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Non-KAM (Kolmogorov-Arnold-Moser) incommensurate states of the discrete Frenkel-Kontorova chain

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Abstract. — The depinning phase transition in the discrete Frenkel-Kontorova model is considered. It is found that there exists a set of irrational periodicities such that the chain is pinned at any periodic potential strength. Every Cantorus describing the pinned phase is shown to belong to the stochastic layer.

Recently pinning effects in pure discrete systems have been extensively theoretically studied [1-6]. Various incommensurate systems such as monolayers of atoms adsorbed on crystal substrates, intercalation compounds, etc., can be described using the discrete Frenkel-Kontorova model. The Hamiltonian is of the form:

$$H = \sum_{n}^{1} \frac{1}{2} (x_{n+1} - x_{n})^2 + \lambda V(x_{n})$$

(1)

where \(V(x + 1) = V(x)\) is a periodic potential. The simplest system described with the Hamiltonian (1) is a chain of particles placed in the periodic substrate potential \(V(x)\) (the lattice constant is put equal to unity). The Hamiltonian (1) has no absolute minimum, but if the mean distance \(l\) between the particles is fixed:

$$l = \lim_{N \to \infty} \frac{x_{N+1} - x_{1}}{N}$$

(2)

the configuration \(\{x_{n}\}\) minimizing the energy (1) exists. It is called the ground state configuration of periodicity \(l\) [2]. One can establish the correspondence between the ground state configuration of the particles \(\{x_{n}\}\) and the trajectory of the standard mapping \(\{(u_{n}, z_{n})\}\) on a cylinder in the usual way:

$$z_{n} = x_{n} - x_{n-1}, \quad u_{n} = x_{n} - \text{Int}(x_{n}) = x_{n} \text{(mod 1)}.$$

(3)
If \( l \) is rational, the chain is in the commensurate state. In this case the system is pinned to the substrate at any potential strength \( \lambda \) [1-5]. If the periodicity \( l \) is irrational the depinning phase transition may occur. According to numerous computer data [3, 5, 7-10] there is a well-defined transition at \( \lambda = \lambda_c(l) \) called depinning transition or transition by breaking of analyticity. For \( \lambda < \lambda_c(l) \) no force must be applied to translate the chain and the gap in the phonon spectrum is zero [3, 4]. The absence of pinning is the consequence of the fact that the corresponding trajectory on the cylinder is a smooth curve (KAM-torus). For \( \lambda > \lambda_c(l) \) the trajectory is a Cantorus [3, 9, 11] so the chain is pinned.

Numerical and qualitative calculations were performed for special \( l \) (golden mean, nobles, etc.). In these cases the critical potential strength \( \lambda_c(l) \) was found to be non-zero. Is it true that \( \lambda_c(l) \neq 0 \) for any irrational \( l \)? The KAM-theory does not give the answer [12]. It only states that for almost all \( l \), \( \lambda_c(l) \) is not zero. Here we want to report that the answer is negative.

**Assertion 1.** There exists a set \( \Omega \) of irrational numbers \( l \) such that \( \lambda_c(l) = 0 \). \( \Omega \) has the cardinality of continuum but its measure is zero.

The exact mathematical formulation and the proof will be published elsewhere. Below we give a qualitative description.

The reason for the existence of such strange numbers is that they are « close enough » to rational numbers. It is well known that \( \lambda_c(l) = 0 \) for all rational \( l \). Thus \( \Omega \) is a set of the numbers which are irrational but physically indistinguishable from rational ones. From the experimental point of view all the periodicities \( l \) can be divided into two classes: incommensurate (unpinned) and « physically commensurate » (pinned). The latter class consists of all rationals and \( \Omega \). We shall call elements of \( \Omega \) as quasi-rationals. The continued fraction expansions of the quasi-rationals are not typical. For typical periodicities \( l \) the integers \( S_i \) in the expansion

\[
l = S_0 + \cfrac{1}{S_1 + \cfrac{1}{S_2 + \cfrac{1}{\ddots + \cfrac{1}{S_i + \cdots}}}}
\]

[4]

do not increase with \( i \) or increase slowly [13]. But in the quasi-rationals the sequences \( \{ S_i \} \) are rapidly increasing. We have constructed them by induction.

Before describing the induction we mention a result concerning the periodicities close enough to rational ones. Let \( l_0 = q/p \) be an arbitrary rational number. We fix \( \lambda \) in equation (1) and consider the states with periodicities \( l \) close to \( q/p \). As it was pointed out by Aubry [1] if \( |l - l_0| \) is small enough the configurations can be described as a superstructure of distantly spaced discommensurations interacting as \( \exp(-x/\xi(p/q)) \), where \( \xi(p/q) \) is a coherence length of the commensurate state \( p : q \). The distance \( x \) between them is of the order of \( q/p^2 |l - l_0| \). Every discommensuration interacts also with a pinning potential \( E_{\text{pin}}(p/q) \) [1, 2, 4] which does not depend on \( |l - l_0| \). It is seen that there is a very small neighbourhood of the point \( l_0 = q/p \) where the interaction between the defects is much weaker than the pinning energy:

\[
E_{\text{int}} \sim \exp\left(-\frac{q}{p^2 |l - l_0| \xi(p/q, \lambda)}\right) \ll E_{\text{pin}}(p/q, \lambda) .
\]

[5]

In this neighbourhood the chain is pinned. More exactly, we have proved the following statement.

**Assertion 2.** For every potential strength \( \lambda \) and for any rational periodicity \( l_0 = q/p \) there exists a small neighbourhood \( |l - l_0| \leq \epsilon(l_0, \lambda) \) of the point \( l_0 \) such that the states with periodicities \( l \) belonging to it are pinned. The corresponding trajectories on the cylinder are Cantori, every such Cantorus is contained in the stochastic layer generated by the heteroclinic trajectory.
of the $p$-cycle. Physically it means that the states can be described as the superstructures of strongly pinned discommensurations.

The width of the neighbourhood $\epsilon(l_0, \lambda)$ can be evaluated using equation (5). It depends strongly on the analytic properties of the potential $V(x)$. For example, if $V(x)$ is an analytic function then $E_{\text{pin}} \sim \exp(-\text{const. } \xi)$ [1, 4], so $\epsilon$ is of the order $\xi^{-2}$. For most $l_0$ and $\lambda$ the coherence length $\xi(l_0, \lambda)$ is large and therefore $\epsilon(l_0, \lambda)$ is very small. It should be noted that distantly spaced discommensurations are not necessarily pinned [4]. Really, the distance between the defects $q/p^2 | l - l_0 |$ is larger than their width $\xi(l_0, \lambda)$ when $| l - l_0 | \ll (p\xi)^{-1}$. If $\xi^{-2} \ll | l - l_0 | \ll \xi^{-1}$ the discommensurations are far from each other but can be unpinned. This region of $| l - l_0 |$ has been considered by Aubry [1]. The small neighbourhood $| l - 1 | \ll \xi^{-2}(1, \lambda)$ of the periodicity $l_0 = 1$ has been considered in [6], where the discommensurations has been shown to form a lattice gas.

Now we shall describe briefly the iteration procedure giving a quasi-rational number $l$. We pick out a sequence $\lambda_i$ tending to zero. If $l$ is a quasi-rational then the state of periodicity $l$ must be pinned at $\lambda = \lambda_i$ for any $i$. We construct the number $l = [S_0, S_1, ..., S_k, ...]$ satisfying stronger condition, namely all the states of the periodicities $l$ of the form $l = [S_0, S_1, ..., S_{k+1}, t_{k+2}, ...]$ with arbitrary integers $t_{k+1}, t_{k+2}, ...$ are pinned at $\lambda \geq \lambda_k$.

The element $S_0$ can be arbitrarily chosen. In the first step of the induction we fix $\lambda_1$ and find the first element $S_1$ of the expansion (4). We make use of Assertion 2 and put $\lambda = \lambda_1$ and $l_0 = S_0$. Note that $| l - l_0 | = 1/(S_1 + 1/(t_2 + 1/(t_3 + ...)) \leq 1/S_1$ so if $S_1$ is large enough all the states of the periodicities $l = [S_0, S_1, t_2, t_3, ...]$ are pinned at $\lambda = \lambda_1$. Then we fix $\lambda_2, S_0, S_1$ and find $S_2$ and so on. Let $\lambda_k, S_0, S_1, ..., S_{k-1}$ be found. We put $\lambda = \lambda_k$ and $l_0 = [S_0, S_1, ..., S_{k-1}]$ in Assertion 2. Because $| l - l_0 | \leq (S_k p^2)^{-1}$ all the states $l = [S_0, S_1, ..., S_k, t_{k+1}, ...]$ are pinned if $S_k$ is sufficiently large. Therefore $l$ is a quasi-rational. Note that $S_k$ must satisfy the inequality $S_k > p^{-2} \times \epsilon(l_0, \lambda_k)$ thus the set $\Omega$ is uncountable.

We have obtained quasi-rational numbers $l$ using Assertion 2. For this reason every such state at fixed non-zero $\lambda = \lambda_k$ can be described as the superstructure of strongly pinned defects. The « background » commensurate configuration has the periodicity $l_0 = q/p = [S_0, S_1, ... S_k]$ which is the truncated continued fraction (4). It is reasonable to conjecture that.

At any $\lambda$ and for every Cantorus of the periodicity $l = [S_0, S_1, ... S_p, ...]$ there exists an integer $k$ such that the Cantorus belongs to the stochastic layer generated by the heteroclinic trajectory of the hyperbolic cycle of the periodicity $l_0 = [S_0, S_1, ... S_k]$. Physically it means that every pinned incommensurate configuration is the superstructure of strongly pinned discommensurations imposed on the commensurate configuration of the periodicity $l_0 = [S_0, S_1, ... S_k]$.

In conclusion we want to note once again that we deal only with the trajectories of the standard mapping which corresponds to ground state configurations of the Hamiltonian (1).

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References