of real numbers, or for a finite sequence containing at least N terms, the discrepancy $D_N(\omega)$ is meant to be the discrepancy of the initial segment formed by the first N terms of ω .

An alternate definition is given by

Definition 2.2. For a finite sequence of real numbers x_1, \ldots, x_N in [0, 1], we define

$$D_N^* = D_N^*(x_1, \dots, x_N) = \sup_{0 < \alpha \le 1} \left| \frac{A([0, \alpha); N)}{N} - \alpha \right|.$$
 (2.2)

This definition is extended as the previous one to infinite sequences. The discrepancies D_N and D_N^* are related by the following inequality, see [19]:

$$D_N^* \le D_N \le 2D_N^*. \tag{2.3}$$

Theorem 2.3 (Koksma's inequality, Theorem 5.1 in [19], p. 143). Let ϕ be a function on [0,1] of bounded variation $\|\phi\|_{TV}$, and suppose we are given N points x_1, \ldots, x_N in [0,1] with discrepancy D_N^* . Then,

$$\left| \frac{1}{N} \sum_{i=1}^{N} \phi(x_i) - \int_0^1 \phi(x) \mathrm{d}x \right| \le \|\phi\|_{\mathrm{TV}} D_N^*.$$
(2.4)

In general, the discrepancy of the sequence generated by iterating an irrational rotation, $x_i = \{i\alpha\} \in \mathbb{T}$ with $\alpha \in \mathbb{R} \setminus \mathbb{Q}$, goes to zero as N goes to infinity thanks to the ergodic theorem. However the order of convergence could be arbitrarily low and depends in general strongly on the number theoretical properties of α . A more precise estimate of the order of convergence can be deduced in an average sense from the following result owing to Kesten [16]:

Theorem 2.4. Let $D_N(\alpha)$ be the discrepancy of the sequence $(\{j\alpha\})_{0 \le j < N} \subset \mathbb{T}$ for $\alpha \in [0,1]$, $N \in \mathbb{N}$. Then:

$$\frac{N \cdot D_N(\alpha)}{\log N \cdot \log \log N} \to \frac{2}{\pi^2} \quad in \ measure \ on \ [0,1] \ as \ N \to \infty.$$
(2.5)

To obtain pointwise estimates, *e.g.*, to bound the error in numerical computations, it is necessary to choose carefully N, the number of atoms in our model. We say that p/q is a rational approximation of a real number α if $p \in \mathbb{Z}$, $q \in \mathbb{N}$ are mutually prime and

$$\left|\alpha - \frac{p}{q}\right| < \frac{1}{q^2}.\tag{2.6}$$

For irrational α , an infinite number of such rational approximations exist and they can be obtained as the convergents from its continued fraction expansion, see *e.g.* [14], p. 61.

Here, we wish to investigate the convergence of series of the type given by the last term in our approximate periodized energy given by (1.12). We are thus led to consider sequences of points that are obtained by iterating a rigid rotation of the circle \mathbb{T} , which is given by the map $R_{\alpha} : \mathbb{T} \mapsto \mathbb{T}, x \to x + \alpha$. Such a rotation is said to have rotation number $\rho(R_{\alpha}) = \alpha$. Equispaced sequences of points are then obtained as iterates of R_{α} , *i.e.*,

$$x_0 + j\alpha = \overbrace{R_\alpha \circ \cdots \circ R_\alpha}^{j \text{ times}} (x_0) = R_\alpha^j(x_0),$$

where the exponent j denotes the number of iterates of the map R_{α} .

Such rotations are particular instances of orientation-preserving homeomorphisms of the circle. These are maps $f : \mathbb{T} \to \mathbb{T}$ that can be lifted onto a homeomorphism of the real line $F : \mathbb{R} \to \mathbb{R}$ such that F(x+1) = F(x) + 1 and $\{F(x)\} = f(\{x\})$ for $x \in \mathbb{R}$. Its rotation number is defined as the limit $\rho(f) = \lim_{j \to \infty} F^j(x)/j$, which can be shown not to depend on the choice of F or $x \in \mathbb{R}$.

Theorem 2.5 (Denjoy–Koksma inequality, Theorem 3.1 in [14], p. 73). Let f be an orientation-preserving homeomorphism of \mathbb{T} with rotation number $\rho(f) = \alpha \in \mathbb{R} \setminus \mathbb{Q}$, and p/q a rational approximation of α in the sense of (2.6). Let $\phi : \mathbb{T} \to \mathbb{R}$ be a function with bounded variation $\|\phi\|_{\mathrm{TV}}$, not necessarily continuous, and let μ be a probability measure on \mathbb{T} invariant by f (i.e., $f_*\mu = \mu$). Then, for all $x_0 \in \mathbb{T}$, we have:

$$\left|\sum_{j=0}^{q-1} \phi \circ f^{j}(x_{0}) - q \int_{0}^{1} \phi \mathrm{d}\mu\right| \le \|\phi\|_{\mathrm{TV}}.$$
(2.7)

This classical result also allows to tackle the general case of homeomorphisms of the circle which are not necessarily rigid rotations, a situation which appears in relaxed configurations as we study in a second paper [7].

Remark 2.6. A typical example of nonuniform homeomorphism is given by the modulated circle map $F : \mathbb{R} \to \mathbb{R}$, $x \mapsto x + \Omega - \frac{K}{2\pi} \sin(2\pi x)$, where Ω is the driving phase and $0 \le K < 1$ a coupling strength. For K = 0, this map reduces to the standard rigid rotation with rotation number Ω .

Remark 2.7. The Denjoy–Koksma inequality implies in particular uniqueness of an invariant probability measure for a given orientation-preserving homeomorphism of \mathbb{T} with irrational rotation number.

In fact, an improved result is obtained for continuous functions, if we restrict ourselves to the situation of a rigid rotation, for which the only invariant measure is the usual Lebesgue or Haar measure dx on \mathbb{T} :

Proposition 2.8 (Proposition 4.8 in [14], p. 189). Let R_{α} be an irrational rotation of \mathbb{T} , and $\frac{p_n}{q_n}$ the sequence of rational approximations of α obtained from its continued fraction expansion. Then if $\phi : \mathbb{T} \mapsto \mathbb{R}$ is an absolutely continuous function, we have

$$\left\|\sum_{j=0}^{q_n-1}\phi \circ R^j_\alpha - q_n \int_0^1 \phi \mathrm{d}x\right\|_\infty \to 0 \quad as \ n \to \infty.$$
(2.8)

The convergence in (2.8) could be arbitrary slow. To improve on this result, we need to introduce a Diophantine condition on α to control the so-called small divisors. We say that an irrational number $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ is of Diophantine type (K, σ) , where K > 0 and $\sigma \ge 0$, when we have for every $k \in \mathbb{Z} \setminus \{0\}$:

$$\inf_{p \in \mathbb{Z}} |k\alpha - p| \ge \frac{K}{|k|^{1+\sigma}}.$$
(2.9)

Note that the set of Diophantine numbers is of full Lebesgue measure in \mathbb{R} . On the other hand, the set of numbers of Diophantine constant type ($\sigma = 0$) is dense, but of measure zero. For ϕ regular enough we can improve on (2.8) and provide an explicit uniform order of convergence. We begin by proving a sharp result where the convergence is measured in a weak sense.

Theorem 2.9. Let R_{α} be an irrational rotation of \mathbb{T} with α of Diophantine type (K, σ) . Let $\phi : \mathbb{T} \mapsto \mathbb{R}$ be of class H^r where $r \geq \sigma + 1$. Then, there exists a function ψ in $H^{r-\sigma-1}$ which solves the linear homological equation

$$\psi \circ R_{\alpha} - \psi = \phi - \int_{0}^{1} \phi dx, \quad with \|\psi\|_{H^{r-\sigma-1}} \le \frac{1}{4K} \|\phi\|_{H^{r}}.$$
(2.10)

For any integer $n \ge 1$, we have the uniform bound on the Birkhoff sums:

$$\left\| \frac{1}{n} \sum_{j=0}^{n-1} \phi \circ R_{\alpha}^{j} - \int_{0}^{1} \phi \mathrm{d}x \right\|_{H^{r-\sigma-1}} \le \frac{1}{2Kn} \|\phi\|_{H^{r}}.$$
(2.11)

Furthermore, if $\frac{p}{q}$ is a rational approximation of α in the sense (2.6) then

$$\left\| \frac{1}{q} \sum_{j=0}^{q-1} \phi \circ R_{\alpha}^{j} - \int_{0}^{1} \phi \mathrm{d}x \right\|_{L^{2}} \leq \frac{\pi}{2Kq^{1+\theta}} \|\phi\|_{H^{r}},$$
(2.12)

where $\theta = \min(1, r - \sigma - 1)$.

Theorem 2.9 is proved in Appendix A. We then obtain as a corollary the following strong result:

Corollary 2.10. Let R_{α} be an irrational rotation of \mathbb{T} with α of Diophantine type (K, σ) . Let $\phi : \mathbb{T} \mapsto \mathbb{R}$ be of class H^r where $r > \sigma + 5/2$. Then, for any integer $n \ge 1$, we have the uniform bound on the Birkhoff sums:

$$\left\| \frac{1}{n} \sum_{j=0}^{n-1} \phi \circ R_{\alpha}^{j} - \int_{0}^{1} \phi \mathrm{d}x \right\|_{C^{1}} \leq \frac{2C}{Kn} \|\phi\|_{H^{r}}.$$
(2.13)

Furthermore, if $\frac{p}{q}$ is a rational approximation of α in the sense (2.6) then

$$\left\| \frac{1}{q} \sum_{j=0}^{q-1} \phi \circ R_{\alpha}^{j} - \int_{0}^{1} \phi \mathrm{d}x \right\|_{C^{0}} \le \frac{C}{Kq^{2}} \|\phi\|_{H^{r}},$$
(2.14)

where C is a universal constant.

Remark 2.11. The bounds (2.13) are not the sharpest which can be obtained in the Hölder scale of strong derivatives. The loss of regularity can be shown to be at most $1 + \sigma$, rather than the $3/2 + \sigma$ suggested by (2.13), for functions of Hölder class C^r with $r > \sigma + 1$, $r - \sigma - 1 \notin \mathbb{Z}$. The proof of such Hölder regularity estimates is however much more technical, using Littlewood–Paley decomposition and Hadamard interpolation inequalities, see *e.g.* Theorem 3.8.1, page 164 in [15] for the case of constant type numbers, $\sigma = 0$.

Proof. Let $\phi : \mathbb{T} \to \mathbb{R}$ be of class H^r where $r > 5/2 + \sigma$. Thanks to Theorem 2.9 and to the Sobolev embedding $H^s \to C^1$ for s > 3/2, there exists a universal constant C > 0 and a function ψ of class C^1 solving the homological equation:

$$\psi \circ R_{\alpha} - \psi = \phi - \int_0^1 \phi \mathrm{d}x, \quad \text{with } \|\psi\|_{C^1} \le \frac{C}{K} \|\phi\|_{H^r}$$

Now, for $x_0 \in \mathbb{T}$ and $n \ge 1$ the Birkhoff sum in (2.13) can be computed as a telescopic sum,

$$\sum_{j=0}^{n-1} \phi \circ R_{\alpha}^{j}(x_{0}) - n \int_{0}^{1} \phi \mathrm{d}x = \psi(x_{0} + n\alpha) - \psi(x_{0}),$$

and the bound (2.13) follows by the triangular inequality. Next, since we know that $|q\alpha - p| < 1/q$ for $\frac{p}{q}$ a rational approximation of α , we obtain directly

$$\left\|\sum_{j=0}^{q-1} \phi \circ R_{\alpha}^{j} - q \int_{0}^{1} \phi \mathrm{d}x\right\|_{C^{0}} = \left\|\psi(\cdot + q\alpha - p) - \psi(\cdot)\right\|_{C^{0}} \le \frac{1}{q} \left\|\psi'\right\|_{C^{0}} \le \frac{C}{Kq} \left\|\phi\right\|_{H^{r}},$$

and we have proved (2.14).

We present in Figure 2 a graphical representation of the behavior of Birkhoff sums for α chosen as the golden mean $\frac{\sqrt{5}-1}{2}$, which is of Diophantine constant type (1/2, 0). For the purpose of illustration, we make the following particular choice of functions ϕ_r where r > 0 is a parameter controlling the regularity of ϕ_r , and we



FIGURE 2. Convergence behavior of the Birkhoff sums for two choices of ϕ (see text) and α chosen as the golden mean. In each case, we plot on the top the function ϕ on [0, 1]. In the middle, we plot the solution ψ to the homological equation. On the bottom is the log-plot for the deviation of the Birkhoff sums, measured in the L^{∞} or L^2 norms and for general n or values n = q satisfying (2.6), as well as the theoretical upper bound (2.13).

introduce the deviation $\Delta_n \phi_r$ of the Birkhoff sums to the mean:

$$\phi_r(x) = \sum_{n=1}^{\infty} \frac{(-1)^n}{q_n^r} \cos(2\pi q_n x), \quad \Delta_n \phi_r(x) = \frac{1}{n} \sum_{j=0}^{n-1} \phi_r(x+j\alpha) - \int_0^1 \phi_r \mathrm{d}\mu,$$

where the $\{q_n\}_{n\geq 1}$ are the denominators of rational approximations of α obtained by the continued fraction algorithm, which is well-known to form the Fibonacci sequence. Such functions ϕ_r belong to $H^{r-\varepsilon}$ for any $\varepsilon > 0$ since the Fibonacci sequence $\{q_n\}_{n\geq 1}$ grows exponentially fast, and we present numerical results for two cases:

- First, a rough potential given by the choice $r = \frac{3}{2}$. The loss of regularity induced by solving the homological equation (2.10) is clear in the comparison of the respective plots of $\phi_{3/2}$ and $\psi_{3/2}$. In this case, the theoretical order of convergence of the deviation $\Delta_q \phi_r$ to zero computed by (2.12) is almost $\frac{3}{2}$, as verified by the numerical results in Figure 2a.
- Second, a smoother potential given by the choice $r = \frac{5}{2}$. The theoretical quadratic order of convergence is also in excellent agreement with the numerical data in Figure 2b.

These results confirm that the weak Denjoy–Koksma inequality (2.12) is a sharp bound on the effective convergence order, while the uniform result (2.14) is not as precise, as discussed in Remark 2.11. In all cases, we observe that the behavior for general N appears chaotic with oscillations spanning several orders of magnitude.

2.3. Error estimates

Using these results, it is straightforward to obtain formulas for the averaged properties of the double chain model from Section 1 and study the order of convergence.

First, thanks to Koskma's inequality (2.4) and the fact that the discrepancy of the sequence $\{\alpha j\}_{0 \le j \le [\alpha^{-1}L]}$ goes to zero as $L \to \infty$, we obtain immediately the uniform convergence of the elastic energies defined in (1.6), (1.12) and (1.14):

Theorem 2.12. Under assumptions (1.8) and (1.9), we have:

$$\begin{cases} \mathcal{E}(\varepsilon; L) \to \mathcal{E}^{\infty}(\varepsilon) \\ \widetilde{\mathcal{E}}(\varepsilon; L) \to \mathcal{E}^{\infty}(\varepsilon) \end{cases} \text{ as } L \to \infty, \text{ in } C^{1}([\varepsilon_{\min}, \infty)). \end{cases}$$
(2.15)

Remark 2.13. Note that the order of convergence in (2.15) could be arbitrarily slow.

Proof. To show (2.15), we need only show that $\|V_{\text{per}}(\cdot,\varepsilon)\|_{\text{TV}}$ and $\|\frac{\partial}{\partial\varepsilon}V_{\text{per}}(\cdot,\varepsilon)\|_{\text{TV}}$ in [0,1] are bounded for $\varepsilon \geq \varepsilon_{\min}$. Then Koskma's inequality (2.4) is sufficient to finish the proof.

Now, from (1.11) we deduce:

$$\begin{split} \|V_{\text{per}}(\cdot,\varepsilon)\|_{\text{TV}} &= \int_0^1 \left|\frac{\partial}{\partial s} V_{\text{per}}(s,\varepsilon)\right| \mathrm{d}s\\ &\leq \int_0^1 \sum_{i\in\mathbb{Z}} \left|(1+\varepsilon)V_{\text{int}}'((s-i)(1+\varepsilon))\right| \mathrm{d}s. \end{split}$$

By a change of variables, this leads to

$$\|V_{\text{per}}(\cdot,\varepsilon)\|_{\text{TV}} \le \int_{\mathbb{R}} |V_{\text{int}}'(s)| \,\mathrm{d}s.$$
(2.16)

Note that $\|V_{\text{int}}\|_{\text{TV}} = \int_{\mathbb{R}} |V'_{\text{int}}(s)| \, ds$ is finite because of the bounds (1.8). Hence $\|V_{\text{per}}(\cdot,\varepsilon)\|_{\text{TV}}$ is uniformly bounded. Similarly,

$$\begin{split} \left\| \frac{\partial}{\partial \varepsilon} V_{\text{per}}(\cdot, \varepsilon) \right\|_{\text{TV}} &= \int_0^1 \left| \frac{\partial^2}{\partial s \partial \varepsilon} V_{\text{per}}(s, \varepsilon) \right| \, \mathrm{d}s \\ &\leq \int_0^1 \sum_{i \in \mathbb{Z}} \left| (1 + \varepsilon)(s - i) V_{\text{int}}''((s - i)(1 + \varepsilon)) \right| + \sum_{i \in \mathbb{Z}} \left| V_{\text{int}}'((s - i)(1 + \varepsilon)) \right| \, \mathrm{d}s \\ &\leq \frac{1}{1 + \varepsilon} \left(\int_{\mathbb{R}} \left| s V_{\text{int}}''(s) \right| \, \mathrm{d}s + \int_{\mathbb{R}} \left| V_{\text{int}}'(s) \right| \, \mathrm{d}s \right). \end{split}$$

Because of the bounds (1.8), $\int_{\mathbb{R}} |sV''_{int}(s)| ds$ is finite, and this concludes the proof.

Corollary 2.14. The sequence of energy functionals $\varepsilon \mapsto \widetilde{\mathcal{E}}(\varepsilon; L)$ Γ -converges to \mathcal{E}^{∞} as $L \to \infty$. In particular, any converging sequence of minimizers $\widetilde{\varepsilon_{eq}}(L)$ of $\mathcal{E}(\cdot; L)$ converges to a minimizer $\varepsilon_{eq}^{\infty}$ of \mathcal{E}^{∞} , and the associated elastic constants converge:

$$\widetilde{\mathcal{K}}(\widetilde{\varepsilon_{\mathrm{eq}}};L) = \frac{\partial^2 \widetilde{\mathcal{E}}}{\partial \varepsilon^2} (\widetilde{\varepsilon_{\mathrm{eq}}}(L);L) \to \mathcal{K}^{\infty}(\varepsilon_{\mathrm{eq}}^{\infty}) = \frac{\partial^2 \mathcal{E}^{\infty}}{\partial \varepsilon^2} (\varepsilon_{\mathrm{eq}}^{\infty}).$$
(2.17)

Remark 2.15. The same results hold also for $\mathcal{E}(\varepsilon; L)$, an associated converging sequence of minimizers $\varepsilon_{eq}(L)$ and the associated elastic constants $\mathcal{K}(\varepsilon_{eq}; L)$ thanks to (2.15).

Remark 2.16. In particular, if the Cauchy–Born energy density $\mathcal{E}_{eq}^{\infty}$ has a unique minimizer at $\varepsilon_{eq}^{\infty} \in (\varepsilon_{\min}, \infty)$ and the minimizers of $\varepsilon \mapsto \mathcal{E}(\cdot; L)$ belong to a bounded set $(\varepsilon_{\min}, \varepsilon_{\max})$ independently of L, then any sequence of minimizers converges to $\varepsilon_{eq}^{\infty}$ and the elastic constants associated with these minimizers also converge to $\mathcal{K}^{\infty}(\varepsilon_{eq}^{\infty})$.

Proof. The uniform convergence of the sequence of functionals $\varepsilon \mapsto \mathcal{E}(\varepsilon; L)$ to the continuous functional \mathcal{E}^{∞} implies its Γ -convergence, see *e.g.* [9]. The Fundamental Theorem of Γ -convergence then implies that the limit of a converging sequence of minimizers $\varepsilon_{eq}(L)$ of $\mathcal{E}(\cdot; L)$ is a minimizer $\varepsilon_{eq}^{\infty}$ of \mathcal{E}^{∞} .

Since $\frac{\partial^2 \tilde{\mathcal{E}}}{\partial \varepsilon^2}$ does not necessarily converge uniformly, we cannot deduce (2.17) directly. By (1.15), we have

$$\lim_{L \to \infty} \frac{\partial^2 \widetilde{\mathcal{E}}}{\partial \varepsilon^2} (\varepsilon_{\text{eq}}^{\infty}; L) = \frac{\partial^2 \mathcal{E}^{\infty}}{\partial \varepsilon^2} (\varepsilon_{\text{eq}}^{\infty}).$$
(2.18)

However, $\frac{\partial^2}{\partial \varepsilon^2} V_{\text{per}}$ is uniformly continuous in a neighborhood of $[0,1] \times \{\varepsilon_{\text{eq}}^{\infty}\}$, so for all $\delta > 0$ there exists $\gamma > 0$ such that if $|\varepsilon_{\text{eq}}(L) - \varepsilon_{\text{eq}}^{\infty}| < \gamma$,

$$\frac{1}{L} \left| \sum_{j=0}^{[L/\alpha]} \frac{\partial^2}{\partial \varepsilon^2} V_{\text{per}} \left(\{ \alpha j \}, \varepsilon_{\text{eq}}^{\infty} \right) - \sum_{j=0}^{[L/\alpha]} \frac{\partial^2}{\partial \varepsilon^2} V_{\text{per}} \left(\{ \alpha j \}, \varepsilon_{\text{eq}}(L) \right) \right| < \delta.$$

Hence, considering (1.12), (2.18) and since $\varepsilon_{eq}(L) \to \varepsilon_{eq}^{\infty}$, there exists $L_{\delta} > 0$ such that

$$L > L_{\delta} \implies \left| \frac{\partial^2 \widetilde{\mathcal{E}}}{\partial \varepsilon^2} (\varepsilon_{\mathrm{eq}}(L); L) - \frac{\partial^2 \mathcal{E}^{\infty}}{\partial \varepsilon^2} (\varepsilon_{\mathrm{eq}}^{\infty}) \right| < 2\delta.$$

This proves (2.17).

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Note that we have obtained in this one-dimensional toy model a closed-form expression (1.14) for the "macroscopic" (limit) energy $\mathcal{E}_{eq}^{\infty}$. In more complex systems, for example in the relaxed configurations we study in the paper [7], such explicit formulae do not exist. It is then necessary to employ numerical simulations, with a finite number of atoms, to determine the macroscopic energy density. When dealing with commensurate systems, this typically leads to solving so-called corrector problems which are set on a unit cell of the commensurate lattice, using periodic boundary conditions. However for incommensurate systems, such unit cells do not exist and the corrector problem, if it is well-posed, is set on the whole space.

Remark 2.17. The same situation arises for example in homogenization of PDEs with periodic vs. quasiperiodic or almost periodic [18], and also stationary random coefficients [25].

It is therefore instructive to study the convergence of the energy density $\widetilde{\mathcal{E}}(\varepsilon; L)$ as $L \to \infty$. By comparing the respective definitions (1.12) and (1.14), we see that this amounts to studying the convergence of the limit

$$\frac{1}{N}\sum_{j=0}^{N-1} V_{\text{per}}\left(\{\alpha j\},\varepsilon\right) \to \int_{0}^{1} V_{\text{per}}\left(s,\varepsilon\right) \mathrm{d}s \quad \text{ as } N \to \infty,$$
(2.19)

where $N = [L/\alpha]$ is the number of atoms in the \mathcal{C}^{α} layer.

Remark 2.18. Note that by studying $\tilde{\mathcal{E}}(\varepsilon; L)$ instead of the exact energy $\mathcal{E}(\varepsilon; L)$, we remove boundary effects limiting the convergence order to linear in L at best, see Lemma 1.4.

Now the left hand term in (2.19) is a Birkhoff sum. The classical results summarized in Section 2.2 enable us to make the following statements:

- From Theorems 2.3 and 2.4, we deduce that the measure of the set of $\alpha \in (0, 1)$ such that, for any $\varepsilon > \varepsilon_{\min}$,

$$\left|\frac{1}{N}\sum_{j=0}^{N-1}V_{\mathrm{per}}\left(\{\alpha j\},\varepsilon\right) - \int_{0}^{1}V_{\mathrm{per}}\left(s,\varepsilon\right)\mathrm{d}s\right| > \frac{2\left\|V_{\mathrm{per}}(\cdot,\varepsilon)\right)\right\|_{\mathrm{TV}}}{\pi^{2}}\frac{\log N \cdot \log\log N}{N},$$

goes to zero as $N \to \infty$. Hence, "on average", we expect to observe almost linear convergence. Still, for a vanishing set of α values the left-hand side could converge arbitrarily slowly.

- A more precise estimate is possible only if α is of Diophantine type (K, σ) and N is chosen as the denominator q of a convergent of α , *i.e.*,

$$\left|\alpha - \frac{p}{q}\right| < \frac{1}{q^2} \text{ for some } p \in \mathbb{Z} \text{ and } \sup_{n \in \mathbb{Z}} |k\alpha - n| \ge \frac{K}{|k|^{1+\sigma}} \text{ for all } k \in \mathbb{Z}.$$

Assuming that $V_{\text{per}}(\cdot, \varepsilon)$ is of class H^r with $r > 5/2 + \sigma$, then by Corollary 2.10, the convergence is quadratic: for all $\varepsilon > \varepsilon_{\min}$,

$$\left|\frac{1}{q}\sum_{j=0}^{q-1}V_{\mathrm{per}}\left(\{\alpha j\},\varepsilon\right)-\int_{0}^{1}V_{\mathrm{per}}\left(s,\varepsilon\right)\mathrm{d}s\right|<\frac{C}{Kq^{2}}\left\|V_{\mathrm{per}}(\cdot,\varepsilon)\right\|_{C^{r}}$$

In each case, the same convergence rate can be obtained for partial derivatives against ε if the corresponding derivative $\frac{\partial^n}{\partial \varepsilon^n} V_{\text{per}}$ is also of class H^r .

We thus obtain rigorous convergence rates for both $\widetilde{\mathcal{E}}(\varepsilon; L)$ and $\frac{\partial}{\partial \varepsilon} \widetilde{\mathcal{E}}(\varepsilon; L)$. Moreover, assuming that

$$\frac{\partial^2 \mathcal{E}^\infty}{\partial \varepsilon^2}(\varepsilon_{\rm eq}^\infty) > 0,$$

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it is readily seen that whenever a sequence of minimizers $\{\varepsilon_{eq}\}_{L>0}$ converges to $\varepsilon_{eq}^{\infty}$, the convergence rate is the same as observed for the energies. Therefore, it is also the case, *e.g.*, for the linearized Cauchy–Born elastic constant around the ground state.

To conclude the analysis of convergence for this toy model, let us point out that the direct computation by simply increasing the number of atoms N achieves a nearly linear order of convergence on average, but a careful choice of the sample size yields a quadratic convergence rate every time. This quite unusual result is a consequence of the incommensurability of the system.

3. Approximation by periodic configurations

Finally, let us construct and analyze a second approximate model based on approximating the incommensurate system by a sequence of periodic configurations. This study is interesting as an elementary example of this very common approach to the computational modeling of incommensurate composites, see e.g. [28]. While everything is explicit in this one-dimensional example, the analysis will be extended in future papers to study the elastic relaxation of incommensurate double chain models.

Let us take a sequence of rational approximants of α , *i.e.*, pairs of mutually prime integers p_n , q_n such that:

$$\frac{p_n}{q_n} \xrightarrow[n \to \infty]{} \alpha$$

We now study the convergence of the energy of configurations where the ratio of the atom spacing in the second chain compared to the first is p_n/q_n instead of α . Interactions between atoms are given by the same potentials ψ_1 , ψ_{α} and V_{int} as before. These new configurations can now be made periodic, such that the period at rest is p_n . Over one period, the first and second chain contain respectively p_n and q_n atoms. Furthermore, the energy per unit length can be written similarly to the previous periodized energy (1.12):

$$\mathcal{E}_n(\varepsilon) = \psi_1(1+\varepsilon) + \frac{q_n}{p_n} \cdot \psi_\alpha \left((1+\varepsilon)\frac{p_n}{q_n} \right) + \frac{q_n}{p_n} \frac{1}{q_n} \sum_{j=0}^{q_n-1} V_{\text{per}}\left(\left\{ j\frac{p_n}{q_n} \right\}, \varepsilon \right).$$
(3.1)

Note that this energy is obtained by averaging over one period. This effectively amounts to taking the limit $L \to \infty$ in this periodic setting. We can further simplify (3.1) by observing that since p_n and q_n are mutually prime, we have equality between discrete sets, up to some reordering:

$$\left(\left\{j\frac{p_n}{q_n}\right\}\right)_{0 \le j < q_n} = \left(\frac{j}{q_n}\right)_{0 \le j < q_n}$$

Therefore,

$$\mathcal{E}_n(\varepsilon) = \psi_1(1+\varepsilon) + \frac{q_n}{p_n} \cdot \psi_\alpha \left((1+\varepsilon) \frac{p_n}{q_n} \right) + \frac{1}{p_n} \sum_{j=0}^{q_n-1} V_{\text{per}} \left(\frac{j}{q_n}, \varepsilon \right).$$
(3.2)

Remark 3.1. By modifying the lattice constant in the second chain, we have obtained a formula which involves only a finite number of atoms. For more complex systems, this allows one to compute easily relaxed configurations or electronic properties. The price for this simplification is that we have introduced some additional, artificial strain in the system.

The following convergence result is proved in Appendix A.

Proposition 3.2. Under assumptions (1.8) and (1.9), we have the error estimate:

$$\left|\mathcal{E}_{n}(\varepsilon) - \mathcal{E}^{\infty}(\varepsilon)\right| \leq C(1+\varepsilon)^{2} \left(\frac{1}{q_{n}^{2}} + \left|\frac{p_{n}}{q_{n}} - \alpha\right|\right).$$

$$(3.3)$$

It is furthermore easy to see that by linearity of the construction, the *i*th derivative of the energy also obeys similar convergence estimates, provided that appropriate bounds furthering the minimal assumption (1.8) on the long-range decay of the derivatives of the inter-layer potential V_{int} are available up to the (i+2)th derivative.

Remark 3.3. Note that, unlike the discrepancy-based estimates constructed for the exact model in Section 2.3, the convergence is always at least linear with no Diophantine conditions on α , under the reasonable assumption $|q_n\alpha - p_n| \leq 1$. The optimal quadratic convergence $\mathcal{O}(1/q_n^2)$ is again recovered for the rational approximations of α .

4. CONCLUSION

In this work, we have studied a Cauchy–Born-type energy density for a coupled system of one-dimensional incommensurate coupled chains. We have shown that it is given by a closed-form formula, equation (1.14), in the thermodynamic limit of infinite system size. This allows to study rigorous estimates of the convergence rate, as a function of either the total length of the system or for periodic approximants to be used in numerical computations.

This study provides a rigorous theoretical foundation for the modeling of incommensurate heterostructures. Work is ongoing on the further development and analysis of more realistic models, including effects such as out-of-plane relaxation of the lattices forming ripples [7], and extension to the two dimensional case to tackle real systems composed of monolayers such as graphene, boron nitride or molybdenum disulfide.

APPENDIX A. PROOFS

In this appendix, we detail the technical proofs of Lemmas 1.2 and 1.4 as well as Theorem 2.9 and Proposition 3.2, which we recall in each case for ease of reading.

Lemma A.1 (Corresponds to Lemma 1.2). If (1.8) and (1.9) are satisfied and $L \ge 2$, there exists $\varepsilon_{\min} > -1$ such that:

$$\varepsilon_{\min} \le \varepsilon_{eq}(L),$$
 (A.1)

where $\varepsilon_{eq}(L)$ is any minimizer of $\mathcal{E}(\varepsilon, L)$ defined by (1.6).

Proof. Since V_{int} is smooth and (1.8) is satisfied, the Riemann sum

$$(1+\varepsilon)\sum_{i\in\mathbb{Z}}|V_{\text{int}}(s-i(1+\varepsilon))|,$$

exists for all $s \in \mathbb{R}$ and converges uniformly to $\int_{\mathbb{R}} |V_{\text{int}}(t)| dt$ as $1 + \varepsilon$ goes to zero. As a consequence, there exists $\varepsilon_0 > -1$ independent of L such that when $-1 < \varepsilon < \varepsilon_0$, we have for all $s \in \mathbb{R}$ and $L \ge 1$:

$$\left|\sum_{i=0}^{[L]} V_{\text{int}} \left(s - i(1+\varepsilon)\right)\right| \le \frac{2}{1+\varepsilon} \int_{\mathbb{R}} |V_{\text{int}}(t)| \mathrm{d}t.$$

Replacing this estimate in (1.6) and using (1.9), we find that for $\varepsilon > -1$ such that $\varepsilon < \varepsilon_0$ and $\varepsilon + 1 < s_0$,

$$\mathcal{E}(\varepsilon;L) \ge \frac{2}{1+\varepsilon} \left(\frac{[L] + [L/\alpha]}{L} \int_{\mathbb{R}} |V_{\text{int}}(t)| \mathrm{d}t - \frac{[L/\alpha] + 1}{L} \int_{\mathbb{R}} |V_{\text{int}}(t)| \mathrm{d}t \right),$$

so for $L \geq 2$,

$$\begin{split} \mathcal{E}(\varepsilon;L) &\geq \frac{1}{1+\varepsilon} \left(\frac{[L]-1}{L/2}\right) \int_{\mathbb{R}} |V_{\text{int}}(t)| \mathrm{d}t \\ &\geq \frac{1}{1+\varepsilon} \int_{\mathbb{R}} |V_{\text{int}}(t)| \mathrm{d}t. \end{split}$$

On the other hand, assumption (1.8) implies that $\mathcal{E}(0; L)$ is bounded from above for $L \ge 1$. Indeed, the series

$$s \mapsto \sum_{i=-\infty}^{\infty} |V_{\text{int}}(s-i)|,$$

is absolutely convergent and defines a smooth 1-periodic function, in particular it is bounded. Substituting in (1.6), we find

$$\mathcal{E}(0;L) \leq \frac{1}{L} \left([L]\psi_1(1) + [L/\alpha]\psi_\alpha(\alpha) \right) + \frac{[L/\alpha] + 1}{L} \left\| \sum_{i=-\infty}^{\infty} |V_{\text{int}}(\cdot - i)| \right\|_{\infty} \leq C,$$

where C > 0 is some constant independent of L. Hence, there exists $\varepsilon_{\min} > -1$ such that, $\mathcal{E}(\varepsilon; L) > \mathcal{E}(0; L)$ for all $L \ge 2$ and $-1 < \varepsilon < \varepsilon_{\min}$. This proves (1.10).

Lemma A.2 (Corresponds to Lemma 1.4). If (1.8) holds, there exists C > 0 independent of L and ε such that for $\varepsilon > \varepsilon_{\min}$ and $n \in \{0, 1, 2\}$:

$$\left| \frac{\partial^{n} \widetilde{\mathcal{E}}}{\partial \varepsilon^{n}}(\varepsilon; L) - \frac{\partial^{n} \mathcal{E}}{\partial \varepsilon^{n}}(\varepsilon; L) \right| < \begin{cases} C/L^{\eta} & \text{if } 0 < \eta < 1, \\ C \cdot \ln(L)/L & \text{if } \eta = 1, \\ C/L & \text{if } \eta > 1. \end{cases}$$
(A.2)

Proof. In this proof, we denote by C any strictly positive constant that does not depend on L and ε . Recall that the periodized energy is defined as

$$\widetilde{\mathcal{E}}(\varepsilon;L) = \psi_1(1+\varepsilon) + \alpha^{-1}\psi_\alpha(\alpha+\varepsilon\alpha) + \alpha^{-1}\frac{1}{[L/\alpha]+1}\sum_{j=0}^{[L/\alpha]} V_{\text{per}}\left(\{\alpha j\},\varepsilon\right),\tag{A.3}$$

where the periodized potential $V_{\rm per}$ is defined by the infinite series

$$V_{\text{per}}: (s,\varepsilon) \mapsto \sum_{i=-\infty}^{\infty} V_{\text{int}} \left((s-i)(1+\varepsilon) \right),$$
 (A.4)

and thus bounded in $C^2(\mathbb{R} \times [\varepsilon_{\min}, \infty))$. We compute explicitly the difference between the exact and periodized energy (n = 0) or first derivatives $(n \in \{1, 2\})$:

$$\frac{\partial^{n} \mathcal{E}}{\partial \varepsilon^{n}}(\varepsilon; L) - \frac{\partial^{n} \widetilde{\mathcal{E}}}{\partial \varepsilon^{n}}(\varepsilon; L) = \left(\frac{[L]}{L} - 1\right) \psi_{1}^{(n)}(1+\varepsilon) + \alpha^{-1} \left(\frac{[L/\alpha]}{L/\alpha} - 1\right) \psi_{\alpha}^{(n)}(\alpha+\varepsilon\alpha) \\
+ \left(\frac{1}{L} - \frac{\alpha^{-1}}{[L/\alpha] + 1}\right) \sum_{j=0}^{[L/\alpha]} \frac{\partial^{n} V_{\text{per}}}{\partial \varepsilon^{n}} \left(\{\alpha j\}, \varepsilon\right) \\
- \frac{1}{L} \sum_{j=0}^{[L/\alpha]} \left(\frac{\partial^{n} V_{\text{per}}}{\partial \varepsilon^{n}} \left(\{\alpha j\}, \varepsilon\right) - \sum_{i=0}^{[L]} (\alpha j - i)^{n} V_{\text{int}}^{(n)} \left((\alpha j - i)(1+\varepsilon)\right)\right). \quad (A.5)$$

We will bound successively each of the terms in the right-hand side of (A.5). First, by assumption $\psi_1^{(n)}(s)$, $\psi_{\alpha}^{(n)}(s)$ are bounded as $s \to \infty$ so that

$$\left|\frac{[L]-L}{L}\psi_1^{(n)}(1+\varepsilon) + \frac{[L/\alpha]-L/\alpha}{L}\psi_\alpha^{(n)}(\alpha+\varepsilon\alpha)\right| < \frac{C}{L}.$$
(A.6)

Second, $\frac{\partial^n V_{\text{per}}}{\partial \varepsilon^n}$ is uniformly bounded on $\mathbb{R} \times [\varepsilon_{\min}, \infty)$ so that

$$\left|\frac{[L/\alpha] + 1 - \alpha^{-1}L}{L} \left(\frac{1}{[L/\alpha] + 1} \sum_{j=0}^{[L/\alpha]} \frac{\partial^n V_{\text{per}}}{\partial \varepsilon^n} \left(\{\alpha j\}, \varepsilon\right)\right)\right| < \frac{C}{L}.$$
(A.7)

For the third and last term, we start by estimating the summand. For $s = \alpha j$, $0 \le s \le L$,

$$\frac{\partial^n V_{\text{per}}}{\partial \varepsilon^n} (s, \varepsilon) - \sum_{i=0}^{[L]} (s-i)^n V_{\text{int}}^{(n)} \left((s-i)(1+\varepsilon) \right) \right|$$
$$\leq \left| \sum_{i<0} (s-i)^n V_{\text{int}}^{(n)} \left((s-i)(1+\varepsilon) \right) \right| + \left| \sum_{i>[L]} (s-i)^n V_{\text{int}}^{(n)} \left((s-i)(1+\varepsilon) \right) \right|.$$

The main argument to bound the two infinite series in the right-hand side is our assumption (1.8), which implies for $\varepsilon \geq \varepsilon_{\min}$,

$$\left| V_{\text{int}}^{(n)} \left((s-i)(1+\varepsilon) \right) \right| \le \frac{C}{(1+|(s-i)(1+\varepsilon)|)^{1+\eta+n}} \le \frac{C'}{(1+|s-i|)^{1+\eta+n}}.$$

We then bound the first series by using integral calculus:

$$\begin{aligned} \left| \sum_{i<0} (s-i)^n V_{\text{int}}^{(n)} \left((s-i)(1+\varepsilon) \right) \right| &\leq \sum_{i<0} \frac{C}{(1+|s-i|)^{1+\eta}} \\ &= \sum_{i'=1}^{\infty} \frac{C}{(s+i'+1)^{1+\eta}} = \int_1^{\infty} \frac{C \mathrm{d}t}{(s+[t]+1)^{1+\eta}} < \int_1^{\infty} \frac{C \mathrm{d}t}{(s+t)^{1+\eta}} < \frac{C}{(s+1)^{\eta}}. \end{aligned}$$

A bound on the second series follows by the same argument:

$$\begin{split} \left| \sum_{i>[L]} (s-i)^n V_{\text{int}}^{(n)} \left((s-i)(1+\varepsilon) \right) \right| &\leq \sum_{i=1}^{\infty} \frac{C}{(1+[L]+i-s)^{1+\eta}} < \sum_{i=1}^{\infty} \frac{C}{(L-s+i)^{1+\eta}} \\ &= \frac{C}{(L-s+1)^{1+\eta}} + \int_1^{\infty} \frac{C \mathrm{d}t}{(L-s+[t]+1)^{1+\eta}} \\ &< \frac{C}{(L-s+1)^{1+\eta}} + \int_1^{\infty} \frac{C \mathrm{d}t}{(L-s+t)^{1+\eta}} < \frac{C}{(L-s+1)^{\eta}}. \end{split}$$

The two previous calculations lead to

$$\begin{split} \sum_{j=0}^{[L/\alpha]} \left| \frac{\partial^{n} V_{\text{per}}}{\partial \varepsilon^{n}} \left(\{ \alpha j \}, \varepsilon \right) - \sum_{i=0}^{[L]} (\alpha j - i)^{n} V_{\text{int}}^{(n)} \left((\alpha j - i)(1 + \varepsilon) \right) \right| \\ &< \sum_{j=0}^{[L/\alpha]} \frac{C}{(\alpha j + 1)^{\eta}} + \frac{C}{(L - \alpha j + 1)^{\eta}} = \sum_{j=0}^{[L/\alpha]} \frac{C}{(\alpha j + 1)^{\eta}} + \sum_{j'=0}^{[L/\alpha]} \frac{C}{(L + \alpha (j' - [L/\alpha]) + 1)^{\eta}} \\ &\leq 2 \sum_{j=0}^{[L/\alpha]} \frac{C}{(\alpha j + 1)^{\eta}} \leq C \left(1 + \sum_{j=1}^{[L/\alpha]} \frac{1}{(\alpha j + 1)^{\eta}} \right) \leq C \left(1 + \frac{1}{\alpha} \int_{\alpha}^{L} \frac{1}{t^{\eta}} dt \right) \\ &\leq C \begin{cases} 1 + \frac{\alpha^{1-\eta} + L^{1-\eta}}{\alpha |1 - \eta|} & \text{if } \eta \neq 1, \\ 1 + \frac{\ln(\alpha) + \ln(L)}{\alpha} & \text{if } \eta = 1, \end{cases} \end{split}$$
(A.8)

where we have used the inequality $L - \alpha[L/\alpha] \ge 0$ and integral calculus again in our estimation. Using the bounds (A.6), (A.7) and (A.8) in (A.5), we now obtain (A.2).

Theorem A.3 (Corresponds to Theorem 2.9). Let R_{α} be an irrational rotation of \mathbb{T} with α of Diophantine type (K, σ) . Let $\phi : \mathbb{T} \mapsto \mathbb{R}$ be of class H^r where $r \geq \sigma + 1$. Then, there exists a function ψ in $H^{r-\sigma-1}$ which solves the linear homological equation

$$\psi \circ R_{\alpha} - \psi = \phi - \int_{0}^{1} \phi dx, \quad with \ \|\psi\|_{H^{r-\sigma-1}} \le \frac{1}{4K} \|\phi\|_{H^{r}}.$$
(A.9)

For any integer $n \ge 1$, we have the uniform bound on the Birkhoff sums:

$$\left\| \frac{1}{n} \sum_{j=0}^{n-1} \phi \circ R_{\alpha}^{j} - \int_{0}^{1} \phi \mathrm{d}x \right\|_{H^{r-\sigma-1}} \leq \frac{1}{2Kn} \|\phi\|_{H^{r}}.$$
(A.10)

Furthermore, if $\frac{p}{q}$ is a rational approximation of α in the sense (2.6) then

$$\left\| \frac{1}{q} \sum_{j=0}^{q-1} \phi \circ R_{\alpha}^{j} - \int_{0}^{1} \phi \mathrm{d}x \right\|_{L^{2}} \leq \frac{\pi}{2Kq^{1+\theta}} \|\phi\|_{H^{r}},\tag{A.11}$$

where $\theta = \min(1, r - \sigma - 1)$.

Proof. Let $\phi : \mathbb{T} \to \mathbb{R}$ be of class H^r where $r \ge \sigma + 1$. First, we seek a function ψ in $H^{r-\sigma-1}$ which solves the linear homological equation (A.9) as a Fourier series and we compute its coefficients:

$$\widehat{\psi}(0) = 0$$
, and for $k \neq 0$, $\widehat{\psi}(k) = \frac{\widehat{\phi}(k)}{e^{2i\pi k\alpha} - 1}$, so that $|\widehat{\psi}(k)| = \frac{|\widehat{\phi}(k)|}{2|\sin(\pi k\alpha)|}$

Now, thanks to the Diophantine condition on α and the inequality $\sin(x) \ge 2x/\pi$ for $|x| \le \pi/2$, we deduce that

$$|\sin(\pi k\alpha)| \ge 2 \inf_{p \in \mathbb{Z}} |k\alpha - p| \ge \frac{2K}{|k|^{1+\sigma}},$$

and thus

$$\|\psi\|_{H^{r-\sigma-1}}^2 = \sum_{k \in \mathbb{Z} \setminus \{0\}} |k|^{2r-2\sigma-2} \frac{|\widehat{\phi}(k)|^2}{4|\sin(\pi k\alpha)|^2} \le \frac{1}{16K^2} \sum_{k \in \mathbb{Z} \setminus \{0\}} |k|^{2r} |\widehat{\phi}(k)|^2 \le \frac{1}{16K^2} \|\phi\|_{H^r}^2$$

Thus ψ belongs to $H^{r-\sigma-1}$ and solves (A.9). For $n \ge 1$, the Birkhoff sum in (A.10) can then be computed as a telescopic sum,

$$\sum_{j=0}^{n-1} \phi \circ R_{\alpha}^{j}(\cdot) - n \int_{0}^{1} \phi \mathrm{d}x = \psi(\cdot + n\alpha) - \psi(\cdot),$$

and this leads immediately to the bound (A.10) by the triangular inequality. Now, by the Parseval identity we have

$$\|\psi(\cdot + q\alpha) - \psi(\cdot)\|_{L^2}^2 = \sum_{k \in \mathbb{Z} \setminus \{0\}} |e^{2i\pi kq\alpha} - 1|^2 |\widehat{\psi}(k)|^2.$$

Let $\theta = \min(1, r - \sigma - 1)$. For $k \in \mathbb{Z} \setminus \{0\}$, an easy computation shows that, since $0 \le \theta \le 1$,

$$|e^{2i\pi kq\alpha} - 1| = 2|\sin\left(\pi k(q\alpha - p)\right)| \le 2\min\left(1, \pi \frac{|k|}{q}\right) \le 2\pi \frac{|k|^{\theta}}{q^{\theta}},$$

since we know that $|q\alpha - p| < 1/q$ for $\frac{p}{q}$ a rational approximation of α , which leads to

$$\left\|\sum_{j=0}^{q-1}\phi\circ R_{\alpha}^{j}(\cdot)-q\int_{0}^{1}\phi\mathrm{d}x\right\|_{L^{2}}^{2} \leq \left(\frac{2\pi}{q^{\theta}}\right)^{2}\sum_{k\in\mathbb{Z}\setminus\{0\}}|k|^{2\theta}|\widehat{\psi}(k)|^{2} \leq \left(\frac{2\pi}{q^{\theta}}\right)^{2}\|\psi\|_{H^{\theta}}.$$

Proposition A.4 (Corresponds to Proposition 3.2). Under assumptions (1.8) and (1.9), we have the error estimate:

$$|\mathcal{E}_n(\varepsilon) - \mathcal{E}^{\infty}(\varepsilon)| \le C(1+\varepsilon)^2 \left(\frac{1}{q_n^2} + \left|\frac{p_n}{q_n} - \alpha\right|\right).$$
(A.12)

Proof. Recall the definition (3.2) of the periodized energy,

$$\mathcal{E}_n(\varepsilon) = \psi_1(1+\varepsilon) + \frac{q_n}{p_n} \cdot \psi_\alpha\left((1+\varepsilon)\frac{p_n}{q_n}\right) + \frac{1}{p_n}\sum_{j=0}^{q_n-1}V_{\text{per}}\left(\frac{j}{q_n},\varepsilon\right).$$

Recall that $\mathcal{E}^{\infty}(\varepsilon)$ is given by (1.14). Let us then consider separately each term in the error, which we decompose as:

$$\begin{aligned} |\mathcal{E}_{n}(\varepsilon) - \mathcal{E}^{\infty}(\varepsilon)| &\leq \left| \frac{q_{n}}{p_{n}} \cdot \psi_{\alpha} \left((1+\varepsilon) \frac{p_{n}}{q_{n}} \right) - \frac{1}{\alpha} \cdot \psi_{\alpha} \left((1+\varepsilon) \alpha \right) \right| \\ &+ \left| \frac{q_{n}}{p_{n}} - \frac{1}{\alpha} \right| \left| \int_{0}^{1} V_{\text{per}}(s,\varepsilon) \mathrm{d}s \right| + \frac{q_{n}}{p_{n}} \left| \frac{1}{q_{n}} \sum_{j=0}^{q_{n}-1} V_{\text{per}} \left(\frac{j}{q_{n}}, \varepsilon \right) - \int_{0}^{1} V_{\text{per}}(s,\varepsilon) \mathrm{d}s \right|. \end{aligned}$$
(A.13)

First, we have for some constant C > 0:

$$\left|\frac{q_n}{p_n} \cdot \psi_\alpha \left((1+\varepsilon)\frac{p_n}{q_n} \right) - \frac{1}{\alpha} \cdot \psi_\alpha \left((1+\varepsilon)\alpha \right) \right| \le C(1+\varepsilon) \left|\frac{q_n}{p_n} - \alpha\right|,\tag{A.14}$$

where we use the fact that ψ_{α} and ψ'_{α} are bounded on the interval $[\varepsilon_{\min}, \infty)$. Next, we estimate the second term by computing:

$$\left|\frac{q_n}{p_n} - \frac{1}{\alpha}\right| \left| \int_0^1 V_{\text{per}}(s,\varepsilon) \mathrm{d}s \right| \le \left| \frac{\alpha - p_n/q_n}{\alpha p_n/q_n} \right| \int_0^1 \sum_{i \in \mathbb{Z}} |V_{\text{int}}((s-i)(1+\varepsilon))| \\ \le \frac{C \left|\alpha - p_n/q_n\right|}{1+\varepsilon} \int_{\mathbb{R}} |V_{\text{int}}(S)| \, \mathrm{d}S,$$
(A.15)

where we used the change of variables $S \equiv (1 + \varepsilon)(s - i)$ in the integral and the boundedness of the sequence q_n/p_n .

Finally, we consider the last term in right-hand side of (A.13). It is clearly a Riemann sum approaching the average of V_{per} over the interval [0, 1] by the periodic trapezoidal rule, for which we recall the standard second order error estimate,

$$\left|\frac{1}{q_n}\sum_{j=0}^{q_n-1}V_{\text{per}}\left(\frac{j}{q_n},\varepsilon\right) - \int_0^1 V_{\text{per}}(s,\varepsilon)\mathrm{d}s\right| \le \frac{C}{q_n^2} \left\|\frac{\partial^2 V_{\text{per}}}{\partial s^2}(\cdot,\varepsilon)\right\|_{\infty}.$$
(A.16)

The required uniform bound on the second derivative of V_{per} is a direct consequence of the definition (1.11) of the periodic potential under the assumptions (1.8):

$$\left|\frac{\partial^2 V_{\text{per}}}{\partial s^2}(s,\varepsilon)\right| \le C(1+\varepsilon)^2,$$

where C > 0 is a constant independent of ε and s. Bringing together estimates (A.14), (A.16) and (A.15) we find the desired result (3.3).

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References

- M. Arroyo and T. Belytschko, An atomistic-based finite deformation membrane for single layer crystalline films. J. Mech. Phys. Solids 50 (2002) 1941–1977.
- [2] M. Arroyo and T. Belytschko, Continuum mechanics modeling and simulation of carbon nanotubes. *Meccanica* 40 (2005) 455–469.
- [3] M. Born, Dynamik der Kristallgitter, Vol. 4. Teubner, Berlin/Leipzig (1915).
- [4] E. Cancès, P. Cazeaux and M. Luskin, Generalized Kubo formulas for the transport properties of incommensurate 2D atomic heterostructures. J. Math. Phys. 58 (2017) 063502.
- [5] R. Car and M. Parrinello, Unified approach for molecular dynamics and density-functional theory. Phys. Rev. Lett. 55 (1985) 2471–2474.
- [6] A.H. Castro-Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov and A.K. Geim, The electronic properties of graphene. *Rev. Mod. Phys.* 81 (2009) 109–162.
- [7] P. Cazeaux, M. Luskin and E. Tadmor, Analysis of rippling in incommensurate one-dimensional coupled chains. *Multiscale Model. Simul.* 15 (2017) 56–73.
- [8] S. Conti, G. Dolzmann, B. Kirchheim and S. Müller, Sufficient conditions for the validity of the Cauchy–Born rule close to SO(n). J. Eur. Math. Soc. 8 (2006) 515–530.
- [9] G. Dal Maso, An Introduction to Γ-Convergence. Springer, Birkhäuser, Boston (1993).
- [10] M. Dobson, There is no pointwise consistent quasicontinuum energy. IMA J. Numer. Anal. 34 (2014) 1541–1553.
- [11] J.L. Ericksen, On the Cauchy–Born rule. Math. Mech. Solids 13 (2008) 199–220.
- [12] G. Friesecke and F. Theil, Validity and failure of the Cauchy–Born hypothesis in a two-dimensional mass-spring lattice. J. Nonlinear Sci. 12 (2002) 445–478.
- [13] A. Geim and I. Grigorieva, Van der Waals heterostructures. Nature 499 (2013) 419–425.
- [14] M. Herman, Sur la conjugaison différentiable des difféomorphismes du cercle à des rotations. Vol. 49 of Publications Mathématiques de l'Institut des Hautes Études Scientifiques (1979) 5–233.
- [15] M. Herman, in Sur les courbes invariantes par les difféomorphismes de l'anneau, With an appendix by Albert Fathi. Vol. 1. Vol. 103 of Astérisque. Société Mathématique de France, Paris (1983).
- [16] H. Kesten, The discrepancy of random sequences {kx}. Acta Arith. 10 (1964) 183–213.
- [17] A.N. Kolmogorov and V.H. Crespi, Registry-dependent interlayer potential for graphitic systems. Phys. Rev. B 71 (2005) 235415.
- [18] S. Kozlov, Averaging differential operators with almost periodic, rapidly oscillating coefficients. Math. USSR-Sbornik 35 (1979) 481–498.
- [19] L. Kuipers and H. Niederreiter, Uniform Distribution of Sequences. Wiley-Interscience, New York (1974).
- [20] X.H. Li, C. Ortner, A. Shapeev and B.V. Koten, Analysis of blended atomistic/continuum hybrid methods. Preprint arXiv:1404.4878 (2014).
- [21] M. Luskin and C. Ortner, Atomistic-to-continuum coupling. Acta Numer. 22 (2013) 397–508.
- [22] I. Nikiforov and I. Tadmor, Continuum model for inextensible incommensurate 1-D bilayer with bending and disregistry manuscript (2015).
- [23] M. Ortiz, R. Phillips and E.B. Tadmor, Quasicontinuum analysis of defects in solids. Philos. Mag. A 73 (1996) 1529–1563.
- [24] C. Ortner and F. Theil, Justification of the Cauchy–Born approximation of elastodynamics. Arch. Ration. Mech. Anal. 207 (2013) 1025–1073.
- [25] G. Papanicolaou and S. Varadhan, Boundary value problems with rapidly oscillating random coefficients, in Rigorous Results in Statistical Mechanics and Quantum Field Theory. Proceedings of Conference on Random Fields, Esztergom, Hungary, 1979, edited by J. Fritz, J.L. Lebaritz and D. Szasz. Seria Colloquia Mathematica Societatis Janos Bolyai, 27. North Holland (1981) 835–873.
- [26] H.S. Park, P.A. Klein and G.J. Wagner, A surface Cauchy-Born model for nanoscale materials. Int. J. Numer. Meth. Eng. 68 (2006) 1072–1095.
- [27] D. Sfyris, Phonon, Cauchy–Born and homogenized stability criteria for a free-standing monolayer graphene at the continuum level. Eur. J. Mech. A/Solids 55 (2016) 134–148.
- [28] H. Terrones and M. Terrones, Bilayers of transition metal dichalcogenides: different stackings and heterostructures. J. Mater. Res. 29 (2014) 373–382.
- [29] G.A. Tritsaris, S.N. Shirodkar, E. Kaxiras, P. Cazeaux, M. Luskin, P. Plecháč, et al., Perturbation theory for weakly coupled two-dimensional layers. J. Mater. Res. 31 (2016) 959–966.
- [30] G. Zanzotto, The Cauchy–Born hypothesis, nonlinear elasticity and mechanical twinning in crystals. Acta Crystallogr. Sect. A 52 (1996) 839–849.