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# JUMP KINETICS ON THE FIBONACCI QUASILATTICE. EXACTLY SOLVABLE MODEL OF THE LAYER GROWTH AND DISLOCATION KINETICS IN QUASICRYSTALS

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The jump kinetics on a quasiperiodic pinning potential is analyzed under small external force in a model of 1D Fibonacci quasilattice. The model describes planar (layer) growth of stable quasicrystals from the melt and is also relevant to the movement of quasicrystal dislocations under small stress. Exact solution is found for the spectrum of jump length as function of the driving force. The solution describes the supercooling dependence of the nucleus heights spectrum on the growing surface of a quasicrystal. The spectrum appears to be universal and its shape has a periodical dependence on the logarithm of supercooling. Resulting quasicrystal growth kinetics agrees well with that found in the computer simulations and in the analysis of continuous thermodynamic models.

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Dynamics of a crystal growth is usualy studied through the kinetic equation for a model Hamiltonian that involves a surface tension along with the pinning term [1, 2]. Supercooling is a thermodynamic driving force and the kinetic coefficient corresponds to the surface mobility. The model describes temperature-induced roughening transition between the smooth and rough states of equilibrium surface as well as dynamic roughening transition separating normal and layer growth mechanisms. A layer (planar) growth proceeds through the thermally activated nucleation of 2D nuclei followed by their lateral expansion via the movement of the surface steps [3]. Thus, surface jumps between the minima of pinning potential with the jump length being equal to the period of pinning potential *i.e.* the lattice period in the direction of growth. The growth rate in this case has an exponential dependence on the supercooling in a contrast with nomal growth where this dependence is linear [2, 3].

In the case of quasicrystals the pinning potential is quasiperiodical due to quasiperiodicity of their atomic structure. The thermodynamic roughening temperature appears to be infinite [4, 5] and, hence, the equilibrium surface remains smooth at any temperature. This corresponds to experimentally observed growth shapes for stable quasicrystals and implies the layer growth at sufficiently small supercoolings [2]. Due to quasiperiodicity the thickness of growing layer of a quasicrystal can take values from a dense set of the "interplane distances" [6]. Thus, during growth of quasicrystal under fixed supercooling there is some spectrum of the thickness of growing layer (nucleus height).

In this paper I present the exact form of this nucleus height spectrum obtained by solving the pinning problem on the 1D Fibonacci quasilattice. The model is also relevant to the movement of dislocations in quasicrystals under small stress due to the fact that intrinsic 'phason' contribution into the energy of dislocation leads to the quasiperiodic

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Peierls potential. The paper is organized as follows. After description of some features of quasicrystal growth and brief analysis of the dislocation mobility in quasicrystals the 1D kinetic problem is formulated. The exact solution of this problem is then presented followed by the discussion of its implications with respect to available experimental data.

For conventional crystals the energy of any perturbation on a flat solid-liquid interface consists of the bulk supercooling term along with the free energy of a linear step that has large entropic contribution [3]. This entropic term makes step free energy negative at the temperatures above thermodynamic roughening transition for conventional crystals. As the quasicrystal structure is not invariant under translations, there is an additional area-proportional contribution to the nucleus energy due to the difference in the surface energy between old and new positions of the surface [7]. The layer of a thickness $h$ can appear during the quasicrystal growth only if corresponding 'effective supercooling' [7]

$$\Delta\mu_{eff}(h,z) = \Delta\mu - \Delta\sigma(h,z)/h \tag{1}$$

is positive. Here $\Delta\mu = \mu_{solid} - \mu_{liquid}$ is the supercooling and $\Delta\sigma$ is the difference in surface energy. $\Delta\mu_{eff}$ depends not only on the nucleus heigh $h$ but on the current location $z$ of a surface as well. The nucleus appearing on the growing surface located at $z$ for a given supercooling $\Delta\mu$ is selected by the smallest height $h$ with positive $\Delta\mu_{eff}(h,z)$ [8].

The surface energy $\sigma(z)$ can be expressed [7] as $\sigma(z_{||}) \propto {z_\perp}^2$ with $z_{||}$ and $z_\perp$ being the 'physical' and 'orthogonal' components of the 6D quasilattice vector $\mathbf{z}$ [9]. Then the 'effective supercooling' takes the form

$$\Delta\mu_{eff}(h) = \Delta\mu - A\frac{\Delta({z_\perp}^2)}{h} \tag{2}$$

where $\Delta({z_\perp}^2) = {(z+h)_\perp}^2 - {z_\perp}^2$. This expression for the 'effective supercooling' leads to the power-law dependency of average nucleus height on the bulk supercooling [7, 8]:

$$h \propto (\Delta\mu)^{-1/3} . \tag{3}$$

The dislocation movement in crystals is described by the thermodynamic model similar to the crystal growth. There are terms in Hamiltonian corresponding to a periodical pinning (Peierls barriers) and to the dislocation line tension. The nuclei correspond to dislocation kinks and the stress component in the sliding plane plays a role of the supercooling. The dislocations in quasicrystals have 6D Burgers vector [10] and their movement involves 'phason' displacements which correspond to diffusion-like atomic rearrangement. Thus, the dislocation movement in quasicrystals is not a sliding but is similar to a 'creeping' [11] which is accompanied by atomic diffusion.

The formation work for a dislocation kink is proportional to the product of the Burgers vector to the kink normal and the translation vector. As Burgers vector has phason component, contribution proportional to perpendicular component of the translation vector appears. Minimization of this work with respect to both the translation length and the orientation of kink normal leads to the expression for activation energy similar to the nucleation barrier for quasicrystal growth. Thus, results for planar growth of quasicrystals are relevant to the dislocation problem as well. Quasiperiodic pinning potential for dislocation movement was obtained in a computer simulation of the quasicrystal dislocations[2].

[2] R. Mikulla, private communication.

The problem has one spatial dimension which is the surface position in the direction of growth and can be analyzed within simplified one-dimensional model. The cut-and-project method of generation of the atomic structure of quasicrystals [9] can be used to generate 1D quasiperiodic sequence of the minima of pinning potential through the projection from a 2D square lattice. The 'physical space' here is a straight line with a slope of the 'golden mean' $\tau = (\sqrt{5}+1)/2$ and the node $(p,q)$ is projected to the point

$$(p,q)_{||} = (p\tau + q)/\sqrt{\tau+2}. \tag{4}$$

in a physical space if $(p,q)$ falls within parallel 'tube' of a width $w$

$$|(p,q)_{\perp}| = \frac{|-p+q\tau|}{\sqrt{\tau+2}} < \frac{w}{2} = \frac{1}{2}\frac{\tau+1}{\sqrt{\tau+2}}\,. \tag{5}$$

The pinning potential at this point is defined similar to $\Delta\sigma(z)$ as $\mathcal{V}((p,q)_{||}) = (p,q)_{\perp}^2$. It might be shown that for sufficiently small supercoolings this model is equivalent to the quasiperiodic pinning potential

$$\mathcal{V}(z) = -V_G\left(\cos(Gz) + \cos(Gz/\tau)\right), \tag{6}$$

used previously in a continuous model [8] and in the Monte-Carlo simulation [12].

The growth process can be fully characterized by a sequence of the surface locations $(p,q)_{||}$ with the nucleus heights $h_{||}$ being the difference between two subsequent positions. At any current point $(p,q)_{||}$ the next surface position is determined by a smallest $h_{||}$ satisfying the condition of positiveness of effective supercooling

$$\Delta\mu_{eff}(h) = \Delta\mu - \frac{((p,q)+\mathbf{h})_{\perp}^2 - (p,q)_{\perp}^2}{h_{||}} > 0\,. \tag{7}$$

Here $h_{||}$ corresponds to a unique 2D lattice vector $\mathbf{h}$ and the supercooling is measured in such units that constant $A$ in the expression (2) for $\Delta\mu_{eff}$ disappears. Due to irrational slope of the projection from 2D square lattice there is a one-to-one correspondence between points of the 'physical' and orthogonal space and, hence, the growth process can be described by the surface locations in the 'perpendicular' space. At every step the minimal jump length $h_{||}$ is selected from all lengths satisfying condition (7) that can be written as

$$h_{\perp}\,(p,q)_{\perp} < \frac{1}{2}\left(\Delta\mu\, h_{||} - h_{\perp}^2\right)\,. \tag{8}$$

Since nodes of 2D square lattice form a dense set of points in the orthogonal space the spectral weight of particular $h_{||}$ is equal to the relative size occupied in this set by those $(p,q)_{\perp}$'s where the condition (8) leads to the selection of $h_{||}$.

The ratio of two subsequent Fibonacci numbers $f_{m+1}/f_m$ are known to give the best rational approximation to the 'golden mean' $\tau$. Then, Eqs.(4) and (5) imply that the vector of 2D square lattice of a kind $\mathbf{h}_m = (f_{m+1},\, f_m)$ has the lowest 'orthogonal' length $h_{\perp}$ from all ones with comparable 'parallel' component $h_{||}$ and corresponding nucleus height is a lowest one satisfying the condition (8). Thus, the nucleus height spectrum in this model of the quasicrystal growth for sufficiently small supercoolings should include only heights $\mathbf{h}_m$ corresponding to the Fibonacci numbers. It has a form of discrete set of peaks and their spectral weight $\{x_m(\Delta\mu)\}$ is determined by the supercooling $\Delta\mu$.

Using the definition of the Fibonacci sequence in recurrent form with $f_0 = 0$ and $f_1 = 1$ we can get from Eqs.(4) and (5)

$$h_{m_{||}} = \frac{\tau^{m+1}}{\sqrt{\tau+2}}, \quad h_{m_\perp} = (-1)^{m-1}\frac{\tau^{-m}}{\sqrt{\tau+2}} . \tag{9}$$

Introducing following set of points in the 'perpendicular' space

$$S_m = \frac{h_{m_\perp}}{2}\left(\Delta\mu\,\tau^{3\,m+1}\sqrt{\tau+2}-1\right) \tag{10}$$

we can get the condition (8) in the form

$$(p,q)_\perp < S_m \quad \text{for} \quad h_{m_\perp} > 0 \tag{11a}$$

$$(p,q)_\perp > S_m \quad \text{for} \quad h_{m_\perp} < 0 . \tag{11b}$$

At every location of the growing surface $(p,q)_{||}$ the nucleus height $h_{m_{||}}$ is selected according to the lowest $m$ that satisfies condition (11).

Using (9) we can obtain from the definition (10) the following recurrent scaling law

$$S_{m+1}(\tau^{-3}\,\Delta\mu) = -\tau^{-1}\,S_m\,(\Delta\mu) . \tag{12}$$

As the jump lengths (9) satisfy similar recurrent relationships $h_{(m+1)_\perp} = -\tau^{-1}\,h_{m_\perp}$, this scaling holds for the set of points $(p,q)_\perp$ representing surface position in perpendicular 'space' satisfying (11). Since the appearance of particular height in the spectrum is determined by the relative size of a subset of points $(p,q)_\perp$ satisfying Eq.(11) for particular $m$, such a scaling imply that the nucleus height spectrum has the following invariance

$$x_{m+1}(\tau^{-3}\,\Delta\mu) = x_m(\Delta\mu) . \tag{13}$$

Thus, we can consider supercooling only within the interval between $\Delta\mu^*\,\tau^{-3}$ and $\Delta\mu^*$ for some particular $\Delta\mu^*$. Spectrum for all other $\Delta\mu$'s can be easily obtained through (13). Let us choose $\Delta\mu_m^*$ that corresponds to an equity $S_m = S_{m-1}$ for some odd $m$. Introducing relative supercooling $\kappa_m$ by $\Delta\mu = \kappa_m\,\Delta\mu_m^*$ we can obtain

$$S_{m+l} = \frac{h_{(m+l)_\perp}}{2}\left(\frac{\kappa_m\,\tau^{3\,(l+1)}}{\sqrt{5}}+1\right) \tag{14}$$

with

$$S_{m-1} + h_{(m-1)_\perp} < S_m < S_{m-1} < S_m + h_{m_\perp} . \tag{15}$$

Direct geometrical analysis of the condition of (11) shows that regardless of the starting point, the perpendicular component of the surface position $(p,q)_\perp$ falls into the interval between $S_{m-1} + h_{(m-1)_\perp}$ and $S_m + h_{m_\perp}$ in a finite number of steps. For $(p,q)_\perp > S_m + h_{m_\perp}$ only jumps with negative $h_{(m+l)_\perp}$ are possible and for $(p,q)_\perp < S_{m-1} + h_{(m-1)_\perp}$ only positive $h_{(m+l)_\perp}$ can occur. Once into this interval the point representing surface remains confined and fills this interval closely due to irrational slope of the projection line. Comparing $\Delta\mu_{eff}(h_{(m+l)_{||}})$ for different $l$ it is easy to see that for jumps of $h_{(m+l)_\perp}$ the surface position in perpendicular space $(p,q)_\perp$ should belong to the following intervals

$$S_{m-1} < (p,q)_\perp < S_m + h_{m_\perp}, \quad l = -1, \tag{16a}$$

$$S_{m-1} + h_{(m-1)_\perp} < (p,q)_\perp < S_m, \quad l = 0, \tag{16b}$$

$$S_m < (p,q)_\perp < S_{m-1}, \quad l = 1, \tag{16c}$$

with only finite possible appearance of other $h_{(m+l)_\perp}$'s. The relative size of these intervals gives us the spectral weight of different peaks:

$$x_{m-1}(\kappa_m) = \frac{\kappa_m - \tau^{-3}}{\kappa_m + 1}\ , \quad x_m(\kappa_m) = \frac{\kappa_m + \tau^{-3}}{\kappa_m + 1}, \quad x_{m+1}(\kappa_m) = \frac{1 - \kappa_m}{\kappa_m + 1}\ . \tag{17}$$

All other $h_{(m+l)_\perp}$'s correspond to finite number of points $(p,q)_\perp$. Such subsets have zero measure in perpendicular space and, thus, do not contribute into the spectrum. Mean nucleus height has the following expression in the spectrum (17)

$$h_{mean}(\kappa_m) = 2\,\tau^{(m-1)}\,\frac{\sqrt{3-\tau}}{\kappa_m - 1}\ . \tag{18}$$

At the borders of the $\kappa_m$ interval there are only two peaks

$$x_{m-1}(\tau^{-3}) = 0\ , \quad x_m(\tau^{-3}) = \frac{2\,\tau^{-3}}{1+\tau^{-3}}, \quad x_{m+1}(\tau^{-3}) = \frac{1-\tau^{-3}}{1+\tau^{-3}} = \tau\, x_m(\tau^{-3}) \tag{19}$$

and

$$x_{m-1}(1) = \frac{1-\tau^{-3}}{2}\ , \quad x_m(1) = \frac{1+\tau^{-3}}{2} = \tau\, x_{m-1}(1), \quad x_{m+1}(1) = 0\ . \tag{20}$$

For $\kappa_m > 1$ a peak at $m-2$ appears as does the $m+2$ peak for $\kappa_m < \tau^{-3}$.

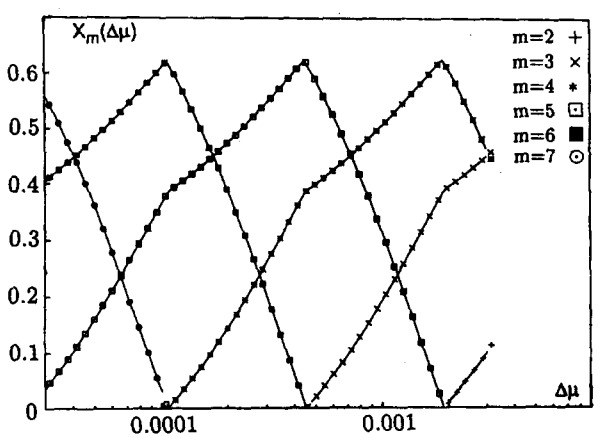


Fig.1. The nucleus height spectrum calculated in the present model as a function of supercooling $\Delta\mu$ (full curves) in a comparison with the results of numerical simulation

Main features of this spectrum agree well with the results of Monte-Carlo simulation [12] where universal discrete spectrum corresponding to three subsequent Fibonacci numbers has been found for the quasiperiodic double-cosine pinning potential. Calculated spectrum is shown at Fig.1 in a comparison with results of numerical calculations [13], where periodical dependence of the spectrum on the logarithm of $\Delta\mu$ was obtained with a period of 3 $\log\tau$. Fig.2 shows periodical dependence of mean nucleus height on supercooling with small deviation from the power-law expression (3) obtained in a continuous model which appears to be a good average approximation for Eq.(18).

The discrete nature of the spectrum of nucleus heights leads to a step-like dependency of the growth rate on supercooling [12]. Since activation barriers for different $h_{m_{||}}$ differs by the orders of magnitude [7] the growth is controlled by the nucleation of the layer with maximal thickness. It means that when the supercooling $\Delta\mu$ varies in the interval between $\Delta\mu^*_{m+1}$ and $\Delta\mu^*_m$ the growt rate experiences small changes. However, when supercooling

passes through $\Delta\mu_m^*$ the highest peak corresponding to $h_{m+2}$ disappears and growth rate undergoes drastic increase.

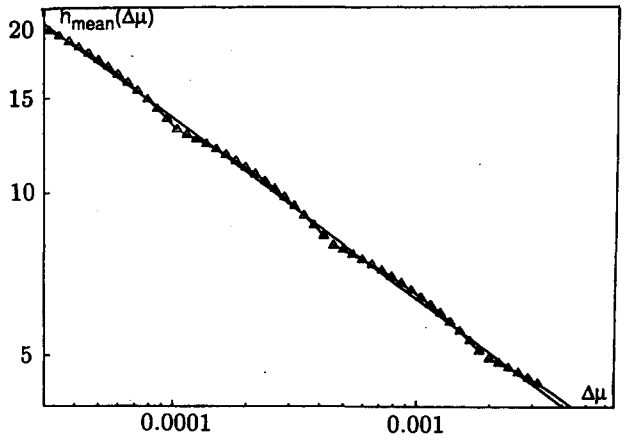


Fig.2. Calculated dependence of the mean step height $h_{mean}$ on $\Delta\mu$ in the present model (full curve) compared with numerical results (triangles). Straight line is a power-law dependency $h_{mean} \propto \Delta\mu^{-1/3}$

Similar pattern should appear in the case of quasicrystal dislocations where growth rate corresponds to the dislocation velocity. It should have small variations for the stress values corresponding to the same peaks in the spectrum with drastic changes around critical stress that leads to the appearance of new peaks in the spectrum. If the quasicrystal has finite density of defects then defects prevent formation of kinks larger than some particular size. Hence, activation-driven dislocation movement would not be possible under the stress level that implies appearance of larger kinks in the spectrum of kink sizes.

Thus, unlike the case of the growth of quasicrystals, the critical stress levels not only correspond to drastic changes in dislocation velocity but the dislocations become frozen for a critical stress corresponding to some $m$. It allows experimental test of the proposed model since the stress level associated with drastic changes in the dislocation velocity should form periodic pattern on a logarithmic scale and the critical stress leading to the dislocation freeze should belong to this pattern as well.


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