Phonon localization in one-dimensional quasiperiodic chains

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Quasiperiodic long-range order is intermediate between spatial periodicity and disorder, and the excitations in one-dimensional (1D) quasiperiodic systems are believed to be transitional between extended and localized. These ideas are tested with a numerical analysis of two incommensurate 1D elastic chains: Frenkel-Kontorova (FK) and Lennard-Jones (LJ). The ground-state configurations and the eigenfrequencies and eigenfunctions for harmonic excitations are determined. Aubry's *transition by breaking the analyticity* is observed in the ground state of each model, but the behavior of the excitations is qualitatively different. Phonon localization is observed for some modes in the LJ chain on both sides of the transition. The localization phenomenon apparently is decoupled from the distribution of eigenfrequencies since the spectrum changes from continuous to Cantor-set-like when the interaction parameters are varied to cross the analyticity-breaking transition. The eigenfunctions of the FK chain satisfy the ''quasi-Bloch'' theorem below the transition, but not above it, while only a subset of the eigenfunctions of the LJ chain satisfy the theorem. [S0163-1829(96)07521-2]

There are surprisingly many examples of quasi-one-dimensional (1D) quasiperiodic incommensurate systems, including quasicrystals, charge-density waves, organic conductors, and various atomic monolayers adsorbed on crystalline substrates. Even high-T_c superconductors show incommensurate 1D modulation. Although embedding these systems in 3D space may change the outcome, understanding the conditions for localization of excitations of the underlying model 1D systems is an essential beginning.

Both electron and phonon localization in 1D incommensurate systems have been studied rather extensively in recent years. Despite considerable efforts and substantial success with several specific models, the problem of formulating necessary and sufficient conditions for localization is still far from being solved. The underlying difficulty seems to be related to the specific position quasiperiodic order takes among various spatial orderings: it is intermediate between periodicity and disorder.[1] On the one hand, since quasiperiodic systems lack periodicity, conventional Bloch theory does not apply. On the other hand, the degree of disorder in quasiperiodic systems is not sufficient for Anderson's arguments about localization in 1D disordered systems[2] to be applied to the case. In fact Levitov showed[3] in a rather general way that the eigenfunctions of the Schrödinger equation for a chain of atoms change from extended to localized when the ''complexity'' of the atomic arrangements in the chain evolves from periodicity to full-fledged disorder. Quasiperiodicity is the boundary between the two regimes, and the eigenfunctions in a 1D quasiperiodic system may be localized, extended, or neither of the two. In the latter case the eigenfunctions are called critical. As described in the following paragraphs, examples of all three behaviors are found in various 1D quasiperiodic systems. That is, the outcome is model and system dependent; even minor modifications to model Hamiltonians or variations in parameters may cause drastic changes in the eigenfunction behavior. Thus, characterizing the solutions of a 1D Schrödinger equation with a quasiperiodic potential is a difficult problem to solve analytically. In this paper we take a numerical approach to demonstrating the dependence of localization on the model and on the parameters. Since there is little difference in the formal descriptions of electron and phonon localization, we study the latter, because it is easier to adapt it to computer calculations without losing essential mathematical details.

An example of extended wave functions in a 1D quasiperiodic system was given in the Dinaburg-Sinai theorem[4] for the differential Schrödinger equation

$$-\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi, \tag{1}$$

where $V(x)$ is a weak analytic quasiperiodic potential. The theorem states that (i) the spectrum is continuous and (ii) the wave functions are extended:

$$\psi_k(x)=u_k(x)e^{ikx}, \tag{2}$$

where the Wannier functions $u_k(x)$ are quasiperiodic. Unfortunately, mathematical constraints, mainly in the required analyticity of $V(x)$, do not allow applying the theorem to many systems of practical interest. Another exactly solvable example is the finite difference (discrete) Mathieu equation:

$$\psi_{n+1}-2\psi_n+\psi_{n-1}+V(n)\psi_n=E\psi_n, \tag{3}$$

$$V(n)=V\cos(\omega n+\alpha), \tag{4}$$

with irrational ω and arbitrary phase α. Aubry and Andre[5] proved that for $V<2$ almost all the wave functions are extended and of the quasi-Bloch form Eq. (2). These two examples indicate that sometimes the Bloch theorem may be applicable and the states be extended even when the Hamiltonian lacks periodicity.

The discrete Mathieu equation, Eqs. (3) and (4), also gives an example of localization in quasiperiodic systems: for $V>2$ all wave functions are localized,[5] and the spectrum is discrete:

$$\psi_n\propto e^{-n/l}, \quad n\to\infty. \tag{5}$$

Critical behavior, i.e., neither localized nor extended, can be found in 1D quasicrystals. They are usually modeled by the discrete Schrödinger equation Eq. (3) with a quasiperiodic crystal potential that takes only two values representative of two atomic species, A and B, constituting the quasicrystal:

$$V(n)=\tilde{V}(\omega n+\alpha),$$

$$\tilde{V}(x+1)=\tilde{V}(x),$$

$$\tilde{V}(x)=V_A, \quad \text{if } 0<x<\omega$$

$$V_B, \quad \text{if } \omega<x<1. \tag{6}$$

This equation was extensively studied by many authors[6–8] who gave rather convincing arguments of critical behavior; the mathematical proof was obtained by Bellisard *et al.*[9] The spectrum is singular continuous, a zero measure Cantor set of nonzero fractal dimension. The wave functions are neither localized nor extended; moreover, they are even divergent:

$$\int [|\psi(x)|^2]^2 dx \Big/ \left[\int |\psi(x)|^2 dx\right]^2 \propto L^{\gamma}, \tag{7}$$

where γ is noninteger and eigenenergy dependent and L is the length of the periodically repeated chain cells.

We believe that solving Eqs. (3) and (6) does not constitute a general solution for 1D quasicrystals. Equation (6) with two undeformable atomic species, A and B, is too crude a model even for a 1D quasicrystal chain. Since the hard-sphere approximation leads to the potential $V(x)$ in Eq. (6) taking only two values, one for each species, this in itself determines the absence of localization for the model. It is a theorem that if a quasiperiodic potential $V(x)$ takes only finite number of values then localization is impossible.[10] To include the possibility of localization, an elastic atomic chain should be examined.

A simple model embodying many of the features of the above systems is the 1D Frenkel-Kontorova (FK) chain:[11]

$$H=\sum_n \left[\frac{1}{2}(x_{n+1}-x_n-a)^2+V\cos(2\pi x_n)\right]. \tag{8}$$

Aubry and LeDaeron[12] showed that the minimal energy configurations are periodic when the interatomic distance a is commensurate with the substrate period and quasiperiodic when a is irrational. However, there are qualitatively different configurations for the two types of incommensurate states separated by *the transition by breaking of analyticity* predicted by Aubry. It is customary to display this transition by plotting trajectories in the phase space $(x_{n+1}-x_n;\ x_n \bmod 1)$ as in Fig. 1. For each irrational a there exists a critical value V_c of the substrate potential amplitude. If $V<V_c$, the trajectory derived from the atomic configuration $\{x_n\}$ is a smooth analytic Kolmogorov-Arnold-Moser (KAM) curve; if $V>V_c$, the atomic configuration $\{x_n\}$ is discontinuous, and the trajectory is represented by a so-called Cantor set torus or Cantorus. The critical value V_c depends on a in a rather complicated manner.[12,13] However, it is known that the largest $V_c=0.02461\ldots$ is achieved when a is equal to the golden mean:[14]

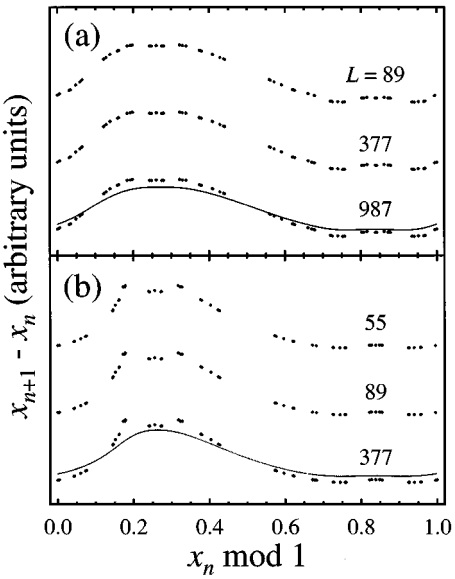

FIG. 1. Phase space trajectories for the FK and LJ chains. The connected KAM curves (small spots) and discontinuous Cantorus curves (large spots) are the trajectories below and above the transition by breaking of analyticity, respectively. The Cantorus results are shown for varying chain sizes and are offset from the KAM curve for clarity. The only discernible difference, as a function of the cell length L, is the addition of spots at x_n mod $1=0.67$ and 1.0 from $L=89$ to 377 in both models. (a) FK chain with $V=0.0207$ and $V=0.0271$ for the small and large spots, respectively; (b) LJ chain with $V_g=-80$ and $V_g=-110$, respectively, and with positions normalized to $R_s=3.25$ Å.

$$a=\frac{1}{2}(\sqrt{5}+1). \tag{9}$$

We have restricted ourselves to this particular value of a in the numerical solutions.

The transition, despite its pure mathematical appearance, has profound physical implications. The smooth KAM configurations keep a vestige of translational symmetry: the chain can slide without any change in energy. The discontinuous configurations are, on the other hand, pinned by the substrate: there is a nonzero Peierls-Nabarro barrier.[15] Thus, the transition by breaking of analyticity coincides with an intrinsic pinning transition. The spectrum of harmonic excitations also changes there: in the KAM regime the lowest eigenfrequency is zero (there is a translational Goldstone mode), whereas in the pinned Cantorus regime it is nonzero.[15] In view of these facts, one is tempted to speculate that some normal modes themselves evolve from extended to localized when the system is driven over the transition by breaking of analyticity. Our numerical results show only a limited correlation between the threshold for localization of the excitations and the analyticity-breaking transition: the correlation does not hold for a chain with anharmonic couplings and only a weak localization arises for the harmonic FK chain, Eq. (8).

We checked two chains for phonon localization: the Frenkel-Kontorova (FK) and the nearest-neighbor Lennard-Jones (LJ). The former is described by Eq. (8), the latter by a similar Hamiltonian with only a modification of the interatomic forces:[16]

$$H=\sum_n [J(x_{n+1}-x_n)+2V_g\cos(2\pi x_n/R_s)],$$

$$J(x)=4\epsilon[(\sigma/x)^{12}-(\sigma/x)^6]. \quad (10)$$

The results presented here are limited to the LJ chain with nearest-neighbor interactions, but tests with the interaction extended to second and third neighbors showed no significant differences. Critical values V_c for the LJ chain depend on σ as well as on the mean misfit.

The first step of the solution was to determine minimum energy configurations for Fibonacci approximations to the golden-mean misfit of both chains[17] for various choices of parameters. For the FK chain, a force-relaxation method was used, following guidance by Aubry and co-workers[12,15] on how to avoid getting trapped in local minima: for an initial configuration with equidistant atoms, with the first atom in the ''proper'' place, the system relaxes to the absolute minimum. For the LJ chain, both the force-relaxation and a gradient search method were used to locate the minimum energy configuration as there was an additional complication of possible fracturing of the chain.[18,19] The transition by breaking of analyticity is clearly observable for both the FK and LJ chains, as shown in Fig. 1. We show the smooth KAM curve for the largest unit cells, $L=987$ and 377 for the FK and LJ chains, respectively. The clumping of the Cantorus is shown there for several values of L to demonstrate that its character is well established at modest values of L.

In the second stage, tridiagonal dynamical matrices were constructed for small-amplitude vibrations about the ground-state configurations $\{x_n\}$ obtained in the first stage. This leads to the following eigenvalue problem for the FK chain for unit cell modes of zero wave vector and atomic mass m

$$\psi_{n+1}-2\psi_n+\psi_{n-1}+V(n)\psi_n=-E\psi_n,$$

$$V(n)=(2\pi)^2V\cos(2\pi x_n), \quad E=m\omega^2, \quad (11)$$

and to a similar result for the LJ chain, where the eigenenergies E are related to the frequency by $E=m\omega^2\sigma^2/4\epsilon$. Equations (11) are an example of a general quasiperiodic Schrödinger equation. However, unlike the case of Eq. (6), the crystal potential $V(n)$ may take an infinite number of values. Thus, possible localization is not immediately evident.[10] The eigenvalues and eigenvectors for the dynamical matrices were obtained using standard (EISPAC) bisection routines.

The minimal eigenvalue for both the LJ and FK chains changes from zero to nonzero when the system is driven over the transition by breaking of analyticity in accordance with earlier observations by Aubry.[15] For both models, the eigenvalue distribution also changes over the transition: at $V<V_c$, the eigenvalues are evenly spaced, densely filling the bands as in the periodic case; at $V>V_c$, however, the distribution is more fragmented. The resulting integrated density of states vs eigenenergy E (i.e., squared frequency ω^2) and the eigenvalue distribution over the energy scale are qualitatively similar for the FK and LJ chains, as shown in Fig. 2. However, the apparent bandwidths for the LJ case are much narrower, and surprising differences arise upon examining the spatial character of the eigenfunctions.

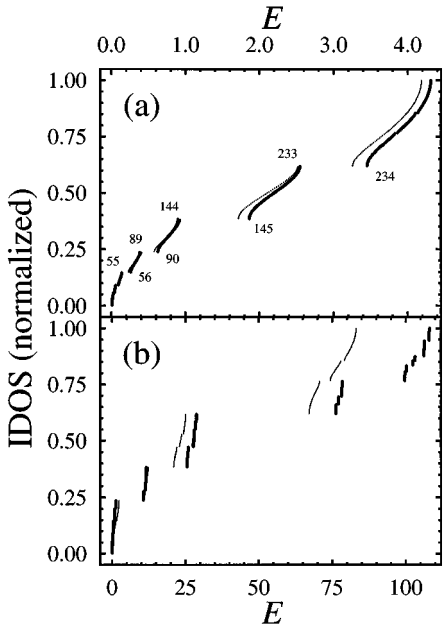

FIG. 2. Integrated density of states for a chain size $L=377$ for (a) the FK chain and (b) the LJ chain. In (a), the integers at the band edges are the count of the eigenenergies plotted from left to right; the right-most numbers of each band are Fibonacci numbers. This coincidence with Fibonacci numbers also applies to (b). Note the narrow width of the bands in (b) for the LJ model as compared with the bands in (a) the FK model. Potential parameters and labelings are as in Fig. 1.

Before presenting the results for localization, we review some of the limitations of a numerical study of the problem. Localization cannot be decided by examining the eigenvectors of the dynamical matrix of one rational approximation to the golden mean misfit. We followed the evolution of results for a series of rational approximants converging to the golden mean. Some properties of the eigenfunctions showed strongly convergent behavior. There were also values of parameters and parts of the eigenvalue spectrum where limitations of accuracy and slow convergence combined to leave the situation undecided. This is the case of our rather weak evidence for critical behavior in localization.

Generally, it is difficult to draw quantitative conclusions about the localization of eigenfunctions by visual inspection because of the volume of information involved and because oscillatory behavior is sometimes mixed with the decay of a weakly localized state. The data were first analyzed for evidence of localization by computing participation ratios (PR):

$$\mathrm{PR}=\frac{1}{L}\frac{(\Sigma_n\psi_n^2)^2}{\Sigma_n\psi_n^4}. \quad (12)$$

If the eigenfunction is extended, PR tends to a finite limit as $L\to\infty$. If an eigenfunction is truly localized, as in Eq. (5), $L\times\mathrm{PR}$ tends to a finite limit as the length L of the unit cell tends to infinity. Critical states might have more bizarre scalings, as in Eq. (7).[20]

We present the results of our localization studies on the Frenkel-Kontorova chain first; participation ratios are shown in Fig. 3. In the KAM regime $V<V_c$, i.e., when the ground state is smooth and unpinned, the PR test shows that all

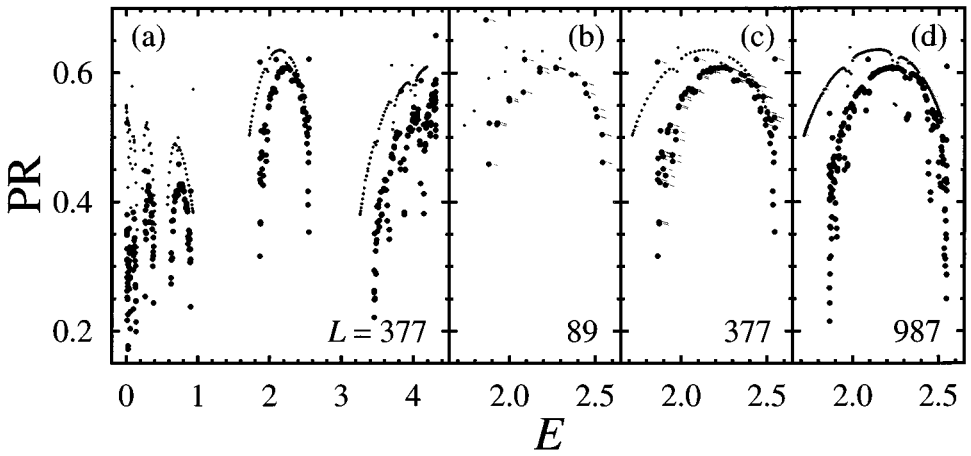

FIG. 3. Participation ratio as a function of eigenenergy for the FK chain. (a) full spectral range for $L=377$; (b)–(d) over a selected range of eigenenergies that corresponds to the central band of (a) for $L=89$, 377, and 987. Note the increase in the length of the ''tails'' of the disconnected Cantorus curves as the length of the chain cell increases. Potential parameters and labelings are as in Fig. 1(a).

eigenfunctions are extended. This is corroborated by demonstrating that the eigenfunctions can be transformed to the quasi-Bloch form Eq. (2). More precisely, any quasiperiodic function [e.g., $u_k(n)$] may be represented as

$$u_k(n)=\tilde{u}_k(\omega n+\alpha),$$

$$\tilde{u}_k(x)=\tilde{u}_k(x+1). \tag{13}$$

The periodic generating function $\tilde{u}_k(x)$ in Eq. (13) is presented in Fig. 4 for three quasimomenta[21] that bracket the band shown in Fig. 3(c). At $V<V_c$, the eigenvalues for $L\to\infty$ become doubly degenerate, as in the usual application of the Bloch theorem: $E(k)=E(-k)$. We determined the value of the quasimomentum k in Eq. (2) by matching to the eigenfunctions of the nearly degenerate eigenvalue pairs. We were able to do this both below and above the transition. Below, the function $\tilde{u}_k$ is smooth. Above, the eigenvalue pair typically differs in the fourth decimal place, but k values could still be identified easily. The function $\tilde{u}_k$ above the transition has a clumping along the abscissa, as in Fig. 1, and also in the ordinate. The departure from the quasi-Bloch theorem becomes very pronounced at the band edge. Above V_c, the participation ratios for states near the band edges decrease with increasing L, as shown in Fig. 3, but true exponential localization was not observed. There may be critical behavior, but more detailed analyses would be required to establish that.

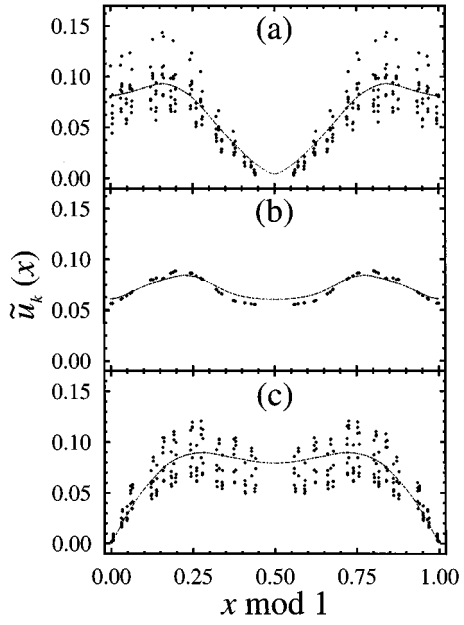

FIG. 4. Quasi-Bloch functions $\tilde{u}_k(x)$ for the FK chain for $L=377$ for three quasimomenta k and configurations below and above the transition, $V=0.0207$ and 0.0271, respectively. Parameters and labelings are as in Fig. 1(a). The values of k (Ref. 21) and the corresponding eigenenergies are (a) $k=1.95$, $E=1.72$ and 1.87; (b) 2.57, 2.13 and 2.22; and (c) 3.11, 2.51 and 2.55. The quasi-Bloch functions that are shown correspond to states from (a) the left tail (b) the middle peak and (c) the right tail of Fig. 3(c). Note the functions above the transition maintain the rough shape of the corresponding functions below the transition but have a smearing that is correlated with the trend of the participation ratios.

Participation ratios for part of the spectrum of the LJ chain are shown in Fig. 5. The behavior is very different from that for the FK chain, even though the behavior of the eigenvalue distribution of the two chains is similar. There is a pronounced high-frequency band of the LJ chain where all eigenfunctions are exponentially localized regardless of the smoothness of the underlying ground state, i.e., localization occurs for both $V>V_c$ and $V<V_c$. The localized upper band is by no measure small: the band contains (golden mean)$^{-2}\sim 38\%$ of all states. The construction $L\times\mathrm{PR}$ in Fig. 5 converges with successive Fibonacci approximations to distinct values that might be called localization lengths. In fact, and in contrast to the results for the FK chain, examination of the corresponding eigenfunctions shows that the probability distributions ψ_n^2 are very narrow and sharply peaked. They extend only a few atomic spacings and their participation ratios seem well specified. The upper branch in Fig. 5(b) is precisely a factor of 2 larger than the lower branch and corresponds to eigenfunctions that are concentrated at two spatial locations rather than one. What we term the upper band is itself a collection of smaller permitted and forbidden bands with gaps at successively finer scales as the golden mean is more closely approximated. The lower band has more similarity to the FK case, both in the trends for the participation ratios and in the behavior of the quasi-Bloch functions, examples of which are shown in Fig. 6. However,

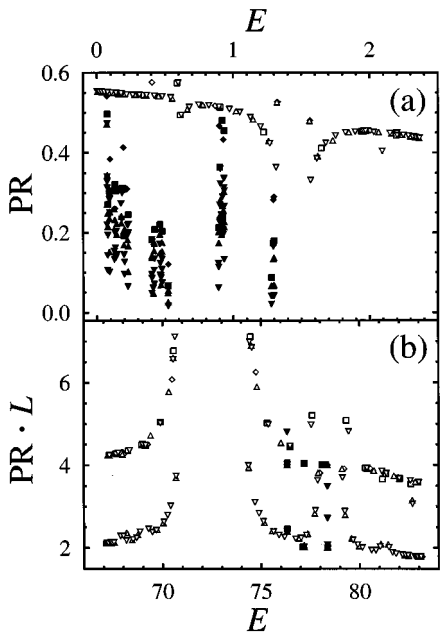

FIG. 5. Participation ratio for the LJ chain over eigenenergies representative of the (a) ''extended'' and (b) ''localized'' regimes. Shown are results for $L=55$ (diamonds), 89 (squares), 233 (triangles) and 377 (inverted triangles). The open and filled symbols correspond to $V_g=-80$ and $V_g=-110$, respectively, for the various chain lengths [these are the same potentials as in Fig. 1(b)]. The participation ratio is shown in (a) whereas the participation ratio times the chain length L is shown in (b) to emphasize the localization over this range of eigenenergies. Note the splitting of the curve in (b) as formed by the renormalized participation ratios for the various chain lengths.

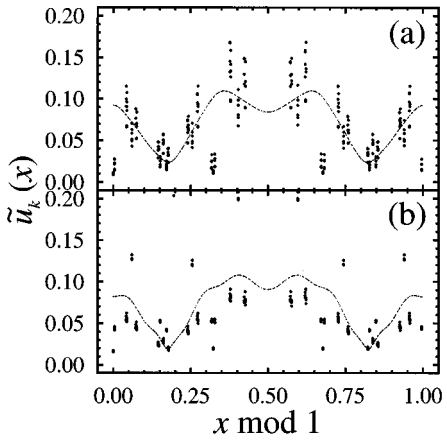

FIG. 6. Quasi-Bloch functions $\tilde{u}_k(x)$ for the LJ chain for $L=377$ at various quasimomenta k, with labelings as in Fig. 1(b). The values of k and the corresponding eigenenergies are (a) $k=0.38$, $E=1.75$ and 0.91 and (b) 0.42, 2.03, and 0.93, for $V_g=-80$ and -110, respectively. These values are chosen from the ''extended'' region of Fig. 5. Above the transition, the functions are smeared out, as in Fig. 4 for the FK chain, again correlated with the participation ratio.

there are some differences between the quasi-Bloch functions of the two models: the LJ quasi-Bloch functions shown for $V<V_c$ have more oscillatory features than those of the FK functions, and the clumping along the abcissa and ordinate for $V>V_c$ is so much more pronounced in the LJ chain than in the FK chain that the remnant of the underlying functions can barely be discerned.

In conclusion, true, strong, phonon localization is observed in the upper band of the nearest-neighbor LJ chain. In fact, the observation of a structure interpreted as a vibration within a domain wall for a uniaxially modulated 2D lattice[22] was a motivation for examining the 1D LJ chain. However, this localization is present regardless of the changes in the level statistics and pinning/unpinning of the chain, i.e., the transition by breaking of analyticity. The behavior of a closely related model, the FK chain, is strikingly different: the transition by breaking of analyticity does affect localization in the system. These results are in accord with the widely held view that quasiperiodic chains lie on the border between localization and delocalization and, thus, are very sensitive to even minor perturbations. Not only is it inadequate to study localization in quasiperiodic systems with models which correspond to hard-core interactions, modest changes to compressible nearest-neighbor interactions may have drastic effects on phonon localization behavior.

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[17] The golden mean Eq. (8) was approximated by a converging series of truncated continued fractions: 2/3, 3/5, 5/8, ... F_n/F_{n+1}, ... , where F_n are Fibonacci numbers: $F_{n+1} = F_n + F_{n-1}$. The longest unit cell in this work corresponded to the ratio 610/987, but most of the analyses were for cells no larger than 233/377.

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[21] The wave numbers were derived by fitting the eigenfunctions of nearly degenerate eigenvalue pairs, in the KAM regime, to Eq. (2). The eigenfunctions in the Cantorus regime were associated with the corresponding eigenfunctions of the KAM regime in an enumeration in order of increasing eigenvalue, and the wave number of the KAM eigenfunction was used to construct an approximation to a quasi-Bloch function. While this procedure has some arbitrariness, it does seem to help systematize the data, as shown in Fig. 4.

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