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Crystallization in a One-Dimensional Periodic Landscape

Manuel Friedrich[1] · **Ulisse Stefanelli**[2,3,4]

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Abstract
We consider the crystallization problem for a finite one-dimensional collection of identical hard spheres in a periodic energy landscape. This issue arises in connection with the investigation of crystalline states of ionic dimers, as well as in epitaxial growth on a crystalline substrate in presence of lattice mismatch. Depending on the commensurability of the radius of the sphere and the period of the landscape, we discuss the possible emergence of crystallized states. In particular, we prove that crystallization in arbitrarily long chains is *generically* not to be expected.

Keywords Crystallization · Hard spheres · Periodic landscape · Ionic dimers · Epitaxial growth

Mathematics Subject Classification 82D25

1 Introduction

The emergence of crystalline states at low temperatures is a common phenomenon in material systems. Its rigorous mathematical description poses severe mathematical challenges even at the quite simplified setting of Molecular Mechanics, where configurations of particles interacting via classical potentials are considered [10,16]. Here, *crystallization* corresponds to the periodicity of ground state configurations, an instance which in many cases is still eluding

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✉ Ulisse Stefanelli
ulisse.stefanelli@univie.ac.at
http://www.mat.univie.ac.at/∼stefanelli

Manuel Friedrich
manuel.friedrich@uni-muenster.de
https://www.uni-muenster.de/AMM/Friedrich/index.shtml

1 Applied Mathematics, Universität Münster, Einsteinstr. 62, 48149 Münster, Germany

2 Faculty of Mathematics, University of Vienna, Oskar-Morgenstern-Platz 1, 1090 Wien, Austria

3 Vienna Research Platform on Accelerating Photoreaction Discovery, University of Vienna, Währinger Str. 17, 1090 Vienna, Austria

4 Istituto di Matematica Applicata e Tecnologie Informatiche E. Magenes, v. Ferrata 1, 27100 Pavia, Italy

Fig. 1 A 4-crystal and a 7-crystal

a complete mathematical understanding. In fact, rigorous mathematical crystallization results are scarce and often limited to very specific choices of data [4]. Specifically, interactions with the environment are usually neglected or assumed to be homogeneous.

We intend to progress in this quest by addressing here the case of finite one-dimensional crystallization in a periodic, possibly nonconstant energy landscape. Given the configuration $\{x_1, \dots, x_n\} \subset \mathbb{R}^n$, we consider the *energy*

$$E = \sum_i v_1(x_i) + \frac{1}{2} \sum_{i \neq j} v_2(|x_i - x_j|). \tag{1}$$

The *landscape potential* $v_1 : \mathbb{R} \to [0, \infty)$ is assumed to be 1-periodic, piecewise continuous, and lower semicontinuous with $\min v_1 = 0$. The *interaction potential* $v_2 : \mathbb{R}_+ \to \mathbb{R} \cup \{\infty\}$ is of *hard-sphere* type at distance $\alpha > 0$, namely $v_2 = \infty$ on $[0, \alpha)$, $v_2(\alpha) = -1$, and $v_2 = 0$ on (α, ∞), see [13]. A collection of n particles is called an *n-crystal* (or, simply, *crystal*) if it is of the form $\{x, x + \alpha, \dots, x + \alpha(n-1)\}$ for some $x \in \mathbb{R}$, see Fig. 1. If all ground-state n-particle configurations are n-crystals, we say that *n-crystallization* holds. We call *crystallization* the case when n-crystallization holds for all n.

The aim of this note is to investigate crystallization under different choices for v_1 and α. Our main result states that crystallization does not *generically* hold. More precisely, we have the following.

Theorem 1.1 (Generic noncrystallization) *For all given α and v_1 as above and each $\varepsilon > 0$, there exist α^ε and v_1^ε as above with $|\alpha - \alpha^\varepsilon| < \varepsilon$ and $\|v_1 - v_1^\varepsilon\|_{L^\infty(0,1)} < \varepsilon$, and a strictly increasing sequence $(n_k)_{k \in \mathbb{N}} \subset \mathbb{N}$ such that n_k-crystallization does not hold for the energy E^ε defined from α^ε and v_1^ε.*

In addition to this generic negative result, which is proved in Sect. 5, we discuss different *nongeneric* settings where crystallization does hold. Two quite different scenarios arise, depending on the rationality of α.

In case α is rational (a nongeneric property), the crystallization problem can be solved by localized arguments. In particular, Theorem 3.1 states that n-crystallization holds under some specific conditions on v_1 which are independent of n but only depend on the irreducible fraction of α. In fact, we are able to present a hierarchy of sufficient conditions entailing crystallization, see Proposition 3.2.

The case of α irrational is tackled in Sect. 4 instead. Here, the ergodic character of the map $x \in [0, 1) \mapsto (x + \alpha)_{\mathrm{mod}\,1}$ comes into play. We resort in using and extending some tools from the theory of *low discrepancy sequences* [5], carefully quantifying the extent at which the potential landscape v_1 is explored by the latter map. Such quantitative information is instrumental in investigating crystallization. Here, we are able to find a specific class of landscape potentials v_1 entailing crystallization, see Theorem 4.4 and the discussion thereafter.

The specific form of the energy E is inspired by the modelization of a *dimer* of elements A and B at zero temperature. By labelling the corresponding atoms as x_i and y_ℓ, a possible choice for the energy of the dimer is

$$\frac{1}{2} \sum_{i \neq j} v_2^A(|x_i - x_j|) + \frac{1}{2} \sum_{\ell \neq k} v_2^B(|y_\ell - y_k|) + \sum_{i,\ell} v_2^{\mathrm{int}}(|x_i - y_\ell|).$$

Here, v_2^A and v_2^B are the intraspecific two-body interaction energies for atoms of type A and B, minimized at the interaction distance $0 < \alpha \neq 1$ and 1, respectively, and v_2^{int} is an interaction energy between types. Assume now that type B has already formed a one-dimensional infinite rigid crystal, say $\mathbb{Z}$, see [7,15] for a similar approach. By removing the self-interacting v_2^B terms, the energy can hence be rewritten as a function of $\{x_1, \dots, x_n\}$ in the form of E by letting $v_2 = v_2^A$ and

$$v_1(x) := \sum_{\ell \in \mathbb{Z}} v_2^{\text{int}}(|x - \ell|).$$

By assuming that the latter series converges for all $x \in [0, 1)$, the resulting landscape potential v_1 is 1-periodic.

Energies of the type of E may also arise in modeling the *epitaxial growth* of a first layer of type A on top of an underlying rigid crystal of type B in presence of lattice mismatch. Here, the potential v_1 represents the effect of the rigid substrate, with periodicity 1. The deposited layer $\{x_1, \dots, x_n\}$ is then expected to optimize intraspecific atomic interactions in a given nontrivial potential landscape.

Crystallization problems have received constant attention in the last decades. The reader is referred to the recent survey by Blanc and Lewin [4] for a comprehensive account on the literature. To the best of our knowledge, crystallization results in periodic landscapes are still currently unavailable. We contribute here in extending the classical one-dimensional crystallization theory [11,12,18] toward the discussion of molecular compounds.

Numerical studies on crystallization in multicomponent systems are abundant, see [1,2,6,15,19], just to mention a few. On the other hand, rigorous crystallization results for such systems are scarce. A first result in this direction is due to Radin [17], who studies a specific multicomponent two-dimensional system showing quasiperiodic ground states. Bétermin et al. [3] investigate conditions for crystallization of *alternating* one-dimensional configurations interacting via a smooth interaction density v_2. Two dimensional dimer crystallization results in hexagonal and square geometries for a hard-spheres interaction v_2 are given in [8,9].

2 Preliminaries

In this section we collect some preliminary discussion and fix notation.

To start with, one can assume with no loss of generality that $\alpha < 1$. Indeed, if $\alpha = 1$, then ground-state configurations are obviously n-crystals with all particles sitting at $x_1 + \mathbb{N}$, where $x_1 \in [0, 1)$ is a minimizer of v_1. Since $\min v_1 = 0$, the corresponding energy is $E = (n-1)v_2(\alpha) = -(n-1)$. On the other hand, if $\alpha > 1$, we can rescale the problem by redefining α as $\alpha/\lceil\alpha\rceil \leq 1$, where $\lceil\alpha\rceil = \min\{z \in \mathbb{Z} : \alpha \leq z\}$, and by replacing $t \mapsto v_1(t)$ with $t \mapsto v_1(\lceil\alpha\rceil t)$. We also use the notation $(x)_{\text{mod}\,1} := x - \lfloor x \rfloor$ for all $x \in \mathbb{R}$, where $\lfloor x \rfloor = \max\{z \in \mathbb{Z} : x \geq z\}$. Given any $A \subset \mathbb{R}$, we indicate by χ_A the corresponding *characteristic function*, namely, $\chi_A(x) = 1$ if $x \in A$ and $\chi_A(x) = 0$ elsewhere.

The total contribution of the landscape potential to the energy of the n-crystal with the leftmost particle sitting at x (i.e., the collection of points $\{x, x+\alpha, \dots, x+\alpha(n-1)\}$) reads

$$V_n(x) := \sum_{j=0}^{n-1} v_1(x + j\alpha).$$

This is indeed the crucial object to study here, for the total energy of the n-crystal with the leftmost particle sitting at x is readily obtained from it as

$$E(\{x, x+\alpha, \dots, x+\alpha(n-1)\}) = V_n(x) - (n-1), \tag{2}$$

see Definition (1) (recall that the n-crystal has $n-1$ bonds, each of which contributes -1 to the energy). Let us introduce the notation $V_n^* := \min V_n$ and indicate with $x_n^* \in [0,1)$ (possibly not uniquely) a minimizer, i.e., $V_n^* = V_n(x_n^*)$. Note that a minimizer exists since v_1 is lower semicontinuous. If an n-particle ground state is an n-crystal, then necessarily its leftmost particle sits at a point x_n^* (possibly not unique). Note that one always has that

$$V_p^* + V_q^* \le V_{p+q}^* \quad \forall\, p, q \in \mathbb{N} \tag{3}$$

as the minimization on the right-hand side is performed under an extra constraint with respect to those on the left-hand side.

Our first aim is to elucidate the role of the somewhat *opposite* relation

$$V_{p+q}^* < V_p^* + V_q^* + 1 \quad \forall\, p, q \ \text{ with } \ p+q \le n. \tag{4}$$

Under condition (4), one has that the splitting of an n-crystal into smaller crystals is energetically not favored. (In the following, we use the term *splitting* to refer to a configuration made of different crystals.) In fact, looking back to (2), condition (4) says that it is not energetically favorable to split a $(p+q)$-crystal into a p-crystal and a q-crystal. This can by generalized to arbitrary splittings. Consider indeed an n-particles configuration made of j different crystals $\{x_1^j, \dots, x_{n_j}^j\}$ with $n_1 + \cdots + n_j = n$. In case $j \ge 2$, one can use (4) and $\min v_2 = -1$ in order to get that

$$E \ge \sum\nolimits_{k=1}^{j} (V_{n_k}^* - (n_k - 1)) \overset{(4)}{>} V_n^* - (j-1) - n + j = V_n^* - (n-1).$$

The above right-hand side is the energy of the n-crystal, which is then favorable with respect to any of its splittings, regardless of the number $j \ge 2$ of splitting parts.

On the other hand, condition (4) is *almost* necessary for n-crystallization to hold. Indeed, if one has

$$V_{p+q}^* > V_p^* + V_q^* + 1 \quad \text{for some } p, q \text{ with } p+q = n, \tag{5}$$

then n-crystals are not ground states as splitting an n-crystal into a p- and a q-crystal lowers the energy. In case equality holds in condition (5) for some $p+q = n$, n-crystals and the union of a p- and a q-crystal are equienergetic. In conclusion, we have checked the following.

Proposition 2.1 (Key condition). *Condition* (4) *implies n-crystallization. On the other hand, n'-crystallization for all $n' \le n$ implies* (4).

Owing to the latter, in order to check for the validity of n-crystallization, one is left with checking the key condition (4). This check is at the core of all our arguments in the remainder of the paper. It will be investigated under different settings for α and v_1. As already mentioned in the Introduction, the analysis depends strongly on α being rational or not. Correspondingly, our discussion is divided in the coming Sects. 3 (α rational) and 4 (α irrational).

Let us conclude this section by some remarks:

(a) At first, we would like to record that, differently from the trivial case $v_1 \equiv 0$, n-crystallization may indeed depend on the number n of particles involved. We present here an example illustrating this fact. Let $\alpha = 1/2$ and v_1 be such that

$$v_1(x) = h(1 - 4(x - 1/2)^2) \qquad \text{for } x \in [0,1)$$

for some $h > 0$. Then, one has that

$$V_n^* = h\lfloor n/2 \rfloor \quad \forall\, n \in \mathbb{N}.$$

In particular, given $p + q = n$, there holds

$$h(k + j) + h\ell = V_n^*, \quad h(k + j) = V_p^* + V_q^*,$$

where $k = \lfloor p/2 \rfloor$, $j = \lfloor q/2 \rfloor$, and $\ell = \lfloor (n - 2k - 2j)/2 \rfloor$. Note that $\ell = 0$ unless both p and q are odd, in which case $\ell = 1$. Then, we conclude that the sufficient condition (4) holds if $h < 1$ whereas, if $h > 1$, then condition (5) implies that ground states are not crystalline for $n \geq 6$ and even.

In case $h = 1$ and n even, crystallized states and noncrystallized states are energetically equivalent. On the other hand, ground states are crystalline for all $n \geq 3$ odd, regardless of the value of h.

(b) One may wonder if the key condition (4) could be weakened to

$$V_{p+q}^* < V_p^* + V_q^* + 1 \quad \forall\, p, q \ \text{ with } \ p + q = n, \tag{6}$$

namely, by restricting to the splitting into exactly two subcrystals at level n only. This is however not the case, as the following simple example shows. Let $\alpha = 1/4$, take $v_1 = 0$ on $A = \{0, 1/4, 3/4\}$, and $v_1 = h > 2$ out of a very small neighborhood of A. One can readily compute that $V_1^* = V_2^* = 0$, $V_3^* = V_4^* = V_5^* = h$. Hence, condition (6) holds for $n = 5$. In particular, no splitting of a 5-crystal into exactly two smaller crystals is favorable. On the other hand, the ground states for $n = 5$ are not crystalline as one can favorably split a 5-crystal into two 2-crystals and a 1-crystal since $V_1^* + 2V_2^* + 2 = 2 < h = V_5^*$.

(c) Eventually, we present an example showing that, in general, the minimizers x_p^* of V_p may depend on p. Let $\alpha = 1/4$, $v_1 = 0$ only on $A = \{0, 1/4\}$, and $v_1 = 1$ out of a very small neighborhood of A. One readily gets that $x_1^* \in \{0, 1/4\}$, $x_2^* = 0$, $x_3^* \in \{0, 3/4\}$, $x_4^* \in \{0, 1/4, 1/2, 3/4\}$, $x_5^* \in \{0, 1/4\}$, and $x_6^* = 0$. In particular, the position of the leftmost particle of a crystal ground state may depend on its length.

3 Crystallization for Rational α

Let α be rational. By possibly rescaling, as explained at the beginning of Sect. 2, one can assume with no loss of generality that $m\alpha = 1$ for some $m \in \mathbb{N}$. Note that in this case

$$V_{pm}^* = pV_m^* \quad \forall\, p \in \mathbb{N}. \tag{7}$$

The aim of this section is that of showing that crystallization, namely n-crystallization *for all* n, can be achieved under some version of the key condition (4) which is *localized* with respect to n. More precisely, we consider the condition

$$(p + q)\frac{V_m^*}{m} < V_p^* + V_q^* + 1 \quad \forall\, p, q \in \mathbb{N} \ \text{ with } \ 1 \leq p, q \leq m - 1. \tag{8}$$

The condition is in the same spirit as the key condition (4), with the difference that on the left-hand side the minimal contribution of the landscape potential to the energy of an $(p + q)$-crystal is replaced by the

minimal per-particle energy V_m^*/m in an m-crystal times the number of particles $p + q$. On the one hand, condition (8) is stronger than (4) since

$$(p + q)V_m^* \overset{(7)}{=} V_{(p+q)m}^* \overset{(3)}{\geq} mV_{p+q}^*,$$

and therefore $(p+q)V^*_m/m \geq V^*_{p+q}$. On the other hand, in comparison with (4), condition (8) involves only the energy of p-crystals of length at most m, and is thus weaker and easier to check. In particular, it is *local* with respect to n.

The main result of this section is the following statement, turning the local condition (8) on crystals of length at most m into crystallization of infinitely large crystals.

Theorem 3.1 (Crystallization). *Condition* (8) *implies crystallization.*

Proof Let us check that (4) holds for any given $n \in \mathbb{N}$. Assume by contradiction that this is not the case, namely that there exist n', h, $\ell \in \mathbb{N}$ and i, $j \in \{0, \dots, m-1\}$ with $(h+\ell)m+i+j = n' \leq n$ such that

$$V^*_{hm+i} + V^*_{\ell m+j} + 1 \leq V^*_{n'}. \tag{9}$$

We first observe that

$$mV^*_{n'} \overset{(3)}{\leq} V^*_{mn'} = V^*_{m(h+\ell)m+mi+mj} \overset{(7)}{=} mV^*_{hm} + mV^*_{\ell m} + iV^*_m + jV^*_m.$$

For the following, it is convenient to set $V^*_0 = 0$. The previous inequality along with (9) (multiplied by m) then yields

$$\begin{aligned} m\big(V^*_{hm} + V^*_i + V^*_{\ell m} + V^*_j + 1\big) &\overset{(3)}{\leq} m\big(V^*_{hm+i} + V^*_{\ell m+j} + 1\big) \leq mV^*_{n'} \\ &\leq mV^*_{hm} + mV^*_{\ell m} + iV^*_m + jV^*_m \end{aligned}$$

and therefore

$$V^*_i + V^*_j + 1 \leq (i+j)V^*_m/m. \tag{10}$$

Note that, if i or j equal zero, they can be replaced by 1 and (10) still holds as $V^*_0 = V^*_1 = 0$. Then, (10) contradicts (8). One hence concludes that the key condition (4) holds for every $n \in \mathbb{N}$, and the assertion follows from Proposition 2.1. □

We close this section by presenting a hierarchy of sufficient conditions entailing (8). Let us start by considering the condition

$$V^*_{sm} < V^*_p + V^*_q + V^*_r + 1 \quad \forall\, p, q, r \ \text{ with } \ p+q+r = sm, \ s = 1, 2 \tag{11}$$

which means that the splitting of an m-crystal or an $2m$-crystal into three splitting parts is energetically not convenient. We check that (11) implies (8). To this end, we preliminarily note that

$$V^*_r/r \leq V^*_m/m \quad \forall\, 1 \leq r \leq m. \tag{12}$$

In fact, there holds

$$rV^*_m \overset{(7)}{=} V^*_{rm} = V_{rm}(x^*_{rm}) = \sum_{i=0}^{m-1} V_r(x^*_{rm} + ir\alpha),$$

and therefore

$$V^*_r \leq \min_{i\in\{0,\dots,m-1\}} V_r\left(x^*_{rm} + ir\alpha\right) \leq m^{-1} \sum_{i=0}^{m-1} V_r\left(x^*_{rm} + ir\alpha\right) = rV^*_m/m,$$

which implies (12). Suppose now that $1 \le p, q \le m-1$ are given. Choose $1 \le r \le m$ such that $p+q+r = sm$, $s \in \{1,2\}$. Then, we get

$$V_p^* + V_q^* + 1 \overset{(11)}{>} V_{sm}^* - V_r^* \overset{(12)}{\ge} V_{sm}^* - rV_m^*/m \overset{(7)}{=} sV_m^* - rV_m^*/m = (p+q)V_m^*/m.$$

This shows (8).

We now consider the following stronger albeit localized version of condition (4)

$$V_{u+v}^* < V_u^* + V_v^* + 1/2 \quad \forall\, u, v \ \text{ with } \ u+v \le 2m. \tag{13}$$

Condition (11) can be deduced from the latter by subsequently splitting the sm-crystal into a $(p+q)$-crystal and an r-crystal and then splitting the $(p+q)$-crystal into a p-crystal and a q-crystal.

We record now different sufficient conditions entailing (13). Let us start by considering a function v_1 with Lipschitz constant

$$\operatorname{Lip} v_1 < \alpha/2. \tag{14}$$

Recall the definition of *oscillation* of a function $f : \mathbb{R} \to \mathbb{R}$ as $\operatorname{osc} f = \sup_{x,y} |f(x) - f(y)|$. As v_1 is nonnegative and $\min v_1 = 0$, we readily have that $\operatorname{osc} v_i = \sup v_1$. Since $|x-y|_{\mathrm{mod}\,1} \le 1/2$ for all $x,\ y \in \mathbb{R}$, we find $\operatorname{osc} v_1 \le \operatorname{Lip} v_1/2$. We then get by (14)

$$\operatorname{osc} v_1 < \alpha/4. \tag{15}$$

Now, by (15) and $m\alpha = 1$ we obtain

$$\operatorname{osc} V_p \le \sum_{j=0}^{p-1} \operatorname{osc} v_1(\cdot + j\alpha) \le 2m \operatorname{osc} v_1 < 2m\alpha/4 = 1/2 \quad \forall\, p \le 2m. \tag{16}$$

Let now $u+v \le 2m$. We have that

$$\begin{aligned} V_{u+v}^* &\le V_{u+v}(x_u^*) = V_u(x_u^*) + V_v(x_u^* + u\alpha) = V_u^* + V_v(x_u^* + u\alpha) \\ &= V_u^* + V_v^* + V_v(x_u^* + u\alpha) - V_v(x_v^*) = V_u^* + V_v^* + r_{u,v} \end{aligned}$$

where

$$r_{u,v} = V_v(x_u^* + u\alpha) - V_v(x_v^*) \le \operatorname{osc} V_v.$$

In particular, (16) implies

$$r_{u,v} < 1/2 \ \ \forall\, u, v \ \text{ with } \ u+v \le 2m \tag{17}$$

which in turn entails (13). We have hence proved the following.

Proposition 3.2 (Sufficient conditions)

$$(14) \ \Rightarrow \ (15) \ \Rightarrow \ (16) \ \Rightarrow \ (17) \ \Rightarrow \ (13) \ \Rightarrow \ (11) \ \Rightarrow (8).$$

Note that all implications in Proposition 3.2 cannot be reversed:

As for (15) $\not\Rightarrow$ (14), the choice $v_1(x) = (\alpha/9)\sin(3\pi x)$ gives $\operatorname{osc} v_1 = 2\alpha/9 < \alpha/4$ but $\operatorname{Lip} v_1 = 3\pi\alpha/9 > \alpha/2$.

As for (16) $\not\Rightarrow$ (15), one can consider $v_1(x) = h(1-xm)^+$ for $\alpha/4 \le h < 1/4$. Then $\operatorname{osc} v_1 = h$ and $\operatorname{osc} V_p \le 2h$ for all $p \le 2m$.

As for (17) $\not\Rightarrow$ (16), one takes the sawtooth function

$$v_1(x) = \frac{2h}{\alpha} \max_{j=0,\dots,m-1} \left(\frac{\alpha}{2} - \left| x + j\alpha - \frac{\alpha}{2} \right| \right)$$

for $h \geq 1/(4m)$ and check that $r_{u,v} = 0$ whereas osc $V_{2m} = 2mh \geq 1/2$.

As for (13) $\not\Rightarrow$ (17), take $\alpha = 1/2$ (i.e., $m = 2$), let v_1 be locally minimized at $0,\ 1/4$, and $1/2$ with $v_1(0) = v_1(1/2) = \varepsilon < 1/6$, $v_1(1/4) = 0$, and $v_1 = h > 1/2$ out of a very small neighborhood of $\{0,\ 1/4,\ 1/2\}$. Note that $V_1^* = 0$ and $V_p^* = \varepsilon p$ for $p \geq 2$. Then, (13) can be readily checked as $V_{u+v}^* \leq (u+v)\varepsilon \leq V_u^* + V_v^* + 2\varepsilon < V_u^* + V_v^* + 1/2$. On the other hand, $V_1^* = 0$ and $x_1^* = 1/4$, so that $r_{1,1} = V_1(x_1^* + \alpha) - V_1(x_1^*) = h - 0 > 1/2$.

As for (11) $\not\Rightarrow$ (13), we take $m = 2$, and take $v_1(0) = 0$ and $v_1 = h$ out of a very small neighborhood of $\{0\}$, for any $h \in (1/2, 1)$. One can easily check that $V_i^* = h\lfloor i/2 \rfloor$ for $i \in \mathbb{N}$. Then, condition (11) holds since $V_4^* = 2h < h + 1 = V_2^* + V_1^* + V_1^* + 1$. On the other hand, one has $V_2^* = h > 1/2 = V_1^* + V_1^* + 1/2$.

As for (8) $\not\Rightarrow$ (11), we let $\alpha = 1/3$ (i.e., $m = 3$), and take $v_1(0) = 0$ and $v_1 = h$ out of a very small neighborhood of $\{0\}$, for any $h \in (1/2, 3/4)$. One can readily compute that $V_p^* = h(p - \lceil p/3 \rceil)$ for all $p \in \mathbb{N}$. Thus, we can check that for $1 \leq p, q \leq 2$

$$(p+q)\frac{V_3^*}{3} = h((p-1)+(q-1)) + h\Big(2 - \frac{p+q}{3}\Big) \leq V_p^* + V_q^* + \frac{4h}{3} < V_p^* + V_q^* + 1.$$

However, there holds $V_3^* = 2h > 1 = V_1^* + V_1^* + V_1^* + 1$.

Let us conclude this discussion by remarking that condition (8) is indeed not necessary for crystallization. More precisely, let us show that (4) $\not\Rightarrow$ (8). Consider the previous example for $h \in (3/4, 1)$. Recall that $V_p^* = h(p - \lceil p/3 \rceil)$ for all $p \in \mathbb{N}$. Therefore, (4) can be checked for all $n \in \mathbb{N}$ by using the fact that $\lceil x/3 \rceil + \lceil y/3 \rceil \leq \lceil (x+y)/3 \rceil + 1$ for all $x, y \in \mathbb{N}$ and $h < 1$. On the other hand, (8) is not satisfied since $(1+1)V_m^*/m = 4h/3 > 1 = V_1^* + V_1^* + 1$.

4 Crystallization for Irrational α

Assume now α to be irrational. Let us start by presenting a necessary condition for crystallization.

Proposition 4.1 (Necessary condition for crystallization) *If $\int_0^1 v_1(t)\,dt \geq 1$, one has no n-crystallization for n large enough.*

Proof The map $x \in \mathbb{T} := \mathbb{R}/\mathbb{Z} \mapsto \alpha x \in \mathbb{T}$ is ergodic. Hence, for all $x \in [0, 1)$ we have that

$$\frac{1}{n} V_n(x) = \frac{1}{n} \sum_{j=0}^{n-1} v_1(x + j\alpha) \to \int_0^1 v_1(t)\,\mathrm{d}t. \tag{18}$$

In case $\int_0^1 v_1(t)\,\mathrm{d}t \geq 1$, one has that $V_n^* > n - 1$ for n large enough. The statement follows because splitting an n-crystal into n isolated particles lowers the energy. □

This already shows the fundamental distinction between the rational and the irrational. An illustration of this difference can be obtained by fixing $m \in \mathbb{N}$ and assuming to be given v_1 such that $v_1(i/m) = 0$ for $i = 0, \ldots, m-1$ and $\int_0^1 v_1(t)\,\mathrm{d}t \geq 1$. Then, for all α such that $m\alpha \in \mathbb{N}$ we obtain crystallization. On the other hand, if α is irrational, there is no n-crystallization for n large enough.

In case the landscape potential v_1 exhibits some quantitative convergence rate in (18), one can deduce n-crystallization under the condition

$$\left| \frac{1}{r} V_r^* - \int_0^1 v_1(t)\,\mathrm{d}t \right| < \frac{1}{3r} \quad \forall\, r \leq n. \tag{19}$$

We anticipate that potentials v_1 fulfilling this condition for all n exist, as we shall see later in Theorem 4.4. Let us start by proving the following result.

Proposition 4.2 (n-crystallization) *Under (19), n-crystallization holds.*

Proof For all $r \leq n$, define the *error*

$$e(r) := \left| V_r^* - r \int_0^1 v_1(t)\,\mathrm{d}t \right|.$$

Condition (19) entails that $e(r) < 1/3$. For all $p,\ q \leq n$ we can hence compute that

$$V_{p+q}^* - V_p^* - V_q^* \leq (p+q)\int_0^1 v_1(t)\,\mathrm{d}t - p\int_0^1 v_1(t)\,\mathrm{d}t - q\int_0^1 v_1(t)\,\mathrm{d}t$$
$$+ e(p+q) + e(p) + e(q) < 1 \quad \forall\, p, q \ \text{ with } \ p+q \leq n.$$

In particular, the key condition (4) holds and n-crystallization follows. □

Note that the positive statement of Proposition 4.2 is compatible with the negative assertion of Proposition 4.1: by assuming (19) for some n and choosing $r = 1 \leq n$, one has that $\int_0^1 v_1(t)\,\mathrm{d}t < 1/3$. The following proposition yields a sufficient condition for (19).

Proposition 4.3 (Control via oscillation) *For all $n \in \mathbb{N}$, there holds*

$$\left| \frac{1}{n} V_n^* - \int_0^1 v_1(t)\,dt \right| \leq \frac{osc\, V_n}{n}.$$

Proof Since v_1 is 1-periodic, we obtain

$$\int_0^1 v_1(t)\,\mathrm{d}t = \frac{1}{n}\sum_{j=0}^{n-1}\int_0^1 v_1(t+j\alpha)\,\mathrm{d}t = \frac{1}{n}\int_0^1 V_n(x)\,\mathrm{d}x.$$

We also observe that

$$\left| \int_0^1 V_n(x)\,\mathrm{d}x - V_n^* \right| \leq \operatorname{osc} V_n.$$

The result follows by combining the two estimates. □

By combining Propositions 4.2 and 4.3 one gets n-crystallization if $\operatorname{osc} V_r < 1/3$ holds for all $r \leq n$. In view of computation (16), this is in particular satisfied if $\operatorname{osc} v_1 < 1/(3n)$. The fundamental difference with respect to the result in Proposition 3.2 consists in the fact that the bound on the oscillation depends on the number of particles n, and is violated for all n large enough. In the following, we seek for conditions entailing n-crystallization *for all* n. We present a result in this direction by focusing on a special family of piecewise constant functions v_1 which are constant on intervals of very specific length.

Theorem 4.4 (Crystallization for a special piecewise constant v_1) *Let $\alpha \in (0,1)$ be irrational. Let $h > 0$. For each $\varepsilon \in (0,1)$, there exists $\gamma \in (0, \varepsilon]$ such that for each open interval $I \subset (0,1)$ with $|I| = \gamma$ the 1-periodic function v_1 defined by $v_1(t) = h\chi_I(t)$ for $t \in [0,1)$ satisfies*

$$\left| \frac{1}{n} V_n(x) - \int_0^1 v_1(t)\,dt \right| \leq \frac{C_\varepsilon h}{n} \quad \forall x \in [0,1) \quad \forall\, n \in \mathbb{N},$$

where C_ε depends on α and ε, but is independent of h and n. In particular, by Proposition 4.2 this implies that crystallization holds if $h < 1/(3C_\varepsilon)$.

It is a standard matter to check that the above assertion holds for functions v_1 resulting from linearly combining indicator functions of the type described in the statement of Theorem 4.4. More precisely, crystallization holds for landscape potentials of the form

$$v_1(x) = \sum_{j=1}^{N} h_j \chi_{(0,\gamma_j)+\mathbb{N}}(x + x_j)$$

for any $x_1, \dots, x_N \in \mathbb{R}$ and any $h_1, \dots, h_N \in \mathbb{R}$ with $\sum_{j=1}^{N} C_{\varepsilon_j} |h_j| < 1/3$, where $\gamma_j \in (0, \varepsilon_j]$ and C_{ε_j} are given from Theorem 4.4, for some $\varepsilon_1, \dots, \varepsilon_N \in (0, 1)$. Apart from the above mentioned linear combinations, the problem of determining more general classes of potentials v_1 entailing crystallization remains open. Note that, even in the case of piecewise constant potentials, the onset of crystallization is triggered by the choice of very specific, nongeneric interval lengths. We expect that the quest for a nontrivial continuous potential v_1 entailing crystallization will be very challenging.

In order to prove Theorem 4.4 we need a technical lemma. Given an interval $I \subset (0, 1)$ and $n \in \mathbb{N}$, the *n-discrepancy* of the sequence $\{(j\alpha) \bmod 1\}_{j\in\mathbb{N}}$ with respect to the interval I is defined as

$$\phi_n(I) = \frac{1}{n} \sum_{j=0}^{n-1} \chi_{\mathbb{N}+I}(j\alpha) - |I|. \tag{20}$$

In the following, if not specified, I may be open, half-open, or closed.

Lemma 4.5 (n-discrepancy control) *Let $\alpha \in (0, 1)$ be irrational. For each $\varepsilon \in (0, 1)$, there exists $\gamma \in (0, \varepsilon]$ such that each interval $I \subset \mathbb{R}$ with $|I| = \gamma$ satisfies*

$$|\phi_n(I)| \le \frac{C_\varepsilon}{n} \quad \forall\, n \in \mathbb{N}, \tag{21}$$

where C_ε depends on α and ε.

Proof Fix $\varepsilon \in (0, 1)$ and let $m \in \mathbb{N}$ be the smallest integer such that

$$\gamma := m\alpha \bmod 1 \in (0, \varepsilon). \tag{22}$$

Note that such m exists uniquely since α is irrational. Consider the interval $I = x_0 + [0, \gamma)$ for some $x_0 \in \mathbb{R}$. By choosing the constant C_ε in the statement sufficiently large, we limit ourselves in proving (21) for $n \ge m\lceil 1/\gamma \rceil$. Fix $k \in \mathbb{N}$ such that

$$m\lceil k/\gamma \rceil \le n < m\lceil (k+1)/\gamma \rceil. \tag{23}$$

Define $J_n = \bigcup_{j=0}^{n-1} \{j\alpha\}$ and the sets

$$J_n^i := \bigcup_{\ell=0}^{\lceil k/\gamma \rceil - 1} \{i\alpha + \ell\gamma\}, \quad \forall\, i = 0, \dots, m-1.$$

In view of (22) and $n \ge m\lceil k/\gamma \rceil$, we obtain

$$(J_n^i) \bmod 1 \subset (J_n) \bmod 1, \quad \forall\, i = 0, \dots, m-1. \tag{24}$$

In a similar fashion, $n < m\lceil (k+1)/\gamma \rceil$ implies

$$\#\left(J_n \setminus \bigcup_{i=0}^{m-1} J_n^i \right) \le m\lceil (k+1)/\gamma \rceil - m\lceil k/\gamma \rceil \le m(1 + 1/\gamma). \tag{25}$$

As $I = x_0 + [0, \gamma)$, it is not hard to see that

$$k = \#\big((\mathbb{N} + I) \cap J_n^i\big) \tag{26}$$

since k consecutive intervals in $\mathbb{N} + I$ contain exactly one element of J_n^i. By (24) we get

$$\sum_{i=0}^{m-1} \#\big((\mathbb{N} + I) \cap J_n^i\big) \le \sum_{j=0}^{n-1} \chi_{\mathbb{N}+I}(j\alpha) \le \sum_{i=0}^{m-1} \#\big((\mathbb{N} + I) \cap J_n^i\big) + \#\left(J_n \setminus \bigcup_{i=0}^{m-1} J_n^i\right).$$

This, along with (25) and (26), shows

$$\left|\sum_{j=0}^{n-1} \chi_{\mathbb{N}+I}(j\alpha) - km\right| \le \#\left(J_n \setminus \bigcup_{i=0}^{m-1} J_n^i\right) \le m(1 + 1/\gamma).$$

Since $|km/n - |I|| = |km/n - \gamma| \le m(1 + \gamma)/n$ by (23), we estimate

$$\begin{aligned} |\phi_n(I)| &\le \left|\frac{1}{n}\sum_{j=0}^{n-1} \chi_{\mathbb{N}+I}(j\alpha) - \frac{km}{n}\right| + \left|\frac{km}{n} - |I|\right| \\ &\le m(1 + 1/\gamma)/n + m(1 + \gamma)/n \le 2m(1 + 1/\gamma)/n \end{aligned}$$

so that the statement follows for $C_\varepsilon = 2m(1+1/\gamma)$. We point out that the proof can be easily adapted for open or closed intervals of length γ since the endpoints of the intervals appear at most once in the sequence $(j\alpha)_{j\in\mathbb{N}}$. □

Proof of Theorem 4.4 Fix $\varepsilon > 0$ and choose $\gamma \in (0, \varepsilon]$ as in Lemma 4.5. Define $I = x_0 + (0, \gamma)$ with $x_0 \in (0, 1 - \gamma)$ and $v_1(t) = h\chi_I(t)$ for $t \in [0, 1)$. For $x \in [0, 1)$, by applying Lemma 4.5 to the interval $I - x$ and recalling (20), we compute

$$\left|\frac{1}{n}V_n(x) - h|I|\right| = \left|\frac{1}{n}\sum_{j=0}^{n-1} v_1(x + j\alpha) - h|I|\right| = h\left|\frac{1}{n}\sum_{j=0}^{n-1} \chi_{\mathbb{N}+I-x}(j\alpha) - |I|\right| \le \frac{C_\varepsilon h}{n}.$$

Since $\int_0^1 v_1(t)\,\mathrm{d}t = h|I|$, the statement follows. □

5 Generic Noncrystallization: Proof of Theorem 1.1

This section is devoted to the proof of Theorem 1.1. In fact, we prove a more precise version of the statement under the assumption that α is algebraic. This in turn entails Theorem 1.1 by recalling that algebraic numbers are dense in the reals. We have the following.

Theorem 5.1 (Generic noncrystallization) *Let $\alpha \in (0, 1)$ be irrational and algebraic. For each $\varepsilon > 0$ and each 1-periodic, piecewise continuous, and lower semicontinuous function v_1 with $\min v_1 = 0$, there exists a 1-periodic, piecewise constant, and lower semicontinuous function v_1^ε with $\min v_1^\varepsilon = 0$ such that $\|v_1 - v_1^\varepsilon\|_{L^\infty(0,1)} \le \varepsilon$ and a strictly increasing sequence $(n_k)_{k\in\mathbb{N}} \in 2\mathbb{N}$ satisfying*

$$\big(V_{n_k}^\varepsilon\big)^* > \left(V_{n_k/2}^\varepsilon\right)^* + \left(V_{n_k/2}^\varepsilon\right)^* + 1,$$

where $(V_{n_k}^\varepsilon)^* := \min \sum_{j=0}^{n_k-1} v_1^\varepsilon(x + j\alpha)$. Consequently, it is energetically favorable to split an n_k-crystal into two $n_k/2$-crystals and no n_k-crystallization holds.

The proof of Theorem 5.1 is split in a series of lemmas. The statement crucially relies on some properties of the n-discrepancy of additive recurrent sequences, recall the definition (20). Firstly, for α irrational, [5, Theorem 1.51] yields a infinite subset $\mathcal{N}_\alpha \subset \mathbb{N}$ such that

$$\sup_{x\in(0,1)} |\phi_n([0,x))| \geq C_0 \frac{\log n}{n} \quad \forall\, n \in \mathcal{N}_\alpha \tag{27}$$

for a universal constant $C_0 > 0$. Secondly, if α is also algebraic, for each $\eta > 0$ there exists $C_\eta > 0$ such that the upper bound

$$\sup_{0<x<y<1} |\phi_n((x,y))| \leq C_\eta n^{-1+\eta} \quad \forall\, n \in \mathbb{N} \tag{28}$$

holds [14, Theorem 3.2 and Example 3.1, pp. 123–124].

Our first task is that of showing that, by possibly changing the constant, a lower bound like (27) holds not only at one single specific point, but that each interval of arbitrarily small length contains at least one point fulfilling (27).

Lemma 5.2 (Lower bound) *Let α be irrational and let $\mathcal{N}_\alpha \subset \mathbb{N}$ as in (27). Let $\varepsilon > 0$. Then there exists $N_\varepsilon \in \mathbb{N}$ such that for all $n \in \mathcal{N}_\alpha$ with $n \geq N_\varepsilon$ each interval $I \subset (0,1)$ with $|I| \geq \varepsilon$ contains a point $x \in I$ with*

$$|\phi_n([0,x))| \geq C_0 \frac{\log n}{2n}. \tag{29}$$

Proof Given $\varepsilon > 0$, choose $\gamma \in (0, \varepsilon]$ as in Lemma 4.5. Select N_ε sufficiently large such that

$$\log N_\varepsilon \geq \frac{6C_\varepsilon}{C_0\gamma}, \tag{30}$$

where C_ε is the constant of Lemma 4.5. Let $n \in \mathcal{N}_\alpha$ with $n \geq N_\varepsilon$. In view of (27), we choose $x_0 \in (0,1)$ satisfying

$$|\phi_n([0,x_0))| \geq C_0 \frac{2\log n}{3n}. \tag{31}$$

Consider the collection of points $x_k = x_0 + k\gamma$, $k \in \mathbb{Z}$, with $x_k \in (0,1)$. Note that $x_k \in (0,1)$ and $x_0 \in (0,1)$ imply $|k| \leq 1/\gamma$. For each $x_k \in (0,1)$, $k \geq 1$, we observe that

$$\phi_n([0,x_k)) = \phi_n([0,x_0)) + \sum_{l=1}^{k} \phi_n([x_{l-1},x_l)).$$

Therefore, since $|\phi_n([x_{l-1},x_l))| \leq C_\varepsilon/n$ for $l = 1,\dots,k$ by Lemma 4.5, we derive from estimates (30), (31), and $k \leq 1/\gamma$ that

$$|\phi_n([0,x_k))| \geq |\phi_n([0,x_0))| - \sum_{l=1}^{k} |\phi_n([x_{l-1},x_l))| \geq C_0 \frac{2\log n}{3n} - \frac{C_\varepsilon}{n\gamma} \geq C_0 \frac{\log n}{2n}.$$

The same estimate holds for each $x_k \in (0,1)$, $k \leq -1$. The result now follows from the fact that each interval in $(0,1)$ of length at least ε contains at least one of the points x_k. □

Next, we show that, by possibly reducing the constant, a point fulfilling a lower bound like (29) can be chosen independently of n.

Lemma 5.3 (Lower bound, independent of n) *Let $\delta \in (0,1)$. There exists a strictly increasing sequence of integers $(n_k)_{k\in\mathbb{N}} \subset \mathbb{N}$ and $x \in (0,\delta)$ such that*

$$|\phi_{n_k}([0,x))| \geq C_0 \frac{\log n_k}{4n_k} \quad \forall\, k \in \mathbb{N}.$$

Proof We define the sequence of integers $(n_k)_{k\in\mathbb{N}}$ iteratively. As first step of the iteration procedure, apply Lemma 5.2 to $(0,\delta)$ with $\varepsilon = \delta$. This gives $x_1 \in (0,\delta)$ and N_ε such that, by letting $n_1 = \min\{n \in \mathcal{N}_\alpha : n \geq N_\varepsilon\}$ one has $|\phi_{n_1}([0,x_1))| \geq C_0 \log n_1/(2n_1)$. In case $\phi_{n_1}([0,x_1)) > 0$, define $I_1 := (x_1, x_1+\delta_1)$ for some $0 < \delta_1 \leq C_0 \log n_1/(4n_1)$ so small that $I_1 \subset (0,\delta)$. We can then compute for all $x \in I_1$

$$\begin{aligned}\phi_{n_1}([0,x)) &= \frac{1}{n}\sum_{j=0}^{n-1} \chi_{\mathbb{N}+[0,x)}(j\alpha) - |[0,x)| \geq \frac{1}{n}\sum_{j=0}^{n-1} \chi_{\mathbb{N}+[0,x_1)}(j\alpha) - |[0,x_1)| - \delta_1 \\ &= \phi_{n_1}([0,x_1)) - \delta_1 \geq C_0 \frac{\log n_1}{2n_1} - \delta_1 \geq C_0 \frac{\log n_1}{4n_1}. \end{aligned} \tag{32}$$

If $\phi_{n_1}([0,x_1)) < 0$ instead, we repeat the argument for $I_1 := (x_1 - \delta_1, x_1) \subset (0,\delta)$ in place of $I_1 = (x_1, x_1+\delta_1)$.

Suppose now that for $\ell \in \mathbb{N}$ there exists a strictly increasing set of integers n_k, $1 \leq k \leq \ell - 1$, and nested intervals $I_{\ell-1} \subset I_{\ell-2} \subset \ldots I_1 \subset (0,\delta)$ such that

$$|\phi_{n_k}([0,x))| \geq C_0 \frac{\log n_k}{4n_k} \quad \forall\, x \in I_{\ell-1} \quad \forall\, 1 \leq k \leq \ell - 1. \tag{33}$$

We have already checked above that (33) can be realized for $\ell = 2$.

We now define n_ℓ and I_ℓ as follows. Fix $\varepsilon \leq |I_{\ell-1}|$.

By applying Lemma 5.2 to interval $I_{\ell-1}$ with ε one finds $x_\ell \in I_{\ell-1}$ and N_ε such that, by letting $n_\ell = \min\{n \in \mathcal{N}_\alpha : n \geq N_\varepsilon \text{ and } n \geq n_{\ell-1}+1\}$ one has

$$|\phi_{n_\ell}([0,x_\ell))| \geq C_0 \frac{\log n_\ell}{2n_\ell}. \tag{34}$$

We now construct I_ℓ by arguing as above: if $\phi_{n_\ell}([0,x_\ell)) > 0$, we define $I_\ell := (x_\ell, x_\ell + \delta_\ell)$ for some $0 < \delta_\ell \leq C_0 \log n_\ell/(4n_\ell)$ so small that $I_\ell \subset I_{\ell-1}$. By arguing as in (32) with the help of (34), we then compute for all $x \in I_\ell$

$$\phi_{n_\ell}([0,x)) \geq C_0 \frac{\log n_\ell}{4n_\ell}.$$

Along with the induction hypothesis (33) for $\ell - 1$, this shows that (33) holds for all $x \in I_\ell$ and all $1 \leq k \leq \ell$. If $\phi_{n_\ell}([0,x_\ell)) < 0$ instead, we repeat the argument for $I_\ell := (x_\ell - \delta_\ell, x_\ell) \subset I_{\ell-1}$ in place of $I_\ell = (x_\ell, x_\ell + \delta_\ell)$.

By performing this construction for each $k \in \mathbb{N}$, we obtain a sequence $(x_k)_{k\in\mathbb{N}}$ and nested intervals $(I_k)_{k\in\mathbb{N}} \subset (0,1)$. Since $|I_k| \to 0$, we have that $x_k \to x$, where x is the point with $\{x\} = \bigcap_{k=1}^{\infty} I_k$. The statement now follows from (33) and the fact that $x \in I_\ell$ for all $\ell \in \mathbb{N}$. □

Next, we construct an approximation of v_1 such that the sufficient condition for n-crystallization (19) is violated.

Lemma 5.4 (Approximation of v_1) *Let $\alpha \in (0,1)$ be irrational. There exists a strictly increasing sequence of integers $(n_k)_{k\in\mathbb{N}}$ such that the following holds: for each $\varepsilon > 0$ and each 1-periodic, piecewise continuous, and lower semicontinuous function v_1 with* $\min v_1 = 0$,

there exists a 1*-periodic, piecewise constant, and lower semicontinuous function* v_1^ε *with* $\min v_1^\varepsilon = 0$ *such that* $\|v_1 - v_1^\varepsilon\|_{L^\infty(0,1)} \le \varepsilon$ *and*

$$\frac{1}{n_k}(V_{n_k}^\varepsilon)^* - \int_0^1 v_1^\varepsilon(t)\,\mathrm{d}t \le -C\frac{\log n_k}{n_k} \quad \forall k \in \mathbb{N}, \tag{35}$$

for some $C > 0$ *only depending on* α, ε, *and* v_1, *where* $(V_{n_k}^\varepsilon)^* := \min \sum_{j=0}^{n_k-1} v_1^\varepsilon(x + j\alpha)$.

Proof Our goal is approximate v_1 by a piecewise constant function with the desired property. Fix $\delta > 0$ small. We apply Lemma 5.3 to get a sequence $(n_k)_{k\in\mathbb{N}}$ and $x_1 \in (0, \delta)$ such that

$$|\phi_{n_k}([0, x_1))| \ge \frac{C_0 \log n_k}{4n_k} \quad \forall\, k \in \mathbb{N} \tag{36}$$

holds. Moreover, we choose $\gamma \in (0, \delta]$ as in Lemma 4.5 (applied for δ in place of ε), and we decompose the interval $(0, 1)$ by means of the points $x_0 = 0 < x_1 < x_2 < \ldots < x_l = 1$ such that

$$x_i - x_{i-1} = \gamma \quad \forall\, i = 3, \ldots, l.$$

Note that $l \le 2 + 1/\gamma$ and that $|x_i - x_{i-1}| \le \delta$ for $i = 1, \ldots, l$. Since Lemma 4.5 implies $|\phi_{n_k}([x_{i-1}, x_i))| \le C_\delta/n_k$ for all $i = 3, \ldots, l$, we find

$$\big|\phi_{n_k}([0, x_1)) + \phi_{n_k}([x_1, x_2))\big| \le \left|\sum_{i=3}^{l} \phi_{n_k}([x_{i-1}, x_i))\right| \le \frac{C_\delta}{\gamma n_k}. \tag{37}$$

Without restriction we treat the case $\phi_{n_k}([0, x_1)) > 0$. The other case is similar but requires a different notational realization. We define a piecewise constant, 1-periodic function v_1^ε by setting

$$v_1^\varepsilon = b_i \quad \text{on } (x_{i-1}, x_i) \quad \text{for } i = 1 \ldots, l \tag{38}$$

for suitable $b_i \in [0, M]$, where $M := \sup v_1$. The values at x_i, $i = 0 \ldots, l - 1$, can be chosen in such a way that the function is lower semicontinuous. Recall $|x_i - x_{i-1}| \le \delta$ for $i = 1, \ldots, l$. Thus, given $\varepsilon > 0$, we observe that by choosing $\delta = \delta(\varepsilon) > 0$ sufficiently small and the values b_i appropriately, we can achieve $\|v_1^\varepsilon - v_1\|_{L^\infty(0,1)} \le \varepsilon$. Moreover, this can be done in such a way that $b_1 < b_2$ and that $\min_i b_i = 0$. We now check (35). First, in view of definition (38) and (20), we compute

$$\begin{aligned}
&\min_{x\in[0,1)} \frac{1}{n_k}\sum_{j=0}^{n_k-1} v_1^\varepsilon(x + j\alpha) - \int_0^1 v_1^\varepsilon(t)\,\mathrm{d}t \le \frac{1}{n_k}\sum_{j=0}^{n_k-1} v_1^\varepsilon(j\alpha) - \int_0^1 v_1^\varepsilon(t)\,\mathrm{d}t \\
&\le \sum_{i=1}^{l} b_i\Big(\frac{1}{n_k}\sum_{j=0}^{n_k-1} \chi_{[x_{i-1},x_i)+\mathbb{N}}(j\alpha) - |x_i - x_{i-1}|\Big) \\
&= \sum_{i=1}^{l} b_i\,\phi_{n_k}([x_{i-1}, x_i)).
\end{aligned} \tag{39}$$

Moreover, by $\max_i b_i \le M$, $b_1 - b_2 < 0$, and $\phi_{n_k}([0, x_1)) > 0$ we obtain from estimates (36) and (37) that

$$\sum_{i=1}^{l} b_i\,\phi_{n_k}([x_{i-1}, x_i)) \le (b_1 - b_2)\phi_{n_k}([x_0, x_1)) + M\big|\phi_{n_k}([x_0, x_1)) + \phi_{n_k}([x_1, x_2))\big|$$

$$+ M \sum_{i=3}^{l} \left|\phi_{n_k}([x_{i-1}, x_i))\right|$$
$$\leq (b_1 - b_2)\frac{C_0 \log n_k}{4n_k} + \frac{2MC_\delta}{\gamma n_k}.$$

This along with (39) shows

$$\min_{x\in[0,1)} \frac{1}{n_k} \sum_{j=0}^{n_k-1} v_1^\varepsilon(x + j\alpha) - \int_0^1 v_1^\varepsilon(t)\,\mathrm{d}t \leq -C\frac{\log n_k}{n_k}$$

for all $k \in \mathbb{N}$ for some suitable $C > 0$ only depending on α, δ, and v_1. □

Eventually, we establish the following upper bound.

Lemma 5.5 (Upper bound) *Let $\alpha \in (0, 1)$ be irrational and algebraic. Let v_1 be a 1-periodic, lower semicontinuous function of the form $v_1 = \sum_{i=1}^k b_i \chi_{I_i}$ for intervals $I_i \subset (0, 1)$. Then there holds*

$$\left|\frac{1}{n}V_n - \int_0^1 v_1(t)\,\mathrm{d}t\right| \leq C_\eta\, n^{-1+\eta} \quad \forall n \in \mathbb{N},$$

for some $C_\eta > 0$ only depending on α, η, and v_1.

Proof Arguing as in the proof of the approximation Lemma 5.4, we calculate

$$\left|\frac{1}{n}V_n - \int_0^1 v_1(t)\,\mathrm{d}t\right| \leq \left(\max_i b_i\right) \sum_{i=1}^k |\phi_n(I_i)|,$$

where $\phi_n(I_i)$ is defined in (20). The statement follows from the fact that $|\phi_n(I_i)| \leq C_\eta n^{-1+\eta}$ for all $n \in \mathbb{N}$, see (28). □

We are finally in the position of proving Theorem 5.1.

Proof of Theorem 5.1 Given $v_1, \alpha \in (0, 1)$ irrational and algebraic, and $\varepsilon > 0$, we define the piecewise constant, lower semicontinuous function v_1^ε as in the approximation Lemma 5.4. We aim at showing that for each $n' \in \mathbb{N}$ we can find $n \in 2\mathbb{N}$ with $n \geq n'$ such that it is energetically favorable to split an n-crystal into two $n/2$-crystals, i.e.,

$$\left(V_n^\varepsilon\right)^* > \left(V_{n/2}^\varepsilon\right)^* + \left(V_{n/2}^\varepsilon\right)^* + 1. \tag{40}$$

For all $r \in \mathbb{N}$, define the *error* as

$$e(r) := \left(V_r^\varepsilon\right)^* - r\int_0^1 v_1^\varepsilon(t)\,\mathrm{d}t. \tag{41}$$

Fix $n' \in \mathbb{N}$. By the approximation Lemma 5.4 we find $n_0 \geq n'$ such that $e(n_0) < -C \log n_0$ for C only depending on α, ε, and v_1. We can suppose that n_0 is chosen large enough such that $e(n_0) \leq -2$. We claim that there exists $k \in \mathbb{N}$ such that

$$2\,e\left(n_0 2^{k-1}\right) + 1 < e\left(n_0 2^k\right). \tag{42}$$

In fact, assume that this was not the case. Then, we would have $2e(n_0 2^{k-1}) + 1 \geq e(n_0 2^k)$ for all $k \in \mathbb{N}$. Consequently, by an iterative application of this estimate and by using $e(n_0) \leq -2$ we get

$$e\left(n_0 2^k\right) \leq 2^k e(n_0) + 2^k - 1 \leq -2^k \quad \forall\, k \in \mathbb{N}.$$

This contradicts the fact that $|e(n_0 m)| \leq C_\eta (n_0 m)^\eta$ for all $m \in \mathbb{N}$, as predicted by the upper bound in Lemma 5.5. Thus, (42) holds for some $k \in \mathbb{N}$. Set now $n := n_0 2^k$ and use (41) to compute

$$(V_n^\varepsilon)^* = e(n) + n \int_0^1 v^\varepsilon(t)\,\mathrm{d}t > 1 + 2\left(e(n/2) + \frac{n}{2}\int_0^1 v_1^\varepsilon(t)\,\mathrm{d}t\right) = 1 + 2\left(V_{n/2}^\varepsilon\right)^*.$$

This shows (40) and concludes the proof. □

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