

Quantum Stabilization in Anharmonic Crystals

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For a lattice model of interacting quantum particles of mass m oscillating in a double-well crystalline field, a mechanism of its stabilization by quantum effects is described. Namely, a stability condition involving the mass m , the interaction intensity and the parameters of the crystalline field is given. It is independent of the temperature and is satisfied if the mass m is small enough and/or the tunneling frequency is big enough. It is shown that under this condition the infinite-volume free energy density is an analytic function of the external field and the displacement-displacement correlation function decays exponentially, hence no critical point anomalies and phase transitions can arise at all temperatures, which qualitatively agree with experimental data. This gives a complete and mathematically rigorous answer to the question about the influence of quantum effects on structural phase transitions, the discussion of which was initiated in the article [8].

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INTRODUCTION

Ordering of interacting localized quantum particles performing anharmonic oscillations may trigger structural phase transitions. A typical example here is the phase transition in *KDP*-type ferroelectrics with hydrogen bonds, in which such particles are protons or deuterons tunneling along hydrogen bounds between double wells [5], [9], [10]. The Hamiltonian of the simplest model describing a system of such particles is

$$H = \sum_l \left[\frac{1}{2m} p_l^2 + \frac{a}{2} q_l^2 + \frac{b}{4} q_l^4 \right] - \frac{1}{2} \sum_{l, l'} J_{ll'} q_l q_{l'}, \quad (1)$$

where the sums run through \mathbf{Z}^d , p_l and q_l are scalar momentum and displacement operators of the particle oscillating around $l \in \mathbf{Z}^d$, m is the particle mass divided by \hbar^2 and $J_{ll'}$ is the interaction potential. We assume that $a \in \mathbf{R}$, $b > 0$, and that $J_{ll'}$ is a function of the distance between the lattice sites, i.e., $J_{ll'} = \phi(|l - l'|)$, such that $J_{ll'} \geq 0$, $J_{ll} = 0$ and

$$\hat{J}(0) = \sum_{l'} J_{ll'} < \infty.$$

The system (1) in an external field $h \in \mathbf{R}$ is described by the Hamiltonian $H - h \sum_l q_l$.

Since the seventies, understanding the influence of quantum effects on phase transitions is one of the main problem in the theory of systems of this kind, see [8], [9], [11]. It has been known that the *KDP*-type ferroelectrics are getting more stable if one replaces deuterons

by protons. On the other hand, high hydrostatic pressure, applied to such a crystal (which increases tunneling by making minima of the wells closer to each other), also decreases the Curie temperature T_C (see p.188 of the book [5]). In the pioneering paper [8] (see also [11] for a rigorous proof) it was shown that the long range order in such systems is suppressed if the particle mass is small. At the same time, no explanation of the influence of pressure was given and the quantum mechanical origin of such stabilization has remained unclear. In the present note we propose a mathematically rigorous description of the mechanism of such stabilization, which explains both these effects and the role of the anharmonism. It may be outlined as follows. If the tunneling between the wells gets intensive (smaller mass or closer minima), the particle “forgets” about the details of the potential energy in the vicinity of the origin (including instability) and oscillates as if its equilibrium at zero is stable. If the potential energy grows at infinity faster than x^2 , the oscillations become more and more rigid as $m \rightarrow 0$, which completely stabilizes the system.

In the harmonic case $b = 0$, the system (1) is stable provided $a > \hat{J}(0)$, which may be written $m\delta_{\text{har}}^2 > \hat{J}(0)$, where $\delta_{\text{har}} = \sqrt{a/m}$ is the difference between the eigenvalues of $H_l^{\text{har}} = p_l^2/2m + (a/2)q_l^2$. For $b > 0$ and $a < \hat{J}(0)$, the equilibrium positions at zero become unstable, which yields a structural phase transition if the mass m and the inverse temperature β are big enough (a proof for the case of $d \geq 3$ and short-range interactions was given in [4]). This phase transition is of *displacive*

type if $a \in [0, \hat{J}(0))$, and it is of *order-disorder type* if $a < 0$ (see [5], [8], [9]). In both cases the mentioned instability causes the appearance of *soft-mode* collective excitations, see p.11-18 in [5]. On the other hand, at the transition point the infinite-volume free energy density, as a function of the external field, becomes nonanalytic at $h = 0$ (see Chapter 5 in [7]), which means, in particular, that the dielectric susceptibility diverges.

In this note we show that under the stability condition

$$m\delta^2 > \hat{J}(0), \quad (2)$$

the free energy density of the model (1) is an analytic function of the external field $h \in \mathbf{R}$, hence no phase transitions can arise at any temperature. This condition also yields that the soft-mode excitations are suppressed at all temperatures. Here

$$\delta = \delta(m, a, b) = \min_{n \in \mathbf{N}} \{E_n - E_{n-1}\}, \quad (3)$$

and E_n are the eigenvalues of the Hamiltonian

$$H_{\mathbf{l}} = p_{\mathbf{l}}^2/2m + (a/2)q_{\mathbf{l}}^2 + (b/4)q_{\mathbf{l}}^4. \quad (4)$$

The proof is performed in the Euclidean approach, which is described in [2].

As was shown in [1], $m\delta^2$ is a continuous function of m , such that $m\delta^2 \sim Cm^{-1/2}$, $C > 0$, as $m \rightarrow 0$. Thus, the condition (2) is satisfied if $m \in (0, m_*)$ for some $m_* = m_*(\hat{J}(0), a, b) > 0$, which depends on $\hat{J}(0)$, a and b only. Since in (2) the parameter $m\delta^2$ plays the same role

as the rigidity of the harmonic oscillator a does in the corresponding stability condition, it may be considered as a measure of *quantum rigidity*.

THE RESULTS AND DISCUSSION

Given a positive integer L , we consider the cube $\Lambda = (-L, L]^d \cap \mathbf{Z}^d$, which contains $N = (2L)^d$ lattice points. For $\mathbf{l}, \mathbf{l}' \in \Lambda$, we set $J_{\mathbf{l}\mathbf{l}'}^\Lambda = \phi(|\mathbf{l} - \mathbf{l}'|_\Lambda)$, where $|\mathbf{l} - \mathbf{l}'|_\Lambda$ is the distance on the torus which one obtains by identifying the opposite walls of Λ . The local Hamiltonians $H_\Lambda(h|b)$, for empty $b = 0$ and periodic $b = p$ boundary conditions, are

$$H_\Lambda(h|b) = H_\Lambda(0|b) - h \sum_{\mathbf{l} \in \Lambda} q_{\mathbf{l}}, \quad (5)$$

$$H_\Lambda(0|0) = \sum_{\mathbf{l} \in \Lambda} H_{\mathbf{l}} - \frac{1}{2} \sum_{\mathbf{l}, \mathbf{l}' \in \Lambda} J_{\mathbf{l}\mathbf{l}'} q_{\mathbf{l}} q_{\mathbf{l}'},$$

$$H_\Lambda(0|p) = \sum_{\mathbf{l} \in \Lambda} H_{\mathbf{l}} - \frac{1}{2} \sum_{\mathbf{l}, \mathbf{l}' \in \Lambda} J_{\mathbf{l}\mathbf{l}'}^\Lambda q_{\mathbf{l}} q_{\mathbf{l}'}. \quad (6)$$

Set

$$Z_{\beta, \Lambda}(h|b) = \text{trace} \exp(-\beta H_\Lambda(h|b)), \quad b = 0, p. \quad (6)$$

$$F_\Lambda(h) = -\frac{1}{\beta N} \ln Z_{\beta, \Lambda}(h|0). \quad (7)$$

Given Λ , $\mathbf{l}_1, \dots, \mathbf{l}_n \in \Lambda$ and $0 \leq \tau_1 \leq \dots \leq \tau_n \leq \beta$, we also set

$$\Gamma_{\mathbf{l}_1 \dots \mathbf{l}_n}^\Lambda(\tau_1, \dots, \tau_n | h, b) = \frac{1}{Z_\Lambda(h|b)} \text{trace} \left\{ q_{\mathbf{l}_1} e^{-(\tau_2 - \tau_1) H_\Lambda(h|b)} \dots q_{\mathbf{l}_n} e^{-(\beta - \tau_n + \tau_1) H_\Lambda(h|b)} \right\}. \quad (8)$$

This function has a symmetric extension to $[0, \beta]^n$, for which we shall use the same notation. Furthermore, we set

$$\begin{aligned} U_{\mathbf{l}_1 \dots \mathbf{l}_4}^\Lambda(\tau_1, \dots, \tau_4) &= \\ &= \Gamma_{\mathbf{l}_1 \dots \mathbf{l}_4}^\Lambda(\tau_1, \dots, \tau_4 | 0, p) - \\ &- \Gamma_{\mathbf{l}_1 \mathbf{l}_2}^\Lambda(\tau_1, \tau_2 | 0, p) \Gamma_{\mathbf{l}_3 \mathbf{l}_4}^\Lambda(\tau_3, \tau_4 | 0, p) - \\ &- \Gamma_{\mathbf{l}_1 \mathbf{l}_3}^\Lambda(\tau_1, \tau_3 | 0, p) \Gamma_{\mathbf{l}_2 \mathbf{l}_4}^\Lambda(\tau_2, \tau_4 | 0, p) - \\ &- \Gamma_{\mathbf{l}_1 \mathbf{l}_4}^\Lambda(\tau_1, \tau_4 | 0, p) \Gamma_{\mathbf{l}_2 \mathbf{l}_3}^\Lambda(\tau_2, \tau_3 | 0, p), \end{aligned} \quad (9)$$

and

$$M_{\mathbf{l}}^\Lambda(h|b) = \Gamma_{\mathbf{l}}^\Lambda(\tau | h, b), \quad (10)$$

$$K_{\mathbf{l}\mathbf{l}'}^\Lambda(\tau, \tau' | h, b) = \Gamma_{\mathbf{l}\mathbf{l}'}^\Lambda(\tau, \tau' | h, b) - M_{\mathbf{l}}^\Lambda(h|b) M_{\mathbf{l}'}^\Lambda(h|b). \quad (11)$$

In the approach [2] the existence of the infinite-volume free energy density

$$F(h) = \lim_{L \rightarrow +\infty} F_\Lambda(h), \quad (12)$$

may be proven for any $\beta > 0$ and $h \in \mathbf{R}$ in a way similar as in the proof of the corresponding result for classical models given in [6]. It may be also proven that the infinite-volume correlation function

$$K_{\mathbf{l}\mathbf{l}'}(\tau, \tau' | h) = \lim_{L \rightarrow +\infty} K_{\mathbf{l}\mathbf{l}'}^\Lambda(\tau, \tau' | h, 0), \quad (13)$$

exists for all $h \in \mathbf{R}$, $\mathbf{l}, \mathbf{l}' \in \mathbf{Z}^d$ and $\tau, \tau' \in [0, \beta]$. Set $\mathcal{N} = \{\nu = (2\pi/\beta)n : n \in \mathbf{Z}\}$ and

$$\hat{J}(\mathbf{k}) = \sum_{\nu \in \mathcal{Z}^d} J_{\mathbf{l}\mathbf{l}'} e^{i\mathbf{k} \cdot (\mathbf{l} - \mathbf{l}')}, \quad \mathbf{k} \in (-\pi, \pi]^d. \quad (14)$$

Theorem. *Let the stability condition (2) be satisfied. Then for any $\beta > 0$, the free energy density (12) is an analytic function of the external field $h \in \mathbf{R}$ and, for*

all $h \in \mathbf{R}$, $\mathbf{l}, \mathbf{l}' \in \mathbf{Z}^d$ and $\tau, \tau' \in [0, \beta]$, the correlation function (13) obeys the estimates

$$0 \leq K_{\mathbf{U}}(\tau, \tau'|h) \leq \frac{1}{\beta(2\pi)^d} \sum_{\nu \in \mathcal{N}} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{\exp[i\nu(\tau - \tau') + i\mathbf{k} \cdot (\mathbf{l} - \mathbf{l}')] }{m\delta^2 - \hat{J}(\mathbf{k}) + \Xi(\nu)} d^d k, \quad (15)$$

where

$$\Xi(\nu) = \Xi(-\nu) \geq m\nu^2, \quad (16)$$

where uniformly in β .

In what follows, the analyticity of the free energy density stated above corresponds to the absence of any critical point anomaly. In case of short-range interactions (i.e., of nearest-neighbor type) the upper bound in (15) implies that, for any $\beta > 0$, there exist $C(\beta) > 0$ and $\xi(\beta) > 0$ such that

$$K_{\mathbf{U}}(\tau, \tau'|h) \leq C(\beta) \exp(-|\mathbf{l} - \mathbf{l}'|/\xi(\beta)),$$

for all $\mathbf{l}, \mathbf{l}' \in \mathbf{Z}^d$, which means that the correlation length remains finite at all temperatures. By (16), the denominator of the expression on the right-hand side of (15) is positive for all ν and \mathbf{k} , including $\nu = 0$, $\mathbf{k} = 0$, if (2) holds. This means that the soft-mode excitations are absent (suppressed) at all temperatures.

The above results may be extended as follows. The theorem remains valid if one replaces in (1) $(a/2)q_{\mathbf{l}} + (b/4)q_{\mathbf{l}}^4$ by the polynomial $v(q_{\mathbf{l}}^2) = (a/2)q_{\mathbf{l}} + (b_2/4)q_{\mathbf{l}}^4 + \dots + (b_r/2r)q_{\mathbf{l}}^{2r}$, $r > 2$, such that $v''(t) > 0$ for all $t \geq 0$. In this case the small mass asymptotics of the quantum rigidity is $m\delta^2 \sim Cm^{-(r-1)/(r+1)}$, $C > 0$ [1], which yields that the stability condition (2) is satisfied for $m \in (0, m_*)$, where m_* depends on $\hat{J}(0)$ and on the parameters a, b_2, \dots, b_r only. A much stronger result of this type has been proven in [3]. For the model (1), it implies that the Euclidean Gibbs state is unique at all temperatures and all $h \in \mathbf{R}$ provided $m[\delta(m, a, b/2)]^2 > \hat{J}(0)$ (c.f., (3)), which holds for $m < m_*(\hat{J}(0), a, b/2)$.

THE SKETCH OF THE PROOF

In the approach [2] one can prove the following inequalities, which hold for all parameters and variables of the functions involved. For any Λ ,

$$0 \leq K_{\mathbf{U}}^{\Lambda}(\tau, \tau'|h, b) \leq K_{\mathbf{U}}^{\Lambda}(\tau, \tau'|0, b), \quad b = p, 0. \quad (17)$$

For any Λ' , such that $\Lambda \subset \Lambda'$,

$$K_{\mathbf{U}}^{\Lambda}(\tau, \tau'|0, 0) \leq K_{\mathbf{U}}^{\Lambda'}(\tau, \tau'|0, 0) \leq K_{\mathbf{U}}^{\Lambda'}(\tau, \tau'|0, p). \quad (18)$$

For a one-point subset $\{\mathbf{l}\}$, the correlation function is

$$K_{\mathbf{U}}^{\{\mathbf{l}\}}(\tau, \tau'|0) = \frac{1}{Z_{\mathbf{l}}} \text{trace}\{q_{\mathbf{l}} e^{-(\tau'-\tau)H_{\mathbf{l}}} q_{\mathbf{l}} e^{-(\beta-\tau'+\tau)H_{\mathbf{l}}}\},$$

where $Z_{\mathbf{l}} = \text{trace}[\exp(-\beta H_{\mathbf{l}})]$. For $\nu \in \mathcal{N}$, we set

$$\kappa(\nu) = \int_0^{\beta} K_{\mathbf{U}}^{\{\mathbf{l}\}}(\tau, \tau'|0) \cos[\nu(\tau - \tau')] d\tau'. \quad (19)$$

Inserting here the above expression one obtains

$$\kappa(\nu) = \frac{1}{Z_{\mathbf{l}}} \sum_{n, n'=1}^{\infty} (q_{nn'})^2 \frac{(E_n - E_{n'})(e^{-\beta E_{n'}} - e^{-E_n})}{\nu^2 + (E_n - E_{n'})^2},$$

where $q_{nn'} = \langle \psi_n | q_{\mathbf{l}} | \psi_{n'} \rangle$ and $H_{\mathbf{l}} | \psi_n \rangle = E_n | \psi_n \rangle$. By symmetry, $q_{nn} = 0$, hence the denominator may be estimated with the help of (3), which yields

$$\begin{aligned} \kappa(\nu) &\leq \frac{1}{\nu^2 + \delta^2} \cdot \frac{1}{Z_{\mathbf{l}}} \text{trace}\{[q_{\mathbf{l}}, [H_{\mathbf{l}}, q_{\mathbf{l}}]] e^{-\beta H_{\mathbf{l}}}\} = \\ &= \frac{1}{m(\nu^2 + \delta^2)}. \end{aligned} \quad (20)$$

Set

$$\hat{J}^{\Lambda}(\mathbf{k}) = \sum_{\nu \in \Lambda} J_{\mathbf{U}}^{\Lambda} \cos[\mathbf{k} \cdot (\mathbf{l} - \mathbf{l}')],$$

and $\Lambda_* = \{\mathbf{k} = (k_1, \dots, k_d) : k_j = -\pi + (\pi/L)s_j, s_j = 1, \dots, L\}$. Let us show now that under the condition

$$\kappa(0)\hat{J}(0) < 1, \quad (21)$$

the following estimate

$$\begin{aligned} K_{\mathbf{U}}^{\Lambda}(\tau, \tau'|0, p) &\leq \\ &\leq \frac{1}{\beta N} \sum_{\mathbf{k} \in \Lambda_*} \sum_{\nu \in \mathcal{N}} \frac{\exp[i\nu(\tau - \tau') + i\mathbf{k} \cdot (\mathbf{l} - \mathbf{l}')] }{[\kappa(\nu)]^{-1} + \hat{J}^{\Lambda}(\mathbf{k})}, \end{aligned} \quad (22)$$

holds for every Λ , all $\mathbf{l}, \mathbf{l}' \in \Lambda$ and $\tau, \tau' \in [0, \beta]$. Indeed, for $t \in [0, 1]$, let $R_{\mathbf{l}_1, \dots, \mathbf{l}_d}(\tau_1, \dots, \tau_d | t)$ (resp., $X_{\mathbf{U}}(\tau, \tau' | t)$) denote the Ursell function (9) (resp., the correlation function $K_{\mathbf{U}}^{\Lambda}(\tau, \tau' | 0, p)$) calculated with the Hamiltonian

$$H_{\Lambda}(t) = \sum_{\mathbf{l} \in \Lambda} H_{\mathbf{l}} - \frac{t}{2} \sum_{\mathbf{l}, \mathbf{l}' \in \Lambda} J_{\mathbf{U}}^{\Lambda} q_{\mathbf{l}} q_{\mathbf{l}'},$$

instead of $H_{\Lambda}(0|p)$. One can show that the functions $X_{\mathbf{U}}(\tau, \tau' | t)$ satisfy the following system of equations

$$\frac{\partial}{\partial t} X_{\mathbf{l}'}(\tau, \tau'|t) = \frac{1}{2} \sum_{\mathbf{l}_1, \mathbf{l}_2 \in \Lambda} J_{\mathbf{l}_1 \mathbf{l}_2}^\Lambda \int_0^\beta R_{\mathbf{l} \mathbf{l}_1 \mathbf{l}_2}(\tau, \tau', \tau_1, \tau_1|t) d\tau_1 + \sum_{\mathbf{l}_1, \mathbf{l}_2 \in \Lambda} J_{\mathbf{l}_1 \mathbf{l}_2}^\Lambda \int_0^\beta X_{\mathbf{l}_1}(\tau, \tau_1|t) X_{\mathbf{l}_2}(\tau', \tau_1|t) d\tau_1, \quad (23)$$

subject to the conditions

$$X_{\mathbf{l}'}(\tau, \tau'|0) = \delta_{\mathbf{l}'} K_{\mathbf{l}'}^{\{\mathbf{l}'\}}(\tau, \tau'|0), \quad (24)$$

$$X_{\mathbf{l}'}(\tau, \tau'|1) = K_{\mathbf{l}'}^\Lambda(\tau, \tau'|0, p). \quad (25)$$

The first term in (23) is non-positive since, by the Lebowitz inequality (see [2]),

$$R_{\mathbf{l}_1 \dots \mathbf{l}_4}(\tau_1, \dots, \tau_4|t) \leq 0. \quad (26)$$

Now let $Y_{\mathbf{l}'}(\tau, \tau'|t)$ be a solution of

$$\frac{\partial}{\partial t} Y_{\mathbf{l}'}(\tau, \tau'|t) = \quad (27)$$

$$= \sum_{\mathbf{l}_1, \mathbf{l}_2 \in \Lambda} J_{\mathbf{l}_1 \mathbf{l}_2}^\Lambda \int_0^\beta Y_{\mathbf{l}_1}(\tau, \tau_1|t) Y_{\mathbf{l}_2}(\tau', \tau_1|t) d\tau_1,$$

$$Y_{\mathbf{l}'}(\tau, \tau'|0) = X_{\mathbf{l}'}(\tau, \tau'|0).$$

By means of monotonicity methods (see [12]) and (26), the solutions of (23) and (27) can be compared

$$X_{\mathbf{l}'}(\tau, \tau'|t) \leq Y_{\mathbf{l}'}(\tau, \tau'|t), \quad t \in [0, 1]. \quad (28)$$

The system (27) may be diagonalized and solved (under the condition (21)). The solution is

$$Y_{\mathbf{l}'}(\tau, \tau'|t) = \quad (29)$$

$$= \frac{1}{\beta|\Lambda|} \sum_{\mathbf{k} \in \Lambda} \sum_{\nu \in \mathcal{N}} \frac{\exp[i\nu(\tau - \tau') + i\mathbf{k} \cdot (\mathbf{l} - \mathbf{l}')] }{[\kappa(\nu)]^{-1} + t\hat{J}^\Lambda(\mathbf{k})}.$$

Inserting it into (28) and taking there $t = 1$ one gets (22) by (25). Passing in (22) to the limit $L \rightarrow +\infty$ and taking into account (18) we arrive at (15) with $\Xi(\nu) = [\kappa(\nu)]^{-1}$. By means of the Lee-Yang theorem (see p.108 in [7]) one may prove that $F(h)$ is analytic in a strip of the complex plane, which includes the real line, if it is differentiable at any $h \in \mathbf{R}$. Obviously, for any Λ , $F_\Lambda(h)$ is analytic in such a strip hence infinitely differentiable at any $h \in \mathbf{R}$. If one has a sequence $\{f_n\}$ of two times continuously differentiable functions, which (a) converges pointwise on \mathbf{R} to a function f ; (b) satisfies the conditions $|f'_n(h)| \leq C_1$, $|f''_n(h)| \leq C_2$ for all $n \in \mathbf{N}$ and $h \in \mathbf{R}$. Then f is differentiable on \mathbf{R} . Thereby, to complete the proof one has to show that the first and second derivatives of $(1/\beta N) \ln Z_\Lambda(h|0)$ are bounded as $N \rightarrow +\infty$. In the approach [2] one obtains

$$\frac{\partial}{\partial h} \left(\frac{1}{\beta N} \ln Z_\Lambda(h|0) \right) = \frac{1}{N} \sum_{\mathbf{l} \in \Lambda} M_{\mathbf{l}}^\Lambda(h|0), \quad (30)$$

$$\frac{\partial^2}{\partial h^2} \left(\frac{1}{\beta N} \ln Z_\Lambda(h|0) \right) = \frac{1}{N} \sum_{\mathbf{l}, \mathbf{l}' \in \Lambda} \int_0^\beta K_{\mathbf{l} \mathbf{l}'}^\Lambda(0, \tau|h, 0) d\tau.$$

By the mean value theorem and (17), one has

$$\left| \frac{1}{N} \sum_{\mathbf{l} \in \Lambda} M_{\mathbf{l}}^\Lambda(h|0) \right| \leq \frac{|h|}{N} \sum_{\mathbf{l}, \mathbf{l}' \in \Lambda} \int_0^\beta K_{\mathbf{l} \mathbf{l}'}^\Lambda(0, \tau|0, 0) d\tau,$$

thus, both derivatives in (30) are bounded if the sequence

$$\left\{ \frac{1}{N} \sum_{\mathbf{l}, \mathbf{l}' \in \Lambda} \int_0^\beta K_{\mathbf{l} \mathbf{l}'}^\Lambda(0, \tau|0, 0) d\tau \right\}_{L \in \mathbf{N}, L \geq L_0}$$

is bounded, which readily follows from (15). Here L_0 is taken in such a way that $\mathbf{l}, \mathbf{l}' \in (-L_0, L_0]^d \cap \mathbf{Z}^d$.

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