Farey Tree and the Frenkel-Kontorova Model

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Abstract

We solved the Frenkel-Kontorova model with the potential $V(u) = -\frac{1}{2}|\lambda|(u - \text{Int}[u] - \frac{1}{2})^2$ exactly. For given $|\lambda|$, there exists a positive integer $q_c$ such that for almost all values of the tensile force $\sigma$, the winding number $\omega$ of the ground state configuration is a rational number in the $q_c$-th level Farey tree. For fixed $\omega = p/q$, there is a critical $\lambda_c$ when a first order phase transition occurs. This phase transition can be understood as the dissociation of a large molecule into two smaller ones in a manner dictated by the Farey tree. A kind of “commensurate-incommensurate” transition occurs at critical values of $\sigma$ when two sizes of molecules co-exist. “Soliton” in the usual sense does not exist but induces a transformation of one size of molecules into the other.

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I. INTRODUCTION

Frenkel-Kontorova (FK) model describe a system of particles moving in an infinite sequence of potential wells. In the limit of shallow wells, the particles are kept at an equilibrium distance by a tensile force $\sigma$. Such models are also widely studied in the context of circle maps when certain periodicity exists in the locations of the potential wells [1]. A stationary configuration in the FK model corresponds to an orbit in the circle map. In the study of FK models, however, one is particularly concerned with the minimum energy configurations. The ground state is a “recurrent” minimum energy configuration [2,3] that is characterized by a winding number $\omega$, the inverse of which, $1/\omega$, gives the average number of particles per well. Hence a ground state with rational $\omega = p/q$ [4] consists of molecules that are composed of $q$ particles and $p$ wells.

It is well-known that two types of phase transitions occur quite generally in FK models [5]. The first type is the commensurate-incommensurate transition which occurs at critical values of $\sigma$ when the enthalpy for the creation of solitons or anti-solitons vanishes [5]. The second type occurs at critical values of $\lambda$ characterizing the strength of the potential wells and corresponds, in the language of circle map, to the breaking of an invariant circle into a cantorus. In the ground state with an irrational winding number $\omega$, the allowed positions of the particles in the potential wells change from being the entire period in the “unpinned” phase to being a cantor set in the “pinned” phase. Correspondingly, the hull function $f_\omega(x)$, from which one obtains the position $u_n$ of the $n$-th particle by $u_n = f_\omega(n\omega)$, turns from a smooth function into a nowhere-differentiable function [2,3,6–8].

These two types of phase transitions, however, are not the only phase transitions that could occur in a FK model. In particular, when the potential possess an “internal structure”, e.g., having multiple local minima in a period, one will encounter first order phase transitions at critical values of the height of a local minimum [9,10]. At the critical point, the filling fraction of the corresponding well (the local minimum) changes from a value sub-commensurate to the winding number $\omega$ to a value non-sub-commensurate to $\omega$ [10]. As in
the case of commensurate-incommensurate transition, this new type of first order transition is nucleated by solitons.[9]

In this letter, we would like to present yet a new type of first order phase transition by solving exactly an FK model with a potential which is concave almost everywhere. The phase transition is not nucleated by solitons. Rather, it can be understood as the breaking up of a large molecule into two smaller ones, in a manner dictated by the Farey tree.

The stationary configuration of an FK model is determined by the equation

\[ u_{n+1} - 2u_n + u_{n-1} = \lambda V'(u_n), \]  

(1)

where \( u_n \) denotes the coordinate of the \( n \)-th particle. The model we consider has the potential

\[ V(u) = \frac{1}{2} \lambda \left( u - \text{Int}[u] - \frac{1}{2} \right)^2, \quad -4 < \lambda < 0, \]  

(2)

where \( \text{Int}[u] \) equals the largest integer not larger than \( u \). The case of \( \lambda > 0 \) had been thoroughly investigated before by several authors[11].

The recurrent stationary configurations are characterized by a winding number \( \omega \) and can be specified by a hull function \( f_\omega(x) \) so that

\[ u_n = f_\omega(n\omega + \alpha), \]  

(3)

where \( \alpha \) is a constant phase. The hull function satisfies \( f_\omega(x + 1) = f_\omega(x) + 1 \).

For \( \omega = p/q \), the hull function is a step function with \( q \) steps in a period. Depending on whether \( f_\omega(x) \) is continuous at integer values of \( x \), there are two solutions:

\[ f_\omega(x) = \sum_{n=0}^{q-1} \nu_n(q) \left( \text{Int}[x + n\omega] - \overline{\text{Int}}[n\omega] \right), \]  

(4)

and

\[ \overline{f}_\omega(x) = \left[ f_\omega(x + \frac{1}{2q}) + f_\omega(x - \frac{1}{2q}) \right]/2, \]  

(5)

where \( \nu_n(q) = \tan \frac{\pi}{2} \csc \frac{\pi}{2} \cos(n - \frac{q}{2}) \chi \), \( \chi = \arccos(1 - |\lambda|/2) \) and \( \overline{\text{Int}}[x] \equiv (\text{Int}[x^+] + \text{Int}[x^-])/2 \). The configuration described by \( \overline{f}_\omega(x) \) has one particle sitting at the potential bottom in a given period. \( \overline{f}_\omega(x) \) can also be expressed as
\[ \tilde{f}_\omega(x) = \sum_{n=0}^{q-1} \tilde{\nu}_n(q) \left( \text{Int}[x + n\omega + \frac{1}{2q}] - \text{Int}[n\omega + \frac{1}{2q}] \right), \quad (6) \]

where \( \tilde{\nu}_n = (\nu_n + \nu_{n'})/2 \) with \( n' \equiv n + q_1 \quad (\text{mod } q) \), \( 0 \leq n' \leq q - 1 \), and \( q_1 \) is determined by the Farey tree in the following way. Given the irreducible fraction \( \omega = p/q \), \( \omega_1 = p_1/q_1 \) and \( \omega_2 = p_2/q_2 \) is the unique irreducible pair such that

\[ p = p_1 + p_2, \quad q = q_1 + q_2, \quad \omega_1 < \omega < \omega_2 \quad (7) \]

and

\[ pq_1 = p_1q + 1, \quad p_2q = pq_2 + 1, \quad p_2q_1 = p_1q_2 + 1. \quad (8) \]

We shall call the “\( q \)-th level Farey tree” to be the Farey tree where irreducible fractions with denominator larger than \( q \) are truncated. The average energy per particle corresponding to the stationary configurations described by \( f_\omega(x) \) and \( \tilde{f}_\omega(x) \) are respectively

\[ \Psi(\omega) = \frac{\omega^2}{2} - \frac{|\lambda|}{4} \sum_{n=0}^{q-1} \nu_n(q) \left\{ \frac{1}{4} - (n\omega - \frac{1}{2} - \text{Int}[n\omega])^2 \right\}, \quad (9) \]

and

\[ \bar{\Psi}(\omega) = \Psi(\omega) - \frac{|\lambda|}{8q} \nu_0(q). \quad (10) \]

One notices that at \( \chi = \chi_q \equiv \pi/q \), \( \nu_0(q) \) vanishes and the two configurations become degenerate. Eq. (10) also indicates that for \( 0 < \chi < \chi_q \), the ground state configuration with winding number \( \omega = p/q \) is given by \( \tilde{f}_\omega(x) \).

It is instructive to learn how the configuration described by \( f_\omega(x) \) evolves as \( \chi \) increases from zero. Let \( u_n = f_\omega(n\omega - 1/2q) \) for \( 0 \leq n \leq q - 1 \). As \( \chi \) increases from zero to \( \chi_q \), the \( \nu_n \)'s change from \( \nu_0 = \nu_1 = \cdots = \nu_{q-1} = 1/q \) to a first zero value occurring at \( \nu_0 \). When this happens, the two particles \( u_0 \) and \( u_{q_1} \) touch the bottom of the potential wells. As \( \chi \) increases further, these two particles are pinned at the bottom and we can no longer use \( f_\omega(x) \), which ceases to be an increasing function, to describe this configuration. Instead, the \( q_1 \) particles from \( u_0 \) to \( u_{q_1-1} \) are described by an “\( \tilde{f}_{\omega_1} \) section”, i.e., a consecutive \( q_1 \) particles
chain with the first particle sitting at the potential minimum in the $\tilde{f}_{\omega_1}$ configuration, while the $q_2$ particles from $u_{q_1}$ to $u_{q-1}$ are described by an $\tilde{f}_{\omega_2}$ section. For a general $\omega = p/q$, if we regard an $\tilde{f}_\omega$ section as a “molecule” of size $(q, p)$, i.e., composed of $q$ particles and $p$ wells, then $\chi_q$ can be seen to be a critical point of a first order transition when a molecule of size $(q, p)$ is just about to break up into two molecules of sizes $(q_1, p_1)$ and $(q_2, p_2)$ respectively. 

There three type of molecules, whose corresponding $\omega_1$, $\omega$, and $\omega_2$ are related as consecutive Farey fractions, co-exist at the critical point.

For $\chi > \chi_q$, $\tilde{f}_\omega(x)$ ceases to describe the ground state configuration with winding number $\omega$. One can show from Eqs. (9) and (10) that

$$q_1 \tilde{\Psi}(\omega_1) + q_2 \tilde{\Psi}(\omega_2) - q \tilde{\Psi}(\omega) = \frac{\lambda}{8} \tan \frac{\chi}{2} \cot \frac{q \chi}{2} \cot \frac{q_1 \chi}{2} \cot \frac{q_2 \chi}{2}$$

(11)

and the right hand side is negative when $\chi > \chi_q$. The molecules of size $(q, p)$ dissociate and the ground state now is a mixture of $\tilde{f}_{\omega_1}$ and $\tilde{f}_{\omega_2}$ sections with the right proportion.

When $\chi$ continues to increase and reaches $\bar{\chi}_q \equiv \pi / \max(q_1, q_2) = \min(\chi_{q_1}, \chi_{q_2})$, say $\bar{\chi}_q = \chi_{q_1}$, the molecule of size $(q_1, p_1)$ starts to dissociate into even smaller molecules of sizes $(q_2, p_2)$ and $(q_1 - q_2, p_1 - p_2)$. Note that $(p_1 - p_2)/(q_1 - q_2)$, $p_1/q_1$, and $p_2/q_2$ are consecutive Farey fractions in the $(q-1)$-th level Farey tree. The process continues until all the particles are located at the bottom of the potential well. This occurs at $\chi > \pi/2$.

It is interesting to observe that for $\chi_q < \chi < \bar{\chi}_q$, even though $\tilde{f}_\omega(x)$ no longer describes the ground state configuration, it remains an increasing function until $\chi$ reaches $\bar{\chi}_q$. Hence molecules of size $(q, p)$ may be regarded as an unstable resonance state of two smaller molecules of sizes $(q_1, p_1)$ and $(q_2, p_2)$ when $\chi$ lies in the interval $(\chi_q, \bar{\chi}_q)$.

In summary, for given $\chi$, there exists a positive integer $q_c$ such that $\pi / (q_c + 1) < \chi \leq \pi / q_c$. The ground state configurations can only be composed of the $\tilde{f}_\omega$ sections with $\omega$ in the $q_c$-th level Farey tree in the following way. For an arbitrary irrational winding number $\omega$ or rational but not in the $q_c$-th level Farey tree, we can find a unique pair of consecutive fractions $\omega_1$ and $\omega_2$ in the $q_c$-th level Farey tree such that $\omega_1 < \omega < \omega_2$. The ground state configuration with this given $\omega$ can be constructed with a fraction $f_1$ of particles associated
with the $\bar{f}_{\omega_1}$ sections and a fraction $f_2$ associated with $\bar{f}_{\omega_2}$ sections such that

$$f_1 + f_2 = 1, \quad f_1 \omega_1 + f_2 \omega_2 = \omega.$$  \hfill (12)

Moreover, the average energy per particle of this ground state configuration is given by

$$\bar{\Psi}_e(\omega) = \frac{\omega - \omega_1}{\omega_2 - \omega_1} \bar{\Psi}(\omega_1) + \frac{\omega - \omega_1}{\omega_2 - \omega_1} \bar{\Psi}(\omega_2).$$  \hfill (13)

Adding or removing one particle from the system will turn $p_1 \bar{f}_{\omega_2}$ sections into $p_2 \bar{f}_{\omega_1}$ sections or vice versa. This can be seen from Eq. (8) which implies that $p_1 p_2 (1/\omega_1 - 1/\omega_2) = 1$. Starting from pure $\bar{f}_{\omega_1}$ sections, i.e., a $\bar{f}_{\omega_1}$ configuration, we can approach a $\bar{f}_{\omega_2}$ configuration by adding particles one by one. Solitons and anti-solitons in the usual sense of local “defects” do not exists. Effort to create them merely induces transitions between $\bar{f}_{\omega_1}$ and $\bar{f}_{\omega_2}$ sections. If we insist on calling “defect” an $\bar{f}_{\omega_1}$ section in a background of $\bar{f}_{\omega_2}$ sections, this “defect” will carry a “fractional charge” $\frac{1}{p_2}$.

It follows from Eq. (11) that

$$\left(\frac{q_1}{q_1 + q_2}\right) \bar{\Psi}(\omega_1) + \left(\frac{q_2}{q_1 + q_2}\right) \bar{\Psi}(\omega_2) > \bar{\Psi}(\omega) \quad \text{for} \quad \chi < \chi_q,$$  \hfill (14)

which indicates that $\bar{\Psi}_e(\omega)$ is a convex function of $\omega$. Indeed, for given $\chi_{q_c+1} < \chi \leq \chi_{q_c}$, this can be shown by making use of Eq. (13) and proving the convexity of $\bar{\Psi}(\omega)$ for any three consecutive fractions $\omega_1 < \omega_0 < \omega_2$ in the $q_c$-th level Farey tree. It follows from Eq. (8) that $p_1 + p_2 = \kappa p_0$ and $q_1 + q_2 = \kappa q_0$ for some positive integer $\kappa$. Similar to Eq. (11) one can derive that

$$q_1 \bar{\Psi}(\omega_1) + q_2 \bar{\Psi}(\omega_2) - \kappa q_0 \bar{\Psi}(\omega_0) = \frac{\lambda}{8} \tan \frac{\chi}{2} \cot \frac{q_0 \chi}{2} \cot \frac{q_1 \chi}{2} \cot \frac{q_2 \chi}{2}.$$  \hfill (15)

The right hand side is positive and this completes our proof.

Up to now, we have been discussing the ground state configuration for given $\omega$ as $\chi$ is varied. Introducing the tensile force term $-\sigma \omega$ into Eq. (13), we obtain the enthalpy of the system. By minimizing this enthalpy with respect to $\omega$, we obtain the phase diagram in the $\chi - \sigma$ plane, as shown in Fig. 1. One can see that there exist tricritical points at
\( \chi_q = \pi/q \), for each \( q \), where three types of molecules co-exist. For \( \chi < \chi_q \), the lowest enthalpy configuration is locked to \( \omega = p/q \) for

\[
\frac{\Psi(\omega) - \Psi(\omega_1)}{\omega - \omega_1} \leq \sigma \leq \frac{\Psi(\omega_2) - \Psi(\omega)}{\omega_2 - \omega},
\]

where \( \omega_1 < \omega < \omega_2 \) are consecutive fractions in the \( q_c \)-th level Farey tree with \( \chi_{q_c+1} < \chi \leq \chi_{q_c} \). When \( \chi = \chi_q \), the step shrinks to a point and we have

\[
\sigma = \frac{\Psi(\omega) - \Psi(\omega_1)}{\omega - \omega_1} = \frac{\Psi(\omega_2) - \Psi(\omega)}{\omega_2 - \omega},
\]

which gives the equations for the tricritical point. In general, for two consecutive Farey fractions \( \omega_1 \) and \( \omega_2 \), \( \sigma = \frac{\Psi(\omega_2) - \Psi(\omega_1)}{\omega_2 - \omega_1} \) gives the equation for the co-existent curve of the two phases corresponding to molecules of sizes \((q_1, p_1)\) and \((q_2, p_2)\).

In conclusion, we have shown that the solvable FK model considered in this work illustrates some important physics accompanying a first order phase transition. In particular, we demonstrate explicitly how the Farey tree dictates the structure of these phase transitions. Even though the model is one-dimensional and the potential is not smooth, the underlying physics could very well be realized in nature.

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FIG. 1. The domains of stability in the $\chi$-$\sigma$ plane. The number in each domain denotes its winding number.