Farey fractions and the Frenkel-Kontorova model

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We solved the Frenkel-Kontorova model with the potential $V(u)=-\lambda(u-\mathrm{Int}[u]-1/2)^2/2$ exactly. For given $\lambda>0$, there exists a positive integer q_c such that the winding number ω of the minimum enthalpy state is locked to rational numbers in the q_cth row of Farey fractions. For fixed $\omega=p/q$, there is a critical λ_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 fractions. [S1063-651X(97)16003-2]

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The Frenkel-Kontorova (FK) model with the Hamiltonian

$$H(\{u_n\})=\sum_n \left[\tfrac{1}{2}(u_{n+1}-u_n)^2+V(u_n)\right], \qquad (1)$$

where u_n denotes the position of the nth particle, describes a system of particles moving in an infinite sequence of potential wells $V(u)$. In the limit of shallow wells, the particles are kept at an equilibrium distance by a tensile force σ. Such models are also widely studied in the context of circle maps when a 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 [2,3], in which H cannot be decreased by altering a finite number of u_n. For smooth potentials, the ground state is a ''recurrent'' minimum energy configuration characterized by a winding number ω, 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 successive ''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 σ when the enthalpy for the creation of solitons or antisolitons vanishes [5]. The second type occurs at critical values of λ 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 ω, 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 nth particle by $u_n=f_\omega(n\omega)$, turns from a smooth function into a nowhere-differentiable function [2,3,6,7].

These two types of phase transitions, however, are not the only phase transitions that could occur in an FK model. In particular, when the potential possesses an ''internal structure,'' e.g., having multiple local minima in a period or subharmonics in a sinusoidal potential, one will encounter different kinds of first order phase transitions at critical values of the height of a local minimum [5,8].

In this paper, we would like to present yet another type of first order phase transition by solving exactly an FK model with a potential which is concave almost everywhere, has cusps at the bottom of the potential well. The possibility of particles being pinned at the cusps leads to many striking results. For given $\lambda>0$, as the tensile force σ is varied, and the winding number of the system is locked at a *finite set* of rational values. Solitons in the usual sense do not exist. Instead, local defects are ''fractionally charged.'' At critical values of σ, the enthalpy for creation of such fractionally charged defects vanishes. As a result, the minimum enthalpy configurations contain not only configurations with irrational winding numbers and rational winding numbers outside of the finite set mentioned above, but also configurations without a well-defined winding number.

For a minimum energy configuration with a given winding number, as λ is increased, a critical value λ_c will be reached, above which the system is no longer stable and a first order phase transition occurs. The phase transition can be understood as the breaking up of a large molecule into two smaller ones, in a manner dictated by the Farey fractions. As a result of the coexistence of two sizes of molecules, the ground state configurations are infinitely degenerate.

At λ_c, a *localized* zero frequency phonon mode exists. As a result, the dissociating molecules can be continuously deformed *individually* and the particles in the minimum energy configuration are ''unpinned'' in some sense. For a given λ, the minimum energy configurations of this model can be completely characterized. It is composed either of molecules of a single size or of two different sizes, corresponding to two consecutive Farey fractions, mixed with an arbitrary proportion, and arranged in an arbitrary spatial order.

The model that we consider has the potential

$$V(u)=-\frac{\lambda}{2}(u-\mathrm{Int}[u]-\tfrac{1}{2})^2, \quad 0<\lambda<4, \qquad (2)$$

where $\mathrm{Int}[u]$ equals the largest integer not larger than u. The case of $\lambda<0$ has been thoroughly investigated by several authors [9]. The derivative of $V(u)$ is not well defined at integer values of u, so that the equation of motion, $u_{n+1}-2u_n+u_{n-1}=V'(u_n)$, should be replaced by

$$-\frac{\lambda}{2}=V'(u_n^-)\leqslant u_{n+1}-2u_n+u_{n-1}\leqslant V'(u_n^+)=\frac{\lambda}{2}, \quad (3)$$

when u_n is an integer and the nth particle is pinned at a cusp.

From Eq. (3) we know that the stationary configurations on the two sides of a cusp need not be symmetrical with respect to those particles pinned at the cusp. The pinned particle can thus play the role of the conjunction of two different stationary configurations, which are not uniquely determined by each other. Therefore, for a configuration with $u_0=0$, $u_q=p$, and none of the in-between particles pinned at the cusps, we will consider these q particles, $\{u_0,u_1,\ldots,u_{q-1}\}$, as a ''$p/q$ section.''

For $\lambda>0$, we have the following two theorems.

Theorem I. For a stationary configuration of the FK model described above, there cannot be $q-1$ consecutive particles, none pinned at the cusps, in a minimum energy configuration for $\chi>\chi_q\equiv\pi/q$, with $\chi\equiv\arccos(1-\lambda/2)$.

This can be proved by considering the phonon spectrum of these $q-1$ particles with all the other particles fixed. It also reveals that at $\chi=\chi_q$, there is a phonon mode with zero frequency for these $q-1$ particles.

Theorem II. In a stationary configuration of the FK model, described above, with $u_0=0$ and $\chi<\chi_q$, u_r is an increasing function of u_s for $0<r<s\leqslant q$.

This can be proved by observing that $\sin(n\chi)>0$ for $0<n\leqslant q$. It implies that the p/q sections are uniquely determined for $\chi<\chi_q$.

For a given winding number $\omega=p/q$ and $\chi<\chi_q$, among the stationary configurations with no particles pinned at the cusps, there exists a unique *recurrent* configuration, given by

$$u_n'=\sum_{m=0}^{q-1}\nu_m(q)\left(\mathrm{Int}\left[(n+m)\omega+\frac{1}{2q}\right]-\mathrm{Int}\left[m\omega+\frac{1}{2q}\right]+\tfrac{1}{2}\delta_{m,0}\right), \quad (4)$$

with $\nu_n(q)=\tan(\chi/2)\csc(q\chi/2)\cos(n-q/2)\chi$. By theorem I, it cannot be a ground state configuration. However, we can use it to construct another recurrent stationary configuration, given by

$$u_n=\frac{u_n'+u'_{n+q_1^0}-p_1^0}{2}, \quad (5)$$

which has one particle pinned at the cusp in each period (e.g., $u_0=0$) and provides the explicit expression for the p/q section defined above. The definition of p_1^0,q_1^0 is related to the ''Farey fractions'' [10], defined as the collection of all irreducible fractions in [0,1], arranged in an ascending order. Irreducible fractions with denominators less than or equal to q, and arranged in ascending order, form the ''qth row of Farey fractions.''

In the q_cth row of Farey fractions, an irreducible fraction $\omega=p/q$ has two nearest neighbors, $\omega_1=p_1/q_1$ and $\omega_2=p_2/q_2$, such that

$$\kappa p=p_1+p_2, \quad \kappa q=q_1+q_2, \quad \omega_1<\omega<\omega_2 \quad (6)$$

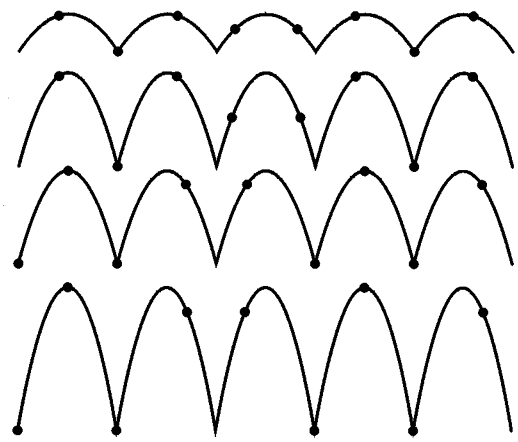

FIG. 1. The ground state configurations for $\omega=3/5$ at (a) $\chi=\pi/8$, (b) and (c) $\chi=\pi/5$ (degenerate), and (d) $\chi=\pi/4$. Note that the configurations in (c) and (d) are composed of $\frac{1}{2}$ and $\frac{2}{3}$ sections. At $\chi=\pi/5$, the ground state configuration in (b) can be continuously deformed to (c). The curves describe $V_{(u)}$ and the black circles indicate the positions of particles.

for some positive integer κ, and

$$pq_1=p_1q+1, \quad p_2q=pq_2+1, \quad p_2q_1=p_1q_2+\kappa. \quad (7)$$

For $q=q_c$, κ is 1, and the corresponding p_i, q_i, and ω_i are denoted by p_i^0, q_i^0, and ω_i^0, respectively.

From theorems I and II, these p/q sections with p/q in the q_cth row of Farey fractions are all the constitutional elements of a minimum energy configuration for $\chi_{q_c+1}<\chi\leqslant\chi_{q_c}$. In the following, we will show that the ground state configuration for fixed ω is composed of the ω sections, if ω is in the q_cth row of Farey fractions, or of ω_1 and ω_2 sections, if ω lies between two successive fractions ω_1 and ω_2 in the q_cth row of Farey fractions.

The average energy per particle of a p/q section, $\Psi(\omega)$, is given by

$$\Psi(\omega)=\frac{\omega^2}{2}-\frac{\lambda}{4}\sum_{n=0}^{q-1}\nu_n(q)\{\tfrac{1}{4}-(n\omega-\tfrac{1}{2}-\mathrm{Int}[n\omega])^2\}-\frac{\lambda}{8q}\nu_0(q). \quad (8)$$

For any three consecutive fractions $\omega_1<\omega<\omega_2$ in the q_cth row of Farey fractions, one can show that

$$q_1\Psi(\omega_1)+q_2\Psi(\omega_2)-\kappa q\Psi(\omega)=\frac{\lambda}{8}\tan\frac{\chi}{2}\cot\frac{q\chi}{2}\cot\frac{q_1\chi}{2}\cot\frac{q_2\chi}{2}, \quad (9)$$

where κ is defined in Eq. (6). The right-hand side is always positive for $\chi<\pi/\max(q,q_1,q_2)$. This indicates that for $0<\chi<\chi_q$, the ground state configuration with winding number $\omega=p/q$ is given by the one composed of p/q sections [see Fig. 1(a) for an example].

From theorem I, we know that the p/q sections will lose their stability for $\chi>\chi_q$. At $\chi=\chi_q$, there is a zero frequency phonon mode assosiated with a p/q section with displacements of each particles $\{\delta u_n\}$ given by

$$\delta u_n = a \sin\frac{n\pi}{q}, \tag{10}$$

where the amplitude a is restricted so that the in-between particles, $\{u_1, u_2, \ldots, u_{q-1}\}$, can only barely touch the cusps and the equation of motion still holds for them. The extreme case happens when either $u_{q_1^0} = p_1^0$ or $u_{q_2^0} = p_2^0$. In either case, say $u_{q_2^0} = p_2^0$, we will regard the q_2^0 particles from u_0 to $u_{q_2^0 - 1}$ as a p_2^0/q_2^0 section, i.e., a consecutive q_2^0 particles chain with the first particle sitting at the cusp, while the q_1^0 particles from $u_{q_2^0}$ to u_{q-1} as a p_1^0/q_1^0 section [see Figs. 1(b) and 1(c) for an example]. For a general $\omega = p/q$, if we regard a p/q section as a molecule of size (q,p), i.e., composed of q particles and p wells, then χ_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_1^0, p_1^0) and (q_2^0, p_2^0), respectively. There the three types of molecules, whose corresponding ω_1^0, ω, and ω_2^0 are related as consecutive fractions in the qth row of Farey fractions, coexist. Moreover, the zero frequency phonon mode allows us to continuously deform the p/q sections into degenerate configurations.

It should be noted that, at this critical point, the cusp can barely provide the force to pin the particle at the conjunction between p_1^0/q_1^0 and p_2^0/q_2^0 sections. When χ increases just above χ_q, the p/q section becomes unstable, and any small perturbation will cause one more particle to roll down to the cusp in each period, resulting in ω_1^0 and ω_2^0 sections. Therefore, the molecules of size (q,p) completely dissociate, and the ground state now is a mixture of ω_1^0 and ω_2^0 sections with the right proportion [see Fig. 1(d) for an example]. One should note that there is a great deal of degeneracy due to the arbitrary ordering of these two kinds of sections.

From Eq. (9), we know that premature dissociations of stable molecules into other kinds of molecules always cost energy. The ground state configuration is thus described by a mixture of ω_1^0 and ω_2^0 sections for $\chi > \chi_q$.

When χ continues to increase and reaches $\overline{\chi_q} \equiv \pi/\max(q_1^0, q_2^0) = \min(\chi_{q_1^0}, \chi_{q_2^0})$, say $\overline{\chi_q} = \chi_{q_1^0}$, the molecule of size (q_1^0, p_1^0) starts to dissociate into even smaller molecules of sizes (q_2^0, p_2^0) and $(q_1^0 - q_2^0, p_1^0 - p_2^0)$. Note that $(p_1^0 - p_2^0)/(q_1^0 - q_2^0)$, p_1^0/q_1^0, and p_2^0/q_2^0 are consecutive fractions in the $(q-1)$th row of Farey fractions. It follows that the ground state configuration with a fixed winding number must be composed of no more than two kinds of sections with fractions consecutive in the q_cth row of Farey fractions for $\pi/(q_c+1) < \chi \leq \pi/q_c$. The dissociating process continues until all the particles are located at the cusps. This occurs at $\chi > \pi/2$.

It is interesting to observe that for $\chi_q < \chi < \overline{\chi_q}$, even though p/q sections no longer describe the ground state configuration, it continues to evolve as an unstable configuration until χ reaches $\overline{\chi_q}$. Hence molecules of size (q,p) may be regarded as a resonance state of two smaller molecules of sizes (q_1^0, p_1^0) and (q_2^0, p_2^0) when χ lies in the interval $(\chi_q, \overline{\chi_q})$.

In summary, for given χ, 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 ω sections with ω in the q_cth row of Farey fractions in the following way. For an arbitrary irrational winding number ω or rational but not in the q_cth row of Farey fractions, we can find a unique pair of consecutive fractions ω_1 and ω_2 in the q_cth row of Farey fractions such that $\omega_1 < \omega < \omega_2$. The ground state configuration with this given ω can be constructed with a fraction ℓ_1 of particles associated with the ω_1 sections and a fraction ℓ_2 associated with ω_2 sections such that

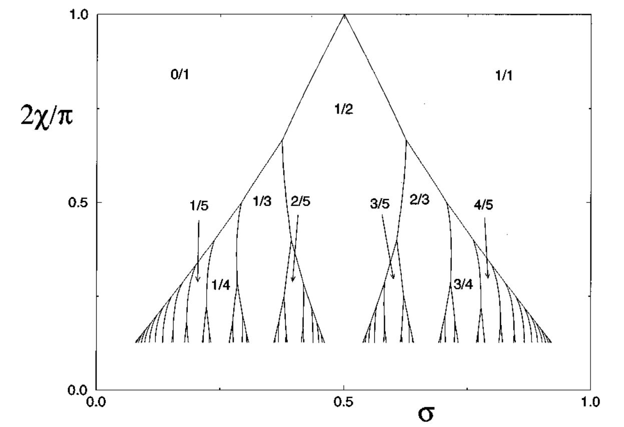

FIG. 2. The domains of stability in the χ-σ plane. The number in each domain denotes its winding number.

$$\ell_1 + \ell_2 = 1, \quad \ell_1\omega_1 + \ell_2\omega_2 = \omega. \tag{11}$$

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

$$\Psi_e(\omega) = \frac{\omega_2 - \omega}{\omega_2 - \omega_1}\Psi(\omega_1) + \frac{\omega - \omega_1}{\omega_2 - \omega_1}\Psi(\omega_2). \tag{12}$$

Equation (9) indicates that $\Psi_e(\omega)$ is a convex function of ω.

Adding or removing one particle from the system will turn p_1 ω_2 sections into p_2 ω_1 sections, or vice versa. This can be seen from $p_1 p_2 (1/\omega_1 - 1/\omega_2) = 1$. Starting from pure ω_2 sections, i.e., the ground state configuration with winding number ω_2, we can approach the ground state configuration with winding number ω_1 by adding particles one by one. Solitons and antisolitons in the usual sense of local ''defects'' do not exist. Efforts to create them merely induce transitions between ω_1 and ω_2 sections. If we insist on calling an ω_1 section in a background of ω_2 sections a defect, this defect will carry a fractional charge $1/p_2$. A general minimum energy configuration may contain an arbitrary number of such defects with an arbitrary spatial arrangement.

Up to now, we have been discussing the ground state configuration for given ω as χ is varied. Introducing the tensile force term $-\sigma\omega$ into Eq. (12), we obtain the enthalpy of this system. By minimizing this enthalpy with respect to ω, we obtain the phase diagram in the $\chi - \sigma$ plane, as shown in Fig. 2. One can see that there exist triple points at $\chi_q = \pi/q$, for each q, where three types of molecules coexist. For $\chi < \chi_q$, the lowest enthalpy configuration is locked to $\omega = p/q$ for

$$\frac{\Psi(\omega)-\Psi(\omega_1)}{\omega-\omega_1}\leqslant\sigma\leqslant\frac{\Psi(\omega_2)-\Psi(\omega)}{\omega_2-\omega}, \tag{13}$$

where $\omega_1<\omega<\omega_2$ are consecutive fractions in the q_cth row of Farey fractions with $\chi_{q_c+1}<\chi\leqslant\chi_{q_c}$. When $\chi=\chi_q$, the step shrinks to a point, and we have

$$\sigma=\frac{\Psi(\omega)-\Psi(\omega_1)}{\omega-\omega_1}=\frac{\Psi(\omega_2)-\Psi(\omega)}{\omega_2-\omega}, \tag{14}$$

which gives the equations for the triple point. In general, for two consecutive Farey fractions ω_1 and ω_2, $\sigma=[\Psi(\omega_2)-\Psi(\omega_1)]/(\omega_2-\omega_1)$ gives the equation for the coexistent curve of the two phases corresponding to molecules of sizes (q_1,p_1) and (q_2,p_2). Different proportions of these two kinds of molecules will lead to varieties of configurations with the same average enthalpy per particle but different winding numbers. Therefore, the winding number of the lowest enthalpy configuration is not uniquely specified, showing that an important result proved by Aubry [3] for smooth potentials does not apply in the present case.

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 fractions dictate 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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