

## Localization Problem in One Dimension: Mapping and Escape

Mahito Kohmoto

*Department of Physics and the Materials Research Laboratory, University of Illinois,  
Urbana, Illinois 61801*

and

Leo P. Kadanoff and Chao Tang

*The James Franck Institute, The University of Chicago, Chicago, Illinois 60637*

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A one-dimensional Schrödinger equation in a discontinuous quasiperiodic potential is reduced to a recursion relation for transfer matrices and then to one for traces of these matrices. When the potential is periodic, the bandwidth goes to zero as an algebraic function of the period with a critical index which depends upon the potential strength. This critical index is also evaluated as the solution to an escape-rate problem for the recursion relations.

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Several authors have recently discussed the localization problem which arises when an electron hops from site to site upon a one-dimensional lattice in the presence of a quasiperiodic potential.<sup>1-5</sup> Let the potential be  $V(n\psi)$ , with  $n$  labeling the lattice site, and the periodicity condition being the statement  $V(t+1) = V(t)$ . If  $\psi_n$  is the wave function at site  $n$ , the resulting Schrödinger equation is  $\psi_{n+1} + \psi_{n-1} + [V(n\psi) - E]\psi_n = 0$ . If  $\psi$  is rational, i.e.,  $p/q$  with  $p$  and  $q$  being relatively prime integers, then the usual band theory applies with there being  $q$  bands of allowed energies and each eigenfunction being extended. If  $\psi$  is irrational, then the eigenvalue equation has quite nontrivial properties. These properties may be of interest both for incommensurate phases of real systems and also because they may be analogous to the behavior of systems in random potentials.<sup>3,6</sup>

For irrational  $\psi$ 's, two different regimes have been studied in some detail. The unbounded potential<sup>3,6</sup>  $V(t) = \lambda \tan 2\pi(t - \omega)$  produces localized eigenstates for "typical" irrational  $\psi$ 's. In this localized regime, rational  $\psi (=p/q)$  leads to bands which have a width proportional to  $\exp(-\gamma q)$  as  $q \rightarrow \infty$ . In contrast, a weak analytic<sup>1,2,5</sup>  $V(t)$  gives extended states for almost all values of  $\psi$ . In this regime rational  $\psi = p/q$  typically gives bands with a width in energy varying like  $q^{-1}$  for large  $q$ . For analytic  $V(t)$ , as the potential strength is increased one tends to move from the extended into the localized regime.

The details of the crossover between localized and extended behavior have heretofore remained unknown. In this Letter, we describe a model problem, whose solution seems to always be in

an intermediate regime between the localized and extended cases described above. In our case  $V(t)$  has two discontinuities within each period, and is thus nonanalytic. For this special potential, a very special behavior arises. For a particular irrational value of  $\psi$ , there exist no wave functions which are either localized or extended in the conventional sense. Furthermore rational  $\psi = p/q$  gives bandwidths for large  $q$  which are on the average of order  $q^{-(1+\delta)}$  with  $\delta > 0$ . The purpose of this Letter is to exhibit this behavior in a special model and to ask whether it might be typical of the crossover between localized and extended regimes.

To see how this special situation arises, write the Schrödinger equation in terms of transfer matrices,  $M$ , as

$$M(n\psi)\Psi_n = \Psi_{n+1},$$

$$M(t) = \begin{bmatrix} E - V(t) & -1 \\ 1 & 0 \end{bmatrix}, \quad \Psi_n = \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}. \quad (1)$$

Notice that  $M(t)$  is a 2 by 2 real matrix with unit determinant which is periodic in  $t$  with period 1. More steps in  $n$  can be generated by a process of matrix multiplication, i.e.,

$$M^{(k)}(n\psi)\Psi_n = \Psi_{n+k}, \quad (2)$$

where  $M^{(k)}$  can be defined recursively via

$$M^{(k_1+k_2)}(t) = M^{(k_1)}(t+k_2\psi)M^{(k_2)}(t). \quad (3)$$

Here  $M^{(1)} \equiv M$ . For rational  $\psi$ ,  $q\psi = p$  is an integer and since  $M^{(k)}(t)$  is periodic in  $t$  with a period 1,  $M^{qj}(t) = [M^q(t)]^j$ . Thus for allowed (forbidden) energies  $|\text{tr} M^q(t)|/2$  is less than (greater than) unity and  $\text{tr} M^{(k)}(t)$  is bounded

(goes to infinity exponentially) as  $k \rightarrow \infty$ .

The barrier to solving Eq. (3) with irrational  $\varphi$  is the  $t$  dependence of  $M^{(k)}(t)$ . If we could choose  $k_2$  such that  $k_2\varphi$  is very close to an integer we might be able to achieve an approximate analysis of this equation. But we can do even better. If we look at the special case in which  $V(t)$  is constant except for discontinuous jumps, then  $M^{(k)}(t)$  would also be constant over intervals of  $t$ . Then a careful choice of interval and of  $k_1$  and  $k_2$  would effectively eliminate all  $t$  dependence.

Consequently, we focus upon an important special case: One in which  $V(t)$  is discontinuous<sup>4,7</sup> and has the particular form

$$V(t) = \begin{cases} V_0 & \text{for } -w < t \leq -w^3, \\ V_1 & \text{for } -w^3 < t \leq w^2. \end{cases} \quad (4)$$

Here,  $w = (\sqrt{5} - 1)/2$  is the inverse of the golden mean. This form has been chosen to make the behavior particularly simple whenever  $\varphi$  is equal to or close to  $w$ . In particular, consider  $M^{(k)}(t)$  when  $k$  is given by the Fibonacci number  $k = F_l$  and  $t$  is equal to zero. Call this matrix  $M_l$ . Equation (3) then becomes the simple statement<sup>8</sup>

$$M_{l+1} = M_{l-1} M_l, \quad (5)$$

where  $M_1$  is  $M(0)$  and  $M_0$  is  $M(-w^3)$ . Equation (5) holds whenever the winding number  $\varphi$  is sufficiently close to the golden mean, i.e., whenever<sup>9</sup>

$$-w^{l+1}(F_l - 1) < (\varphi - w)(-1)^l < w^{l+2}/(F_{l+1} - 1). \quad (6)$$

Therefore when  $\varphi$  is chosen to be exactly  $w$ , Eq. (5) holds for all  $l$ 's.

The reason for using this formula is that Eq. (5) can be converted into a very simple recursion relation for  $x_l = \frac{1}{2} \text{tr} M_l$ , by taking the trace of the equation

$$M_{l+1} + (M_{l-2})^{-1} = M_{l-1} M_l + M_{l-1} M_l^{-1}$$

to obtain

$$x_{l+1} = 2x_l x_{l-1} - x_{l-2}, \quad (7)$$

with the initial conditions

$$x_1 = \frac{1}{2}(E - V_1), \quad x_0 = \frac{1}{2}(E - V_0), \quad x_{-1} = 1, \quad (8)$$

Now we can state a simple approach to determining the band structure. Consider first the case  $\varphi = \varphi_m = F_{m-1}/F_m$ . In this situation, the basic problem is periodic with period  $F_m$ . If the  $x_m$  determined by recursion relations (7) and (8)

lies in the interval  $[-1, 1]$ , then  $E$  is an allowed energy for an extended state. If  $|x_m| > 1$ , then  $E$  is forbidden.

To describe the solution more precisely, use the quantity<sup>10</sup>

$$\lambda^2 = -1 + x_l^2 + x_{l-1}^2 + x_{l-2}^2 - 2x_l x_{l-1} x_{l-2} = \frac{1}{8} \text{tr}[M_l, M_{l-1}]^2. \quad (9)$$

Whenever the recursion relation (7) is satisfied this quantity is independent of  $l$ . From the initial condition (8),  $\lambda = \frac{1}{2}|V_1 - V_0|$ . For  $\lambda = 0$ , the solution is trivial. If  $E - V_0 = E - V_1 = 2 \cos \theta_0$  with  $\theta_0$  real we are in an allowed region of the spectrum since  $x_l = \cos(F_l \theta_0)$ . However, if  $|E - V_0| > 2$ , i.e., if  $E - V_0 = 2 \cosh u_0$  with  $u_0$  real, then  $x_l = \cosh(F_l u_0)$  grows as  $\exp(w^{-l})|u_0|/(1+w^2)$  and this energy is forbidden.

Figure 1 shows forbidden and allowed energies as a function of  $m$  for  $\lambda = 0.6$ . This band structure is similar to the one obtained by Hofstadter<sup>11</sup> for sinusoidal  $V(t)$ . Notice that, for large  $m$ , the allowed regions get narrower and narrower. In fact, the total width of the allowed regions in energy goes down as  $F_m^{-\delta(\lambda)}$ .<sup>12</sup> Figure 2 is a plot of the index  $\delta$  vs  $\lambda$ .

Hence as  $\varphi \rightarrow w$ , what we see is an infinite number of very narrow bands which have self-similar structures of typical Cantor sets.

One can analyze the case  $\varphi = w$  quite directly. For almost any starting choice of  $x_{-1}, x_0, x_1$  having  $\lambda$  real and different from zero, for large  $l$ ,  $x_l$  will grow very rapidly. In particular, the

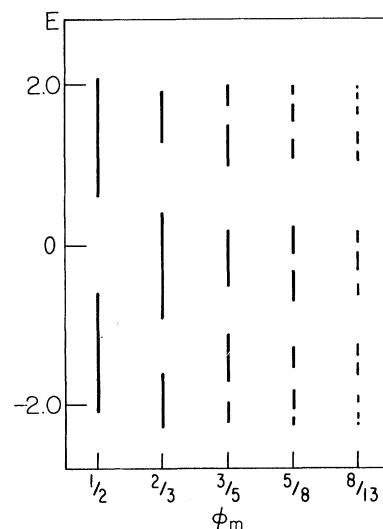


FIG. 1. The allowed energies for  $\lambda = V_0 = -V_1 = 0.6$ . The band structures for  $m = 2, 3, 4, 5$ , and  $6$  are shown.

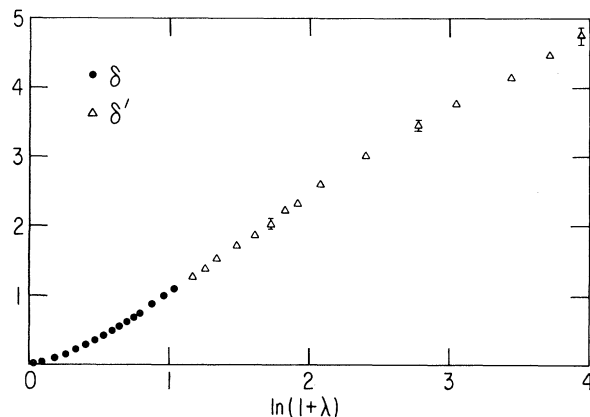


FIG. 2. The critical indices  $\delta(\lambda)$  (of band structure) and  $\delta'(\lambda)$  (of escaping problem). The two data sets agree well. For example, we have  $\delta = 0.22096$  and  $\delta' = 0.2202 \pm 0.0007$  at  $\lambda = 0.4$ ; and  $\delta = 0.4271$  and  $\delta' = 0.423 \pm 0.004$  at  $\lambda = \sqrt{2}/2$ .

growth will have the form in which  $|x_i| \sim \cosh(F_i \times u_0)$ . These "escaping" energies are the direct extension of the forbidden states in the commensurate case. However, for some specially chosen energies escape will not occur and  $|x_i|$  will remain bounded for all  $l$ . These "nonescaping" situations are the extension of the extended states in the commensurate case. They are themselves of two kinds: cyclic, in which  $x_{i+q} = x_i$  for some period  $q$ ; and aperiodic, in which  $x_i$  shows no periodic behavior but nonetheless remains bounded.<sup>13</sup>

We ask the question how do points  $r_i = (x_i, x_{i-1}, x_{i-2})$  evolve after many iterations of the recursion relation

$$\vec{r}_{i+1} = T(\vec{r}_i) = (2x_i x_{i-1} - x_{i-2}, x_i, x_{i-1}).$$

If  $\lambda$  is pure imaginary and  $-1 < \lambda^2 \leq 0$ , then any initial point  $\vec{r}_1$  near the origin will remain near the origin for all subsequent iterations. However, if  $\lambda$  is real and different from zero, almost all initially chosen points will escape. This statement is equivalent to saying that the total bandwidth (the Lebesgue measure of the spectrum) for the incommensurate system  $\varphi = w$  is zero. To show this escape process, choose a set of initial points  $r_1 = (x_1, x_0, x_{-1})$  with  $x_1$  and  $x_0$  each uniformly distributed between  $-1$  and  $1$  and  $x_{-1}$  chosen to produce a fixed value of  $\lambda^2$ . We say that escape has occurred once the  $x$ 's obey  $|x_i| > 1$  and  $|x_{i+1}| > 1$ , since from this iteration on  $\ln|x_i|$  will grow exponentially. We then find that the number of points which have not escaped

after  $l$  iterations decays algebraically in  $F_l$  as

$$N_l \sim N_0 F_l^{-\delta'(\lambda)}.$$

Within our measurement error the escape-rate index  $\delta'(\lambda)$  is the same as the bandwidth index  $\delta(\lambda)$  (see Fig. 2).

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<sup>1</sup>B. Simon, Adv. Appl. Math. **3**, 463 (1982), and references therein.

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<sup>8</sup>M. J. Feigenbaum and B. Hasslacher, Phys. Rev. Lett. **49**, 605 (1982).

<sup>9</sup>To derive Eq. (5) from Eq. (3) set  $k_1 = F_{l-1}$ ,  $k_2 = F_l$  so  $k_1 + k_2 = F_{l+1}$ . Conditions (6) are a consequence of  $wF_l = F_{l-1} - (-w)^{l+1}$  and the demand that  $M^{(k_1)l}$  has no discontinuity between  $t=0$  and  $t=k_2\varphi - F_{l-1}$ .

<sup>10</sup>The conservation of the quantity given in Eq. (9) was derived independently by S. Ostlund, R. Pandit, D. Rand, H. J. Schellnhuber, and E. D. Siggia [following Letter, Phys. Rev. Lett. **50**, 1873 (1983)] based upon their parallel work on recursion relations of the forms (3) and (5).

<sup>11</sup>D. R. Hofstadter, Phys. Rev. B **14**, 2239 (1976).

<sup>12</sup>This behavior of the Lebesgue measure of the spectrum has been observed at a critical point of a class of continuous potential models. However, in those models the Lebesgue measure behaves differently away from the critical point. See Ref. 5 for details.

<sup>13</sup>Even if  $x_i$  remains bounded,  $M^{(k)}(0)$  will not. The best one can say is that the magnitude of matrix elements of  $M^{(k)}$  will be less than or of the order of  $\beta^k$  where  $\beta > 1$ . In one limiting process for finding the wave function,  $\psi_k$ , the magnitude of  $\psi_k$  will similarly be bounded by an algebraically increasing envelope. However, this result depends upon the limiting process. See for comparison Ref. 10, which uses a different limiting method. More details will follow in a later publication.