Localization in an Incommensurate Potential: An Exactly Solvable Model

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The exact eigenstates of a one-dimensional tight-binding model with a periodic diagonal potential that can be commensurate or incommensurate with the lattice are found. If the period is incommensurate, all the eigenstates are localized. The localization length and the density of states are identical to those of a related disordered system. The case of a commensurate potential, for which all the states are extended, and the approach to the incommensurate case are also discussed. The solution is achieved by mapping the model into a time-dependent quantum problem in which the potential is periodic in time.

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Quantum particles (electrons) subject to a sum of potentials which are periodic but incommensurate with one another present an interesting theoretical and experimentally realizable problem. Systems for which this problem is relevant include[1] incommensurate superlattices, charge-density waves, the electronic properties of the mercury chains in $Hg_{3-\delta}AsF_6$, and the problem of two-dimensional electronic systems in a magnetic field. An intriguing theoretical aspect is that such an incommensurate potential presents a case that is intermediate between a random potential and a perfectly ordered crystal. In one dimension, a random potential is known to localize all states (Anderson localization).[2] In an incommensurate potential there can be, in principle, both localized and extended states with the interesting possibility of a metal-insulator transition as a function of energy and/or strength of the potential. Aubry and Andre[3] have produced a self-dual model that exhibits this behavior. In their model all the states are either localized or extended depending on the strength of the potential as measured by the bandwidth. Other models have also been studied by a variety of numerical and analytical techniques[4] with similar results. In this Letter we present exact solutions for a class of problems for which the incommensurate potential always localizes all the states.

We study a one-dimensional tight-binding model with the Schrödinger equation

$$Hu_m = T_m u_m + \sum_{r\neq 0} W_r u_{m+r} = \epsilon u_m. \tag{1}$$

The lattice sites, m, are specified by integers and tacitly have period unity while T_m is a "diagonal" potential which can be chosen in several ways. If the T_m's are taken to be random from a distribution $P(T)$ and W_r is restricted to nearest-neighbor hopping, Eq. (1) is the well-known Anderson model with diagonal disorder.[2] T_m can also be chosen to be periodic in m with a period that is either commensurate or incommensurate with the underlying lattice. For example, if T_m is chosen to be proportional to $\cos(\tau m)$ and $\tau/2\pi$ is irrational, Eq. (1) becomes the case of an incommensurate potential recently studied in Ref. 3.

No exactly solvable case of Eq. (1) with random T_m is known, and indeed, one may not exist, if by exactly solvable it is meant that the wave functions $\{u_m\}$ and energies ϵ are given. The case of a general periodic but incommensurate potential seems just as intractable. We have recently pointed out,[5] however, that there are special choices of the potential for which much progress can be made. In particular we have shown that if, for fixed ω and τ, the T_m's are taken as $T_m = \tan[(\omega - m^2\tau/2)/2]$ (which makes them pseudo-random rather than random in the measure theoretic sense), the *static* problem posed by Eq. (1) can be mapped into the *dynamical* problem of a periodically kicked quantum rotator.[6] The kinetic energy of the rotator is $H_0 = \tau L^2/2$ where the angular momentum operator $L = -i\partial/\partial k$ and $-\pi \leq k \leq \pi$. The potential energy, which gives the rotator a δ-function kick at integer times, is $V(k)\Delta(t)$, with $\Delta(t) = \sum_{-\infty}^{\infty}\delta(t-s)$ and $V(k)$ a periodic function of k related to the Fourier transform of the hopping potential in Eq. (1), $W(k)$ (see below).

In the present paper we consider Eq. (1) with $T_m = \tan[(\omega - m\tau)/2]$. This corresponds to a potential that is periodic but not necessarily commensurate with the underlying lattice. By applying to this case the methods of our previous paper this problem can be shown to be equivalent to another periodically kicked quantum system

for which we are able to find an exact solution. This new dynamical problem is defined by an unperturbed Hamiltonian that is linear in the angular momentum, i.e., $H_0 = -i\tau\partial/\partial k$. The time-dependent Schrödinger equation is

$$i\frac{\partial}{\partial t}\psi(k,t) + i\tau\frac{\partial}{\partial k}\psi(k,t) = V(k)\Delta(t)\psi(k,t). \qquad (2)$$

If we choose $W(k) = \kappa\cos(k)$ the corresponding tight-binding problem involves only nearest-neighbor hopping with strength $\kappa/2$ and, for simplicity, we confine ourselves to this potential in most of what follows. We show that all the eigenstates of (1) are localized when $\tau/2\pi$ is irrational and extended when it is rational. The localization length γ^{-1} in the irrational case is identical to that in the Lloyd model[7,8] for disorder, for most values of τ. As $\tau/2\pi$ approaches a rational p/q, however, there is a tiny region, of size proportional to $e^{-\gamma q}$, for which the eigenstates have a much larger localization length. This set of values of τ giving anomalous localization lengths has the property that it is open and everywhere dense, although small in total measure. It is thus not a set of a type very often encountered in physics, although it is very closely related to the so-called resonance condition encountered in Kolmogorov-Arnold-Moser theory.[9]

To establish the connection between Eqs. (1) and (2) we start by noting that the potential in Eq. (2) is periodic in time. Therefore, we only need to consider solutions of definite quasienergy,[6] ω_ν, of the form

$$\psi_\nu(k,t) = \exp(-i\omega_\nu t)u_\nu(k,t),$$

where $u_\nu(k,t) = u_\nu(k,t+1)$. Furthermore, as we noted in Ref. 5, it suffices to consider the values $u_\nu^{\pm}(k)$ just after (before) a kick. The relationship $u_\nu^{+}(k) = e^{-iV(k)}u_\nu^{-}(k)$ holds. Another relation may be obtained by integrating the Schrödinger equation between kicks to find

$$u_\nu^{-}(k) = (2\pi)^{-1}\int_{-\pi}^{\pi}dp\sum_m \exp[im(k-p)] \times \exp(iE_m)u_\nu^{+}(p)$$

with $E_m = \omega - m\tau$. We now choose $V(k) = -2\times\arctan[W(k)-\epsilon]$, eliminate from the previous equations $u^{\pm}$ in favor of $\bar{u}_\nu(k) = u_\nu^{\pm}(k)/[1 \pm iW(k)]$, and write the equation of motion for its Fourier transform,

$$u_{n\nu} = (2\pi)^{-1}\int_{-\pi}^{\pi}dk\,\exp(ink)\bar{u}_\nu(k).$$

It is easily found that $u_{n\nu}$ satisfies Eq. (1) with $T_m = \tan(E_m/2)$. For finite-range hopping W_r the long-distance behavior of $\bar{u}$ and $u^{\pm}$ is similar. In what follows we concentrate on $u_\nu^{+}(k)$.

The feature that makes Eq. (2) exactly solvable is that its general solution for integral time s can be obtained by iteration of

$$\psi^{+}(k,s+1) = \exp[-iV(k)]\psi^{+}(k-\tau,s). \qquad (3)$$

States of definite quasienergy then satisfy

$$u_\nu^{+}(k) = \exp\{i[\omega_\nu - V(k)]\}u_\nu^{+}(k-\tau). \qquad (4)$$

The properties of the solutions u_ν depend on whether $\tau/2\pi$ is rational or irrational. We consider the latter case first. Since $|u_\nu^{+}(k)| = |u_\nu^{+}(k-\tau)|$ and, for integral n,m, $(n\tau + 2\pi m)$ covers densely the interval $[-\pi,\pi]$, we may write

$$u_\nu^{+}(k) = \exp[i\varphi_\nu(k)]. \qquad (5)$$

The real quantity $\varphi_\nu(k)$ must satisfy $\varphi_\nu(k+2\pi) = \varphi_\nu(k) + 2\pi\nu$ with ν an integer in order for the wave function to be single valued. From Eqs. (4) and (5) and this condition we find

$$\varphi_\nu(k) = \nu k + \sum_{n=1}^{\infty} V_n\frac{\sin n(k-\tau/2)}{\sin n\tau/2}, \qquad (6)$$

where $V_n \equiv V_n(\epsilon) = (1/2\pi)\int_{-\pi}^{\pi}dk\,V(k)\exp(ink)$. The allowed values of ω are discrete and given by $\omega_\nu = [V_0(\epsilon_\nu) + \nu\tau] \bmod(2\pi)$. For a given choice of ω, this is an implicit equation for the energy levels ϵ_ν of the tight-binding problem. Thus, for $\tau/2\pi$ irrational the eigenvalues of Eq. (1) are denumerable (although everywhere dense). From Eq. (5) we conclude that

$$(2\pi)^{-1}\int_{-\pi}^{\pi}dk\,|u_\nu^{+}(k)|^2 = \sum_{n=-\infty}^{\infty}|u_{n\nu}^{+}|^2 < \infty,$$

i.e., all the states are normalizable and, consequently, localized. Notice that so far we have not specified the hopping matrix elements. In order to make further progress the V_n's must be specified. For the nearest-neighbor model a tedious but straightforward calculation gives

$$V_n = (2/n)\exp(-\gamma n)\cos[\mu n + \tfrac{1}{2}(n-1)\pi] \qquad (7)$$

for $n \neq 0$, and $V_0 = 2\mu$, where

$$2\kappa\cosh\gamma = [1+(\epsilon+\kappa)^2]^{1/2} + [1+(\epsilon-\kappa)^2]^{1/2}, \qquad (8)$$

$$\sin\mu = \epsilon/(\kappa\cosh\gamma). \qquad (9)$$

The series in Eq. (6) is absolutely convergent for almost all irrational values of $\tau/2\pi$. The exception is for a Liouville number for which there exists an infinite sequence of integers q_j such that $d(q_j) \equiv q_j\sin(\tau q_j/2) \leq \exp(-\gamma q_j)$. These numbers, however, form a set of measure zero and

we discuss them no further. If $\tau/2\pi$ is not too close to a rational number (in a sense to be defined below), $d(n) \sim O(1)$ for all n and one may show, by Fourier transformation of Eq. (5), that $\ln|u_{n\nu}|/|n-\nu| \to -\gamma$ for $|n-\nu| \to \infty$; i.e., $u_{n\nu}$ is exponentially localized around the νth site with inverse localization length γ given by Eq. (8). As an illustration, we compare in Fig. 1 numerical solutions of Eq. (1) for various values of the hopping matrix element with a pure exponential decay with exponent γ. The agreement is excellent. Notice that this value of γ is the same as the one obtained for the Lloyd[7,8] model of disorder for which the T_m's are independent random variables with the Cauchy distribution, i.e., $P(T) = 1/\pi(1+T^2)$. It can be shown from the eigenvalue equation that the density of states per site is $\rho(\epsilon) = (2\pi)^{-1}\partial V_0/\partial\epsilon$. Not surprisingly this expression turns out to be identical to the average density of states of the Lloyd model. These two facts support the intuitive notion that incommensurate and random potentials may produce similar physical effects. That a discontinuous incommensurate potential may localize all the states was suggested in Ref. 3 on the basis of heuristic arguments.

If $\tau/2\pi$ is very close to a rational number p/q, i.e., $d(q) < e^{-\gamma q}$ for but one q (with, say, $\gamma q \gg 1$), then it can be shown that the wave function consists of exponentially localized pieces of size γ^{-1} which almost repeat themselves at intervals of q for about $\exp(-\gamma q)/d(q)$ times. Thus, as τ approaches a rational multiple of 2π, the wave functions become more and more extended. The total measure $M(L)$ of the set of values of τ giving localization lengths $L > \gamma^{-1}$ is small, however, with $M(L) < [(e^{\gamma}-1)L]^{-1}$. We turn now to the case of rational $\tau/2\pi = p/q$ with integral and relatively

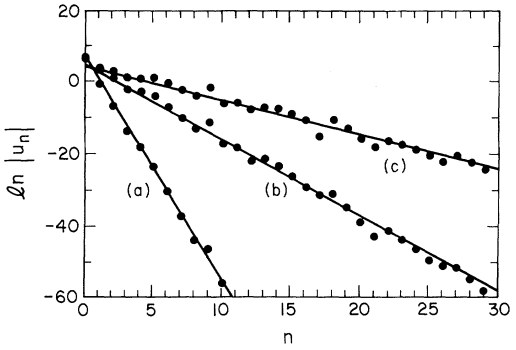

FIG. 1. The wave function u_n (full circles) for $\tau = 4.867$, $\omega = 0$, $\epsilon = 0$, and (curve *a*) $\kappa = 0.005$, (curve *b*) $\kappa = 0.25$, and (curve *c*) $\kappa = 0.95$. The straight lines are the corresponding envelopes as calculated from Eq. (8).

prime p and q. We give here only an outline, reserving the details for future publication. We were able to show that a solution of fixed quasienergy is nonvanishing only at exactly q points in $[-\pi,\pi]$, i.e.,

$$u_{\alpha\lambda}{}^{+}(k) = \sum_{m=0}^{q-1} A_m{}^{\lambda}(\alpha)\Delta(\alpha + m\tau - k), \tag{10}$$

where the amplitudes $A_m{}^{\lambda}(\alpha)$ satisfy certain recursion relations. These solutions are labeled by an integral index $\lambda = 0,1,2,\ldots,q-1$ and a continuous parameter α confined to the interval $[-\pi/q, \pi/q]$. In terms of these quantum numbers the quasienergies are, up to multiples of 2π,

$$\omega_{\lambda}(\alpha) = V_0(\epsilon) + 2\sum_{r=1}^{\infty} V_{rq}(\epsilon)\cos(rq\alpha) + \lambda\tau. \tag{11}$$

For fixed ϵ the quasienergies fall into q bands with uniform separation $2\pi/q$, and width proportional to $\exp(-\gamma q)$, if q is large. Alternatively, for fixed ω, Eq. (11) gives the eigenvalues of the tight-binding problem which also form continuous bands, in sharp contrast with the irrational case. The wave functions in Eq. (10) are localized but nonnormalizable in k space. They are extended and nonnormalizable in real space. When $\tau/2\pi$ approaches an irrational number ($p, q \to \infty$ with p/q finite), however, the bandwidth vanishes exponentially, i.e., faster than the separation between bands, and then, one recovers the discrete (but dense) spectrum of the irrational case. It can be shown that in this limit all the solutions of type (10) with a fixed λ become degenerate. We have explicitly checked that by forming appropriate linear combinations one recovers the localized solutions of Eqs. (5) and (6).

So far we have presented results for the nearest-neighbor model. However, more general potentials can be treated in the same way. For example if $V(k) = \kappa\cos k + \epsilon$ the corresponding hopping W_r becomes complicated (although still approximately nearest neighbor for small κ). For this case the dynamical problem is particularly simple since the only nonvanishing V_n's are V_0 and V_1. For this potential and irrational $\tau/2\pi$ the eigenfunctions of Eq. (1) can be given in closed form:

$$\bar{u}_{n\nu} = \cos[(n-\nu)\tau/2]J_{|n-\nu|}(\kappa/2\sin(\tfrac{1}{2}\tau)), \tag{12}$$

where $J_r(x)$ is a Bessel function. For large r it falls off faster than exponentially. For rational $\tau/2\pi$, there are again bands, but of precisely zero width, i.e., there are only q different energies, each of which is infinitely degenerate.

In summary, we have solved exactly a class of one-dimensional tight-binding models with a diagonal potential that can be incommensurate with the underlying lattice. We found that in the incommensurate case and for nearest-neighbor hopping, all the states are localized with the same localization length as that of a related disordered system for most values of the parameters, and the density of states coincides with that of the disordered system. Thus, all the physical properties that depend on the density of states are identical for both systems. It will be of interest to investigate in what aspects this similarity between disordered and incommensurate systems manifests itself for other incommensurate potentials. The explicit solutions obtained should also be useful for the calculation of observables, such as transport coefficients, in our model.

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