Hidden Dimer in the Frenkel-Kontorova Model

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The incommensurability of the supercritical Frenkel-Kontorova model is decomposed into a family of dimer type “defects” by appropriate decimations. Interestingly, this hidden dimer results in Bloch-wave type excitations of the renormalized chain which appear in the disguised form of multi-step phonon modes for the original system. We call these intriguing excitations stepon modes and conjecture that they play a key role in determining the localization boundary in systems exhibiting Anderson localization.

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In this paper, we describe a very interesting relationship between two seemingly different models that have been in the forefront of theoretical physics: the Frenkel-Kontorova (FK) model and the random dimer model. This relationship establishes the existence of propagating Bloch-type phonons in the pinned phase of the FK model and resolves the mystery of novel multi-step excitations found recently.

The incommensurate FK model consists of a chain of balls connected by Hooke’s springs in a periodic sinusoidal potential of the strength $K$ where the average spacing $\sigma$ between the balls is incommensurate with the periodicity of the potential. The equilibrium positions of the balls $x_n$ are given by the iterates of the standard map

$$x_{n+1} + x_{n-1} - 2x_n = -\frac{K}{2\pi} \sin(2\pi x_n).$$

For small $K$, the iterates $x_n$ are confined on an invariant circle of the standard map. The breakup of the invariant circle at the critical value $K_c$ corresponds to the pinning transition in the FK model accompanied with the disappearance of the zero frequency phonon mode. The phonon modes are linear excitations of the equilibrium configurations of the balls satisfying the equation

$$\psi_{n+1} + \psi_{n-1} + \epsilon_n \psi_n = E \psi_n,$$

where the eigenvalue $E$ is related to the phonon frequency $\omega$ as $E = -\omega^2 + 2$, and $\epsilon_n = K \cos(2\pi x_n)$ is the onsite phonon potential.

At the so-called anti-integrable limit $K \to \infty$, the balls sit at the bottom of the potential wells and therefore $\epsilon_n$ is constant for all sites $n$. When $K$ decreases, the limiting uniform phonon potential splits into more and more distinguishable levels. As shown in Fig. 1, this splitting generates a symbolic representation of the lattice. It turns out that by expanding the potential up to any order $1/K^p$ the resulting incommensurate lattice with no apparent short range clustering can be decimated into a lattice with dimer and tetramer “defects”. As $p$ increases, the decimated structure becomes more and more complex. The discovery of a hidden dimer helps in tracing the origin of intriguing “stepon” excitations with multi-step eigenfunctions that were found in our recent numerical study of the supercritical parameter region $K > K_c$. The central result of this paper is that the stepon modes of the FK model are in fact propagating Bloch waves on the renormalized lattice.

The models with dimer type defects attracted a great deal of attention a few years ago due to the discovery of subtle delocalization mechanisms which explained the conduction in polymers. The delocalized modes originated from special resonance conditions where the reflected waves from neighboring defect sites interfered destructively resulting in the ballistic transport in the system. Detailed theoretical studies showed that a variety of extended defects with reflection symmetry could be made to exhibit this resonance by tuning a control parameter so that the resonance condition was satisfied by an energy close to the Fermi energy. This turns out to be true also for the dimer and tetramer defects in the renormalized lattices of the supercritical FK model.

For our analysis, we study a generalized version of the FK model with two independent parameters $K$ and $\lambda$ so that in Eq. (2) $\epsilon_n = \lambda \cos(2\pi x_n)$. The model reduces to the FK model when the two parameters are equal. This extension of parameter space is analogous to the analytic continuation into complex plane and will turn out to be crucial in understanding the stepon modes. In the 2-parameter model, the parameter $\lambda$ controls the strength while $K$ determines the smoothness of the onsite “phonon” potential as the underlying invariant circle of the standard map undergoes the transition by breaking of analyticity at the critical value $K = K_c$. In the region $K < K_c$, the potential $\epsilon_n$ is a smooth function of the effective phase $\theta = \{nx + \phi\}$ where the brackets denote the fractional part. In this case the model falls into the universality class of the famous Harper equation which exhibits a transition from extended to localized states. On the other hand, for $K > K_c$ the phonon potential is
determined by an underlying invariant Cantor set (cantorus) of the standard map. Therefore, the 2-parameter model provides one with a new class of quasiperiodic systems that interpolates nicely between the Harper equation \((K = 0)\) and the FK phonon equation. As seen later, this important feature helps in understanding the absence of Anderson localization for the FK phonons.

Fig. 2 shows the phase diagram of the model obtained using an exact decimation scheme discussed in our earlier papers \([3, 4]\). The model exhibits an extended phase, a localized phase as well as a critical phase with self-similar eigenfunctions. A novel aspect of the model is the emergence of infinitely many curves from the “corner” \(\lambda, K \to \infty\) along which the eigenfunctions are represented by an infinite series of step functions of the effective phase \(\theta\) (see Fig. 3). We call these solutions stepon modes. All except the right most curve intersect the standard FK limit \(K = \lambda\). We referred to these intersections as degeneracy points in our earlier numerical work \([3]\) because at these parameter values, the nontrivial scaling properties of critical phonons “degenerated” into the trivial scaling of the stepon modes. It is interesting to note that the degeneracy curves accumulate at the critical parameter value \(K = K_c\) for the circle-cantorus transition of the standard map. The parameter region outside these curves consists of either the critical or localized phase. The localized phase for large values of \(\lambda\) intertwines with the degeneracy curves. The fact that the localized modes reside inside the tongues of the degeneracy curves suggests that the stepon modes play a special role in the localization phenomenon in models where the underlying potential is not smooth. However, the specifics of that role remains eluded to us at present.

The above phase diagram suggests a perturbative approach to understand the origin of the stepon modes. We develop a perturbation theory near the anti-integrable limit by expanding the equilibrium configurations of the balls \(x_n\) with \(\kappa = 1/K\) as the expansion parameter. In the cantorus regime, the hull function \(X\) defined by \(x_n = X(n\sigma + \phi)\) is a convergent series of step functions \([2]\). We write \(X(\theta) = X_0(\theta) + X_1(\theta)\kappa + X_2(\theta)\kappa^2 + \ldots\), where \(X_0(\theta) = \frac{1}{2} + \text{Int}(\theta)\). Substituting the above expansion into Eq. \([1]\), we generate a similar expansion for the “phonon” potential \(\lambda \cos[2\pi X(\theta)]\). Truncating this expansion at the order \(\kappa^p\) leads to a potential with a finite number of steps. This in turn leads to symbolic representation of the lattice of the type shown in Fig. 1, where the number of required symbols increases with the order of perturbation.

For general \(p\), the symbolic representation can be very complex. However, it turns out that by an appropriate decimation, the lattice can always be represented by one of the two possible forms which happen to be the ones found at \(p = 2\) and \(p = 3\). Different \(p\) cases are distinguished from each other by different renormalized onsite “energies” and coupling terms. In the following, we summarize the essential features of the symbolic representation.

Each symbol (except the one for the potential minimum) is associated with two symmetrically placed \(\theta\)-intervals where the potential takes the corresponding constant value. For example, for \(p = 2\) the symbol \(a\) is attached to the \(\theta\)-intervals \([0, \sigma), [1 - \sigma, 1)\) and the symbol \(b\) to the interval \([\sigma, 1 - \sigma)\). As \(p\) increases, these intervals split into subintervals in a systematic way. The borders of intervals, which are discontinuities of the potential, are obtained as the first \(p - 1\) forward and backward iterates of the map \(\theta_{j+1} = \theta_j + \sigma\) (mod 1) with \(\theta_0 = 0\). The splitting of the levels as \(p\) increases can be shown to follow two possible patterns depending upon whether the new discontinuities land within the middle interval or not. If the two new discontinuities at the order \(p\) land inside order- \((p - 1)\) intervals other than the middle one, both intervals are split into two parts whose relative lengths are determined by the golden mean. We label the longer ones of these new subintervals by \(a\) and the shorter ones by \(b\).

The rest of the intervals can be labeled in an arbitrary way. This pattern emerges for \(p = 3, 4, 6, 7, \ldots\). The other possibility is that both new discontinuities land inside the middle interval which breaks up into three parts \(a, b, a\). In this case the total length of the \(a\)-subintervals is related to the length of the \(b\)-subinterval by the square of the golden mean. This happens to be the case for \(p = 2, 5, 18, \ldots\).

It turns out that the lattice sites which are not labeled as \(a\) or \(b\) can be decimated. In the renormalized lattice, the complexity of the original symbol dynamics manifests itself in the renormalization of the onsite energies as well as the coupling terms. Because of the symmetric alignment of the decimated blocks \([4]\), the renormalized couplings between the \(a\)-type sites alternate between two values. Thus, the whole problem reduces to showing the existence of propagating wave solutions for the lattice with dimer and tetramer “defects”.

It suffices to discuss the \(p = 3\) perturbation theory in detail (\(p = 2\) gives the trivial solution) as the other renormalized lattices have a similar form. The truncated potential in the \(p = 3\) case takes three distinct values \(\epsilon_a, \epsilon_b, \epsilon_c\) as shown in Fig. 1. Here \(\epsilon_a = \lambda(-1 + 2\pi^2\kappa^2(1 - 6\kappa)), \epsilon_b = \lambda(-1 + 2\pi^2\kappa^2(1 - 8\kappa)),\) and \(\epsilon_c = -\lambda\). The decimation of the sites \(c\) results in the renormalized lattice \(\ldots\text{aaaaabbb}\ldots\) with the renormalized onsite energy \(\epsilon_a = (1 - (E - \epsilon_a)(E - \epsilon_c)),\) while the renormalized couplings between two neighboring \(a\)-sites alternate between \(V_1 = 1\) and \(V_2 = (E - \epsilon_c)\). The decimated lattice can be shown to have a traveling wave solution provided the parameters satisfy the condition

\[(\epsilon_b - \epsilon_a)(E - \epsilon_a)(E - \epsilon_c) = (\epsilon_b - \epsilon_a) + (\epsilon_c - \epsilon_a).\]  

(3)

Each decimated \(c\)-site gives rise to the phase shift \(\Omega\) given by
\[ e^{i\Omega} = (\epsilon_b - \epsilon_a)e^{-ik} + 1 \]
\[ \frac{1}{(\epsilon_b - \epsilon_a)e^{ik} + 1}, \]  
\[ (4) \]

where \( E = \epsilon_b + 2\cos(k) \). Assuming that these phase shifts amount to the total phase shift \( \Omega(n) \) at the \( n \)th site of the renormalized lattice, the traveling wave solution can be expressed as \( e^{i[kn + \Omega(n)]} \).

It should be noted that within the defects, the form of the wave is rather complicated. However, by decimating the sites labeled by \( c \), the complexity has been absorbed into the renormalization of the onsite energies and the coupling terms. For \( k = 0 \), we always have \( \Omega = 0 \) except when \( \epsilon_b - \epsilon_a = -1 \) for which the \( k = 0 \) solution corresponds to \( \Omega = \pi \). This special solution is actually very similar to the one obtained by Dunlap et al. [3] in their study of the random dimer model. We would also like to point out that our general solution is valid for the type of defects we discuss irrespectively of whether they originate from quasiperiodic, chaotic or correlated random processes.

The existence of numerically obtained stepon modes of the type described in Fig. 3 implies that delocalized modes exist also for the system obtained by taking into account the full expansion up to infinite order. In this case, the stepon eigenfunction is represented by an infinite series of step functions. Therefore, the stepon modes of the FK model can be thought of as Bloch waves on an infinitely many times renormalized lattice.

Another important result of our analysis is the fact that it predicts the asymptotic form of the degeneracy curves shown in Fig. 2. Using the explicit values of the onsite energies results in the following relationship between the two parameters \( \kappa \) and \( \lambda \) for the three rightmost branches:

\[ \lambda = \frac{1}{4\pi^2}\kappa^{-3} + O(\kappa^{-2}) \]  
\[ (5) \]
\[ \lambda = \frac{1}{4\pi^2}\kappa^{-4} - \frac{1}{4\pi^2}\kappa^{-3} + O(\kappa^{-2}) \]  
\[ (6) \]
\[ \lambda = \frac{1}{4\pi^2}\kappa^{-4} + O(\kappa^{-2}) \]  
\[ (7) \]

Eq. (5) was obtained using the \( p = 3 \) perturbation theory (Eq. (3)) while the \( p = 4 \) theory gives all three solutions (5-7). We conjecture that the rest of degeneracy curves can be explained by the higher order perturbation theory.

In summary, our numerical results along with the decimation and the systematic perturbation theory demonstrate that the incommensurate FK model in the pinned phase is related to the class of models with correlated defects and exhibits propagating wave solutions on the renormalized lattice. Moreover, the extended two-parameter model is the first known case which exhibits both correlated defects and the localization transition. The propagating stepon modes seem to play a special role in determining the onset to Anderson localization. Proper understanding of how the stepon modes determine the localization boundary may be difficult as the perturbation theory in any finite order does not predict the existence of exponentially localized modes in the model.

The study of the two-parameter model helps one to understand an important distinction between the FK model and the Harper equation. First of all, the absence of localization in the FK model is due to the fact that the nonlinear potential is not strong enough to localize the phonons. The extended FK model, where the strength and the smoothness are controlled independently, does exhibit the localization transition for \( \lambda >> K \). However, the localized phase for \( K > K_c \) exhibits an important distinction from that of the Harper equation. The localized eigenfunctions (once the exponentially decaying part is factorized out) for \( K < K_c \) exhibit universal self-similar fluctuations characterized by a unique strong coupling renormalization fixed point [8]. In contrast, these fractal fluctuations in the cantorus regime \( K > K_c \) appear irregular and defy any simple renormalization explanation.

After the completion of this work, we found other papers where extended states have been seen in other aperiodic lattices [4]. However, the propagating modes in the FK model are somewhat unique as the aperiodicity of the FK model comes from a mismatch of the continuous sinusoidal potential with the periodicity of the lattice. The existence of propagating modes in the pinned FK model suggests the possibility of extended states in other pinned systems such as pinned flux and vortex lattices. Finally, the FK model describes a variety of systems such as adsorbed monolayers on substrates and charge density wave conductors [12-2], and we hope that our study will provide a new direction of research in complex aperiodic systems.

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\( aCaAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBbAaCaAbBb
Ketoja and Satija, Fig. 1
