Cascade of Metal-Insulator Transitions for Electrons in the Frenkel-Kontorova Chain

H. J. Schellnhuber and H. Urbschat
Fachbereich Physik, Universität Oldenburg, D-2900 Oldenburg, West Germany
(Received 20 November 1984)

Novel behavior of the one-dimensional incommensurate Schrödinger equation when the potential is derived from a Kolmogorov-Arnol'd-Moser torus is found by exploitation of univeral scaling properties. Our numerical investigation reveals in particular that nearly torus-breaking electronic states undergo series of back-and-forth localization transitions in sensitive dependence on the potential strength.

PACS numbers: 71.55.Jv, 03.20.+i, 71.30.+h

Incommensurate systems may be conceived as being generated from higher-dimensional commensurate ones by restriction of the degrees of freedom.[1] The resulting "hybrid" translational symmetry no longer guarantees wave propagation of elementary excitations by constructive interference. As a consequence, localization lengths and transport properties depend sensitively on various system parameters as well as on the algebraic character of the discommensuration.[2]

Recent work exploring this field has concentrated on the continuous one-dimensional (1D) quasiperiodic (qp) Schrödinger equation

$$[-d^2/dx^2+\lambda V(x,x/\sigma)]\Psi(x)=E\Psi(x) \qquad (1)$$

and its tight-binding version or Poincaré map

$$\Psi_{n+1}+\lambda v(n/\sigma)\Psi_n+\Psi_{n-1}=E\Psi_n. \qquad (2)$$

Here V and v are 1-periodic in their arguments, σ is irrational, and λ controls the strength of the potential.[3] Equations (1) and and (2) constitute the most simple realizations of the incommensurate quantum dynamics, yet model a number of interesting physical situations such as 2D Bloch electrons in irrational magnetic fields.[4]

One prominent feature of the now widely accepted picture of this subject is the Aubry-André transition (AAT).[5] Given, for example, some analytic v in (2), there is a critical amplitude λ_c, either common to all electronic states or varying with the states considered (if mobility edges exist[6]): The states are extended below their λ_c and exponentially localized above; precisely at λ_c they are exotic (self-similar with respect to dilation).[7,8] Associated with the latter case is a singular-continuous component in the spectrum (see Ref. 2 for a clear account). Another interesting finding is that for certain classes of discontinuous potentials in (2) all states are critical, described by λ-dependent nonuniversal scale factors.[7,9]

These and much more information on qp Schrödinger operators have been extracted from very special systems, often tailored ingeniously for solvability. Thus the results may be atypical or, at least, incomplete. By way of contrast we have studied a model which is characterized by a highly nontrivial qp potential, has a direct physical interpretation, and connects various qualitatively different situations through continuous change of parameters. Extensive numerical work reveals unexpected intricate phase diagrams exhibiting a cascade of AAT's and possibly suggesting a new "road to localization."

We consider the generalized Kronig-Penney Hamiltonian

$$H=-d^2/dx^2+\lambda\sum_{n\in Z}\delta(x-x_n), \qquad (3)$$

with $\lambda>0$ and $0<M_1\leq(x_{n+1}-x_n)\leq M_2$ for all n. We choose configurations $\{x_n\}$ representing σ-incommensurate ground states of the Frenkel-Kontorova model.[5,10] That is, $\{x_n\}$ minimizes, in a well defined way, the functional

$$\phi(\{x_n\})=\tfrac{1}{2}\sum_{n\in Z}(x_{n+1}-x_n)^2+\Lambda[1-\cos(2\pi x_n)] \qquad (4)$$

under the boundary condition

$$\lim_{\substack{L\to\infty\\ L'\to-\infty}}(x_L-x_{L'})/(L-L')=\sigma.$$

Such a configuration is described by

$$x_n=n\sigma+\alpha+g(n\sigma+\alpha), \qquad (5)$$

with an arbitrary phase α and a 1-periodic strongly Λ-dependent hull function g: Given a generic σ, g is analytic for $0<\Lambda<\Lambda_c(\sigma)$ and discontinuous for $\Lambda>\Lambda_c(\sigma)$.[10,11] In dynamical-system language the ground states (5) correspond to recurrent trajectories of the standard map[12] lying on the Kolmogorov-Arnol'd-Moser torus with classical rotation number σ when Λ is small enough. At $\Lambda_c(\sigma)$ this torus breaks to a Cantorus.[13]

Altogether, H is a qp operator specified by the parameters σ, α, Λ, and λ and possessing two incommensurate characteristic lengths 1 and σ.[14] It may serve as a simple model Hamiltonian to describe the electronic properties of a quasi-1D metal below the Peierls transition.[15] The Schrödinger equation

$H(\sigma,\alpha,\Lambda,\lambda)\Psi = k^2\Psi$ can be solved numerically and various interesting questions may be addressed. Here we focus on σ and α fixed and ask how the nature of the eigenstates of H changes as the underlying Kolmogorov-Arnol'd-Moser torus evolves towards criticality.

For convenience the notorious golden torus is chosen, i.e., $\sigma = \frac{1}{2}(\sqrt{5}-1) = \sigma_G$, and $\alpha = 0$. In our units $\Lambda_c(\sigma_G) = 0.4922\ldots$.[12] σ_G is optimally approximated by rationals $\sigma_N = F_{N-1}/F_N$, where F_N is the Nth Fibonacci number. The corresponding commensurate approximants $\kappa_N(k)$ to the quantum rotation number $\kappa(k)$[8,16] will provide us with all the information we need to construct phase diagrams. κ is a continuous monotonic increasing function of k. Its points of growth are the spectral values of H, while its plateaus occurring at

$$\kappa_{r,s} = \pi(r + s/\sigma_G) \geq 0, \quad r,s \in Z \tag{6}$$

represent the gaps. κ allows one to identify individual parts of the spectrum.

κ_N is found by familiar techniques. The appropriate minimizing periodic orbit of length F_N in the standard map is determined by searching symmetry lines[12,13] and the transfer matrix $M_N(\Lambda,\lambda;k)$ for transporting an electron through the corresponding array of δ potentials is constructed.[6] From $\mathrm{Tr}M_N(\Lambda,\lambda;k)$, $\kappa_N(k)$ is obtained directly. κ_{N+1}, in general, contains all the gaps of κ_N plus additional ones opening in the bands of κ_N. From the way the new gaps decrease with growing N locally the nature of the eigenstates of H can be deduced (see also below).

For subcritical Λ and small λ there seem to be infinitely many mobility edges in contrast to exquisite models such as Harper's equation.[5] So, to get a clear picture, we have to work with fixed rotation number κ, i.e., treat each part of the spectrum separately. For computational reasons we concentrate on states at major gap edges labeled as $\kappa_{r,s}^{\pm}$ with r and s small.[7]

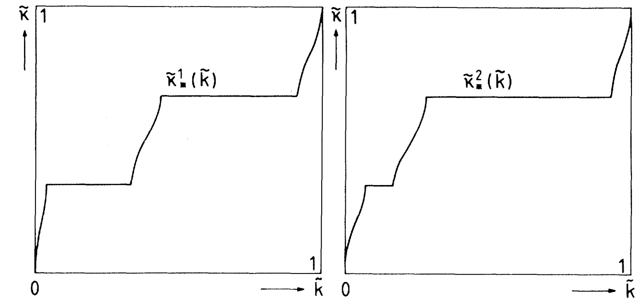

FIG. 1. The universal dispersions $\tilde{\kappa}^1_*$ and $\tilde{\kappa}^2_*$. Three bands and two gaps adjacent to a fixed major gap edge are taken into account and normalization to the unit square is chosen.

$0 < \Lambda < \Lambda_c(\sigma_G)$.—When, for fixed small Λ, λ is increased, the states adjacent to the gap edge considered undergo a single AAT at $\lambda_c(\Lambda)$. A powerful criterion to determine this phase boundary is a scaling property of AAT which we found to be universal for σ_G-incommensurate models: At λ_c the functions $\kappa_N(k)$, when properly normalized, for large N *locally* assume one of the two archetypal forms $\tilde{\kappa}^1_*(\tilde{k})$ and $\tilde{k}^2_*(\tilde{k})$, shown in Fig. 1. These invariant band structures alternate with N according to a pattern (e.g., 112 112. . .) which depends on $\kappa_{r,s}^{\pm}$ but not on Λ. We define

$$R_N(\Lambda,\lambda) = [k_3^{(N)}(\Lambda,\lambda) - k_2^{(N)}(\Lambda,\lambda)]/[k_2^{(N)}(\Lambda,\lambda) - k_1^{(N)}(\Lambda,\lambda)],$$

where $k_i^{(N)}(\Lambda,\lambda)$ is the ith zero of $|\mathrm{Tr}M_N(\Lambda,\lambda;k)-2|$ as counted (inclusively) from the major gap edge in the Nth approximation. Then $\tilde{\kappa}^1_*$ and $\tilde{\kappa}^2_*$ are typified by $R_N(\Lambda,\lambda_c) = 7.83\ldots$ and $1.37\ldots$. The universality of $\tilde{\kappa}^1_*$ and $\tilde{\kappa}^2_*$ was checked in various, quite different models[17]: δ-pulse trains [see Eq. (3)], where the x_n are simply sine modulated or are generated from the dissipative standard map; corresponding square-well arrays; tight-binding models such as Harper's equation, etc. As a practical consequence, an AAT is easily detected in σ_G-incommensurate systems by determining for suitable N the λ where R_N and R_{N+1} are *both* in the set $\{7.83\ldots, 1.37\ldots\}$.

Returning to our model we now discuss as an example the case $\kappa_{0,0}$, which poses the least numerical problems. λ_c first decreases with growing Λ but eventually a minimum is reached. Then the situation drastically changes: Instead of a single AAT an (possible infinite) alternating series of metal-insulator and insulator-metal transitions appears, i.e., the phase boundary $\lambda_c(\Lambda)$ becomes multiple valued! The global Λ-λ phase diagram for states at $\kappa_{0,0}$ gives a clear view of what happens (Fig. 2). Large channels, where states are extended, open in the localized regime, but in each channel peninsulas, where states are localized again, protrude and this process seems to continue *ad infinitum* as Λ goes to Λ_c. This is reminiscent of Cantor set construction: The phase diagram has self-similar structure (see inset in Fig. 2) and there is strong evidence that the surviving channels have total measure zero at Λ_c. Different phase boundaries in Fig. 2 are characterized by different sequential patterns (line I: 112 112. . . , line II: 222 . . . , for example). We emphasize that quantitatively the phase diagrams for other $\kappa_{r,s}^{\pm}$ deviate, in part considerably, from the one for $\kappa_{0,0}$. Our data indicate, however, that the qualitative nature is the same, though the cascade generally has to

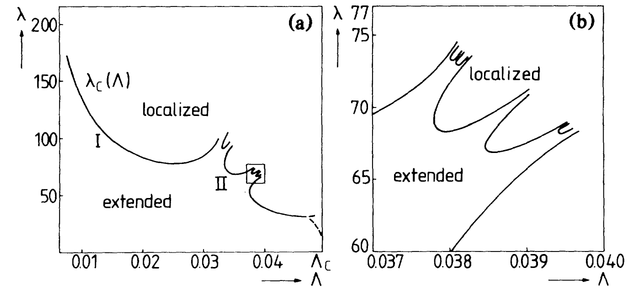

FIG. 2. (a) Phase diagram for $\kappa_{0,0}$. (b) Inset magnified, revealing the cascade structure.

unfold in an extremely narrow Λ interval adjacent to Λ_c. Things have been checked with the actual wave functions; these are perfectly self-similar and thus algebraically localized at $\lambda_c(\Lambda)$.[17]

$\Lambda = \Lambda_c(\sigma_G)$.—Our system should be capable of criticality in at least a second way caused by the torus breaking at $\Lambda_c(\sigma_G)$, where the Fourier components of g decay roughly as ω^{-1}.[12] A crucial question is whether the envelope of localized peninsulas in the phase diagram for a given gap edge $\kappa_{r,s}^{\pm}$ (see Fig. 2) hits the analyticity edge $\Lambda = \Lambda_c$ at a finite value $\lambda_*(\kappa_{r,s}^{\pm})$: Then on the interval $\{0 < \lambda < \lambda_*;\ \Lambda = \Lambda_c\}$ monocritical behavior different from AAT can be expected and complex multicritical behavior near the limit point (Λ_c, λ_*). Examination of the analyticity edge for fixed $\kappa_{r,s}^{\pm}$ by small to intermediate commensurate approximants ($N \lesssim 15$) indeed suggests finite $\lambda_*(\kappa_{r,s}^{\pm})$: For small λ, states seem to be exotic and corresponding scale factors vary continuously with λ similar to the models studied in Refs. 7 and 9. Unlike there these factors are also strong $\kappa_{r,s}^{\pm}$ dependent.[17]

These observations do not stabilize, however, when N is further increased: The behavior described appears to be transient and may persist in the incommensurate limit only for $\lambda \to 0$. On the basis also of our data for $\Lambda < \Lambda_c$ we conjecture that the envelope bends down (probably with infinite slope) to $\lambda = 0$ at Λ_c, enclosing, together with the analyticity edge, an extremely fine structure of localized and extended domains. Then a possible scenario for the extinction of conductivity in a physical system like ours is "Cantorization" of the Λ-λ phase plane with the consequence that almost every electronic state eventually lands on a localized peninsula as Λ approaches Λ_c. In any case not one of the states investigated remains extended at Λ_c for any λ: Thus the analyticity edge is a global boundary for usual conduction mechanisms.

One general conclusion from our results is that the behavior of qp models changes even qualitatively when higher harmonics in the potential become significant. So the conductivity for realistic systems, where very-low-order truncation of the Fourier expansion is unjustified, will be quite difficult to predict.[18] On the other hand, the universality of the critical phenomena involved is remarkable, in particular the role of $\tilde{\kappa}_*^1$ and $\tilde{\kappa}_*^2$. Deeper analysis of this has to rely on a renormalization scheme, probably along the lines of Ref. 8, acting on a parameter space which contains all the models (of given discommensuration σ) derived from analytic potentials. The models are represented by λ trajectories (all other external parameters fixed) in this space, intersecting the critical surface for AAT at λ_c. Within this picture our system has trajectories oscillating through this surface with a "wavelength" approaching zero as $\Lambda \to \Lambda_c$.

Many useful discussions with D. Rand, S. Ostlund, and E. D. Siggia and with W. Kohn in the early stage of this work are gratefully acknowledged.

[1]T. Janssen and A. Janner, Physica (Utrecht) **126A**, 163 (1984).

[2]R. E. Prange, D. R. Grempel, and S. Fishman, Phys. Rev. B **29**, 6500 (1984).

[3]B. Simon, Adv. Appl. Math. **3**, 463 (1982).

[4]Pioneering work was done by M. Ya. Azbel', Zh. Eksp. Teor. Fiz. **46**, 929 (1964) [Sov. Phys. JETP **19**, 634 (1964)], and Phys. Rev. Lett. **43**, 1954 (1979).

[5]G. André and S. Aubry, Ann. Isr. Phys. Soc. **3**, 133 (1980); J. Avron and B. Simon, Bull. Am. Math. Soc. **6**, 81 (1982).

[6]J. B. Sokoloff and J. V. José, Phys. Rev. Lett. **49**, 334 (1982); J. Bellissard, A. Formoso, R. Lima, and D. Testard, Phys. Rev. B **26**, 3024 (1982); C. de Lange and T. Janssen, Phys. Rev. B **28**, 195 (1983).

[7]S. Ostlund, R. Pandit, D. Rand, H. J. Schellnhuber, and E. D. Siggia, Phys. Rev. Lett. **50**, 1873 (1983).

[8]S. Ostlund and R. Pandit, Phys. Rev. B **29**, 1394 (1984).

[9]M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983); M. Kohmoto, Phys. Rev. Lett. **51**, 1198 (1983).

[10]S. Aubry and P. Y. Le Daëron, Physica (Utrecht) **8D**, 381 (1983); J. E. Sacco and J. B. Sokoloff, Phys. Rev. B **18**, 6549 (1978).

[11]See, however, S. E. Burkov and Ya. G. Sinai, J. Phys. (Paris), Lett. **45**, L409 (1984).

[12]B. V. Chirikov, Phys. Rep. **52**, 263 (1979); J. M. Greene, J. Math. Phys. **20**, 1183 (1979); S. J. Shenker and L. P. Kadanoff, J. Stat. Phys. **27**, 631 (1982).

[13]R. S. MacKay, J. D. Meiss, and I. C. Percival, Physica (Utrecht) **13D**, 55 (1984).

[14]A similar model was discussed by J. B. Sokoloff, Phys. Rev. B **25**, 5901 (1982).

[15]A self-consistent approach was made by P. Y. Le Daëron and S. Aubry, J. Phys. C **16**, 4827 (1983).

[16]R. Johnson and J. Moser, Commun. Math. Phys. **84**, 403 (1982).

[17]For details see H. J. Schellnhuber and H. Urbschat, unpublished.

[18]See R. E. Prange, D. R. Grempel, and S. Fishman, Phys. Rev. Lett. **53**, 1582 (1984).