A Frenkel-Kontorova Model with Two Spring Constants: New Phases and Phase Transitions

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Abstract

A discrete Frenkel-Kontorova model with two alternate spring constants $k_1$ and $k_2$ is studied. It is found that this model has many surprising behaviours. The continuum version of this model is different from the sine-Gordon equation, the continuum version of the standard FK model. More interestingly, it has an unpinned commensurate phase which is translationally invariant. A phase transition takes place on a lattice point in the parameter space. We have also predicted another interesting phase transition in which an unlocked commensurate phase breaking translational invariance will take place as the strength of the substrate potential is increased.

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Many years ago Frenkel and Kontorova \[1\] proposed a discrete version of the sine-Gordon equation, which is now known as the Frenkel-Kontorova (FK) model. It has been widely studied as a model for many solid-state systems \[2, 3, 4, 5\] such as crystal dislocations, absorbed epitaxial monolayers and incommensurate structures, etc. This simple classical one-dimensional model consists of a group of particles connected by springs subject to an external sinusoidal potential. It has a rich phase diagram \[5, 6\]. Its commensurate phase is separated by infinitesimal gaps of incommensurate structure. In a commensurate phase, translational invariance is broken and no zero-frequency phonon mode exits. However, an incommensurate phase is translational invariant and has a zero-frequency phonon mode. There is a “transition by breaking of analyticity” \[6\] for an incommensurate phase as the strength of substrate potential is increased. However, there is no symmetry breaking in this transition.

Many generalized FK models \[7, 8, 9, 10, 11\] have been studied for different purposes. In this paper, we propose to study the following generalised FK model,

\[
U = \frac{1}{4} \sum_n f(n, k_1, k_2)(X_{n+1} - X_n - f(n, a, b))^2 - \frac{V_c}{2\pi} \sum_n \cos\left(\frac{2\pi}{c} X_n\right).
\]

(1)

Here \(f(n, l, m) = l(1 - (-1)^n) - m(1 + (-1)^n)\). \(X_n\) is the position of the \(n\)th particle. \(a\) and \(b\) are the equilibrium lengths of the two springs with spring constants \(k_1\) and \(k_2\). They satisfy the balance equation \(k_1 a = k_2 b\) that is the ground state solution of Eq. (1) with \(V = 0\). \(c\) is the period of the sinusoidal substrate potential. The system consists of particles connected alternately by two kinds of springs. Obviously, in the absence of a substrate potential, the ground state is a dimerized state, as shown in Fig. 1. In many real quasi-one-dimensional systems \[4\] of solid state physics, such dimerization often occurs due to lattice distortion as in the case of Peierls instability.

Differentiating the potential function (1) with respect to \(X_n\), we obtain the equations for the equilibrium states:
We rewrite them as

\[ k_1X_{n+1} - (k_1 + k_2)X_n + k_2X_{n-1} - V\sin\left(\frac{2\pi}{c}X_n\right) = 0 \]

\[ k_2X_{n+2} - (k_1 + k_2)X_{n+1} + k_1X_n - V\sin\left(\frac{2\pi}{c}X_{n+1}\right) = 0 \]

We rewrite them as

\[
(X_{n+1} - 2X_n + X_{n-1}) + (2g - 1)(X_{n+1} - X_n) - \\
(X_n - X_{n-1}) - \frac{2V}{k_2}\sin\left(\frac{2\pi}{c}X_n\right) = 0 
\]

\[
(X_{n+2} - 2X_{n+1} + X_n) + (2g^{-1} - 1)(X_{n+2} - X_{n+1}) - \\
(X_{n+1} - X_n) - \frac{2V}{k_1}\sin\left(\frac{2\pi}{c}X_{n+1}\right) = 0 
\]

Here \( g = k_2/k_1 \). We introduce fields \( X \) for a particle with \( n = \text{even} \) and \( Y \) for a particle with \( n = \text{odd} \). In this way, the continuum version of Eq. \((3)\) can be written as,

\[
\frac{d^2X}{dn^2} + (2g - 1)\frac{dX}{dn} - \frac{dY}{dn} = \frac{2V}{k_2}\sin\left(\frac{2\pi}{c}X\right) 
\]

\[
\frac{d^2Y}{dn^2} + (2g^{-1} - 1)\frac{dY}{dn} - \frac{dX}{dn} = \frac{2V}{k_1}\sin\left(\frac{2\pi}{c}Y\right) 
\]

They are two coupled nonlinear equations. When \( g = 1 \), Eq. \((3)\) becomes the sine-Gordon equation \([3]\). Intuitively, we expect our model to behave like the FK model when \( k_1 - k_2 \) is small. However, we find this is not always the case and we will discuss this point in later sections.

From previous studies \([3, 6, 8]\), we know the locked and unlocked phases of the FK model are related to the distribution of the particles in the external potential wells. For a commensurate phase \([8]\), the particles are symmetrically placed about the bottom of a well or the top of a well, i.e., there is a symmetric point. It is just because of this symmetric point that a commensurate phase is pinned to the substrate. To reach another degenerate ground state of the system, it must move its symmetric point over the top of a well to the other side of the well. It has to overcome an energy barrier; therefore, the system chooses to be locked to the substrate. In contrast to a commensurate phase, an incommensurate phase does not have such a
symmetric point. Therefore, an incommensurate phase is unlocked and is translationally invariant. In this sense, we can regard an incommensurate phase as the phase that breaks the symmetry of a commensurate phase. Obviously, the nonuniformity of the spring constants in our model also has the same effect. It makes all the phases less symmetric. Intuitively an incommensurate phase of our model is more asymmetric than that of the FK model. So a stronger substrate potential is expected to lock our model. Besides, due to the nonuniformity, a commensurate phase possibly does not have a symmetric point because it only can exist in some special cases. This means our model could have a new commensurate phase which is translationally invariant and unpinned. Now we prove it in a more rigorous manner by a perturbative study.

For a small amplitude $V$ of a substrate potential, we can view it as a perturbation to a uniform ground state of $X_n - X_{n-1} = a$ or $b$. $V$ is treated as the perturbation parameter. Then $X_n$ can be rewritten as

$$X_n = E_n + \delta_n + \theta$$

Here $E_n$ is the position of the $n$th particle when $V = 0$, $\theta$ is an overall phase shift factor and $\delta_n = 0$ is equivalent to $V = 0$. Putting Eq. (5) into Eq. (2), we have

$$k_1 \delta_{n+1} - (k_1 + k_2) \delta_n + k_2 \delta_{n-1} - V \sin \left[ \frac{2\pi}{c} (E_{n+1} + \delta_{n+1} + \theta) \right] = 0$$

$$k_2 \delta_{n+2} - (k_1 + k_2) \delta_{n+1} + k_1 \delta_{n} - V \sin \left[ \frac{2\pi}{c} (E_{n+2} + \delta_{n+2} + \theta) \right] = 0$$

Expanding $\delta_n$ in orders of $V$, we have

$$\delta_n = \delta^1_n(V) + \delta^2_n(V^2) + \delta^3_n(V^3) + \ldots$$

To first order in $V$, we get
Unlike the standard FK model, this divergence can simply be eliminated by

\[ k_2\delta_n^1 - (k_1 + k_2)\delta_{n-1}^1 + k_1\delta_{n-2}^1 - V\sin\left[\frac{2\pi}{c}(E_{n-1} + \theta)\right] = 0 \]

\[ k_1\delta_{n+1}^1 - (k_1 + k_2)\delta_n^1 + k_2\delta_{n-1}^1 - V\sin\left[\frac{2\pi}{c}(E_n + \theta)\right] = 0 \]  
(7)

\[ k_2\delta_{n+2}^1 - (k_1 + k_2)\delta_{n+1}^1 + k_1\delta_n^1 - V\sin\left[\frac{2\pi}{c}(E_{n+1} + \theta)\right] = 0 \]

Eliminating \( \delta_{n+1}^1 \) and \( \delta_{n-1}^1 \), we have

\[ \delta_{n+2}^1 - 2\delta_n^1 + \delta_{n-2}^1 = A\sin\left[\frac{2\pi}{c}(E_n + \theta)\right] + B\cos\left[\frac{2\pi}{c}(E_n + \theta)\right] \]  
(8)

where

\[ A = \frac{\sqrt{V}}{k_1k_2}[k_1\cos(\frac{2\pi}{c}a) + k_2\cos(\frac{2\pi}{c}b) + k_1 + k_2] \]

\[ B = \frac{\sqrt{V}}{k_1k_2}[k_1\sin(\frac{2\pi}{c}a) - k_2\sin(\frac{2\pi}{c}b)] \]

To obtain these results, we have made use of \( E_{n-1} = E_n - b \) and \( E_{n+1} = E_n + a \). The solution to Eq. (8) is

\[ \delta_n^1 = \frac{A\sin\left[\frac{2\pi}{c}(E_n + \theta)\right] + (-1)^nB\cos\left[\frac{2\pi}{c}(E_n + \theta)\right]}{2(\cos\left[\frac{2\pi}{c}(a + b)\right] - 1)}. \]  
(9)

Putting this solution into Eq. (8), we obtain

\[ \delta_n^2 = \frac{A_1\sin\left[\frac{4\pi}{c}(E_n + \theta)\right] + (-1)^nB_1\cos\left[\frac{4\pi}{c}(E_n + \theta)\right]}{8(\cos\left[\frac{4\pi}{c}(a + b)\right] - 1)(\cos\left[\frac{4\pi}{c}(a + b)\right] - 1)}. \]  
(10)

with

\[ A_1 = \frac{2\pi\sqrt{V}}{k_1k_2}[B(k_1\sin(\frac{4\pi}{c}a) - k_2\sin(\frac{4\pi}{c}b)) + A(k_1 + k_2 + k_1\cos(\frac{4\pi}{c}a) + k_2\cos(\frac{4\pi}{c}b))] \]

\[ B_1 = \frac{2\pi\sqrt{V}}{k_1k_2}[A(k_1\sin(\frac{4\pi}{c}a) - k_2\sin(\frac{4\pi}{c}b)) + B(k_1 + k_2 - k_1\cos(\frac{4\pi}{c}a) - k_2\cos(\frac{4\pi}{c}b))] \]

It is not difficult to know to order \( V^n \) the denominator of \( \delta_n^1 \) is the multiplication of \( \cos[\frac{2\pi}{c}(a + b) - 1], \cos[\frac{4\pi}{c}(a + b)] - 1\), ..., \( \cos[\frac{2n\pi}{c}(a + b)] - 1\). We immediately know that \( \delta_n \) is always divergent for any rational \( (a + b)/c \). Unlike the standard FK model, this divergence can simply be eliminated by
fixing the phase factor to 0 or \( c \) because the numerator of \( \delta_n^\alpha \) is a sum of a sine and a cosine functions. It seems that perturbation theory \([8]\) would not work; however, this is not the case. In the following, we will show how it works perfectly. This divergence only implies there is a new commensurate phase which is translationally invariant and unlocked.

First, we group the solutions ..., \( \delta_{n-1} \), \( \delta_n \), \( \delta_{n+1} \), ..., etc. with two in a group: \((\delta_{n-2}, \delta_{n-1})(i-1), (\delta_n, \delta_{n+1}), (\delta_{n+2}, \delta_{n+3})(i+1), \) etc. We define a new sequence \( t_i = \delta_n + \delta_{n+1} \). To first order in \( \delta_n \), we have \( t_1^1 = \delta_1^1 + \delta_1^{n+1} \). From Eq. (11), we get

\[
t_1^1 = \frac{(A\cos(\frac{\pi a}{c}) + B\sin(\frac{\pi a}{c}))\sin[\frac{2\pi}{c}(i \theta + \frac{\pi a}{c})]}{\cos[\frac{2\pi}{c}(a + b) i - 1]} \quad (11)
\]

By setting \( \theta + a/2 = 0 \) or \( c \), the divergence can be eliminated and \( t_1^1 \) is locked to be identically zero. However, this does not mean the particles are pinned to the external potential. It only shows that the two nearest particles move in a different direction, i.e., \( \delta_1^1 = -\delta_1^{n+1} \), etc. Imposing this condition on Eq. (11), we get the finite and nonzero solutions

\[
\delta_n^1 = \frac{V\sin[\frac{2\pi}{c}(E_n + \theta)]}{2(k_1 + k_2)} \quad (12)
\]

From Eq. (12), we can extend the above conclusions to second order in \( \delta_n \). It is obvious that to any order the divergence in \( \delta_n \) can be eliminated in this way and we can find a finite and nonzero solution like Eq. (12). Summing over all these terms, we can write the solution to Eq. (6) for any rational value of \((a+b)/c\) as

\[
\delta_n = \sum_l \{f_l \sin[\frac{2\pi l}{c}(E_n + \theta)] + (-1)^n t_l \cos[\frac{2\pi l}{c}(E_n + \theta)]\} + \sum_m \frac{p_m}{2(k_1 + k_2)} \sin[\frac{2\pi m}{c}(E_n + \theta)] \quad (13)
\]

Here \( l(a+b)/c \neq \text{integer} \), \( m(a+b)/c = \text{integer} \), and \( m(\theta + a/2)/c = \text{integer} \). \( f_l \) is the sum of the solutions to Eq. (6) to all orders that contain the function \( \sin[\frac{2\pi l}{c}(E_n + \theta)] \); \( t_l \) is the sum of solutions to Eq. (6) to all orders that contain
the function \( \cos \left[ \frac{2\pi l}{c} (E_n + \theta) \right] \). For example, to second order in \( V \), \( f_1 = A/[2(\cos \left[ \frac{2\pi}{c} (a+b) \right] - 1)] \), \( f_2 = A_1/[8(\cos \left[ \frac{2\pi}{c} (a+b) \right] - 1)(\cos \left[ \frac{4\pi}{c} (a+b) \right] - 1)] \) and \( t_1 = B/[2(\cos \left[ \frac{2\pi}{c} (a+b) \right] - 1)] \), \( t_2 = B_1/[8(\cos \left[ \frac{2\pi}{c} (a+b) \right] - 1)(\cos \left[ \frac{4\pi}{c} (a+b) \right] - 1)] \).

In high orders in \( V \), they are a very complex sum. \( p_m \) is the coefficient of the function of \( \sin \left[ \frac{2\pi m}{c} (E_n + \theta) \right] \) in Eq. (6) just as shown in Eq. (12). It is easy to show

\[
\sin \left[ \frac{2\pi m}{c} (E_n + \theta) \right] = (-1)^n \sin \left[ \frac{2\pi m}{c} \theta \right]
\]

from the conditions \( m(a + b)/c = integer \), and \( m(\theta + a/2)/c = integer \). So the second sum is independent of the the particle’s positions; otherwise, this term has different signs for the particles at even and odd sites. This shows that all particles with \( n = even \) move the same distance in the same direction and particles with \( n = odd \) move in the opposite direction with the same distance. In other words, the two sublattices have a relative parallel movement. The distance of the movement is dependent on the overall phase factor \( \theta \). \( \theta \) is determined by the condition \( m(\theta + a/2)/c = integer \). It is related to the parameter \( a \). However, the parameter \( a \) is completely free because the equation \( b = ga \) does not impose any restriction on it. Therefore, the overall phase factor \( \theta \) has a lot of freedom in our model.

Before we go further, let us recall some interesting properties of the standard FK model. In the FK model, the perturbative solution \([8]\) for a commensurate phase can be written as

\[
\delta_n = \sum_l h_l \sin \left[ \frac{2\pi l}{c} (E_n + \theta) \right]
\]

Here \( E_n = a_0 n \), \( la_0/c \neq integer \). This solution can be viewed as a special case of Eq. (13) at \( g = 1 \). It is an odd function. Therefore, a commensurate phase always has a symmetric point. Now let us inspect a more specific case. For \( a_0/c=M/N \), \( \theta/c \) can take the value \( n_0/N \) with \( n_0 = 0, ..., N \). We have

\[
\frac{E_n + \theta}{c} = \frac{na_0}{c} + \frac{\theta}{c} = \frac{nM + n_0}{N}
\]
It is not difficult to find that there is an infinite set of $n$ values that make $(nM + n_0)/c$ equal to an integer for any group of $M$, $N$ and $n_0$. This means that there is an infinite set of particles that never move with a sinusoidal potential $V$ for any commensurate phases and any overall phase factor in the standard FK model. They stay at their initial positions for ever no matter how $\theta$ is changed. Hence a commensurate phase in the standard FK model is always pinned to the substrate and is not translationally invariant.

Now let us return to our model. The most obvious feature of Eq. (13) is that there is no obvious symmetry because it is a sum of an odd function and an even function. Thus there is a symmetry breaking in our model. A commensurate phase in our model does not have any symmetric point. It breaks the symmetry of a commensurate phase in the standard FK model. This is similar to an incommensurate phase in the FK model. Another interesting property is that no particles are pinned to their initial positions. This is because there is no way to make a sine function and a cosine function to be equal to zero at the same value of their variables. Moreover, all particles are related through the overall phase factor $\theta$. Its effect cannot be simply eliminated as shown in Eq. (16) or otherwise. Any value of $\theta$ has an effect on all the particles. Any change in $\theta$ will make all particles move. There is no position that a particle is favoured. We have shown that $\theta$ has much freedom. Therefore, a commensurate phase in our model is translationally invariant and unpinned. However, the movement revealed in Eq. (13) is not trivial. As we have shown, the second sum in Eq. (13) indicates a relative parallel movement of the two sublattices. The first sum also shows the trend of two sublattices moving in two different directions because there is a change of sign for $n = odd$ and $n = even$. So the basic movement in our model is a relatively sliding between two sublattices. As a result a commensurate phase is not expected to have a zero frequency phonon mode for the whole system because it requires the whole system to move in the same direction. So far we have shown that our model has a new commensurate phase which is translationally invariant and unpinned.
Except for the new phase, our model also has the usual FK model-like commensurate phase for the special rational \( \frac{a+b}{c} \). When \( k_1 \sin(\frac{2\pi}{c}a) = k_2 \sin(\frac{2\pi}{c}b) \), \( k_1 \sin(\frac{4\pi}{c}a) = k_2 \sin(\frac{4\pi}{c}b) \), etc., the solutions \( \delta_n^1, \delta_n^2 \), etc. become

\[
\delta_n^1 = \frac{A \sin[\frac{2\pi}{c}(E_n + \theta)]}{2(\cos[\frac{2\pi}{c}(a + b)] - 1)}
\]

\[
\delta_n^2 = \frac{A_1 \sin[\frac{4\pi}{c}(E_n + \theta)]}{8(\cos[\frac{4\pi}{c}(a + b)] - 1)(\cos[\frac{4\pi}{c}(a + b)] - 1)}
\]

e tc., which are just the same as the solutions \( \text{[8]} \) of the FK model. The only way to meet these conditions is \( a/c \) and \( b/c \) are the two non-zero and non-negative solutions of the equation \( \sin(2\pi X) = 0 \), i.e., they are integers or half integers greater than 1/2. In this case, our model behaves like the standard FK model. All the conclusions of the FK model can directly be applied to it. These commensurate phases are locked and are not translationally invariant.

Now we turn to an irrational \( (a + b)/c \). Like the FK model, the perturbation theory works well and there is no locking phenomenon for any irrational \( (a + b)/c \). Therefore, an incommensurate phase of our model is translationally invariant and has a zero-frequency phonon mode. For a small \( k, B_1, B_2, \ldots \approx 0 \), and \( A \) and \( A_1 \), \( \ldots \approx \frac{2}{k_1}(1 + \cos[\frac{2\pi}{c}(a + b)]) \) and \( \frac{8\pi V}{k_2^2}(1 + \cos[\frac{2\pi}{c}(a + b)])(1 + \cos[\frac{4\pi}{c}(a + b)]) \), etc.. The solutions (12) and (13) become the same as the standard FK model \( \text{[8]} \). Aside from this, there is no way to make our model behave like the FK model for an irrational \( (a + b)/c \).

We plot the phase diagram of our model for small \( V \) in \( a/c \) versus \( b/c \), as shown in Fig. 2. Phases in the parameter space that form a square lattice with the lattice constant 1/2 are the locked phases which are not translationally invariant and do not have a zero-frequency phonon mode. The others in the phase space represent unlocked phases which are translationally invariant. So a phase transition breaking translational symmetry must happen on the square lattice in the parameter space \( (a/c, b/c) \).

How this phase diagram changes with the amplitude \( V \) of the external potential is an interesting question. For an irrational \( (a + b)/c \), no new
things are expected to happen: an unlocked incommensurate phase is simply locked to a translationally invariant incommensurate phase. However, for an unlocked commensurate phase, a new phase transition is expected to occur. It will definitely be locked to the external potential with the increase of $V$. It is very possible that an unlocked commensurate phase is locked to a phase on the square lattice in the parameter space. If this happens, the phase transition would break translational symmetry.

In summary, we have proposed a new generalised FK model. Its continuum version is different from the sine-Gordon equation. Under certain conditions, our model is the same as the discrete sine-Gordon equation. Surprisingly, it occurs at a large difference of $(a - b)/c > 1/2$ instead of a small one for a rational $(a + b)/c$. More interestingly, our model has a translationally invariant commensurate phase which is unpinned. It has a rich phase diagram, which is to be explored in the future. A phase transition breaking translational symmetry take place on a square lattice in the parameter space. Furthermore, we predict another new phase transition would happen for large $V$.

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Figure Captions:

1. Frenkel-Kontorova model with two spring constants $k_1$ and $k_2$.

2. Phase diagram $a/c$ vs. $b/c$. A dot represents a locked phase; the others represent unpinned phases.
