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Chaos, Quantum Recurrences, and Anderson Localization

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A periodically kicked quantum rotator is related to the Anderson problem of conduction in a one-dimensional disordered lattice. Classically the second model is always chaotic, while the first is chaotic for some values of the parameters. With use of the Anderson-model result that all states are localized, it is concluded that the *local* quasienergy spectrum of the rotator problem is discrete and that its wave function is almost periodic in time. This allows one to understand on physical grounds some numerical results recently obtained in the context of the rotator problem.

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In this note we show that certain quantum systems showing chaotic behavior in the classical limit and the system of electrons in a disordered lattice are closely related.

That the motion of nonlinear classical systems can display random characteristics is well known.¹ The solutions of the equations, although they may statistically be definite, are stochastic and behave as if they contain a random number generator. This may occur even though the equations themselves are deterministic and even simple. Indeed, the pseudorandom numbers used in computation are generated in just this way.

The classical equations are often approximations to a more fundamental wave equation, e.g., the Schrödinger equation, in the eikonal sense. The issue of whether the wave equation is as chaotic as its classical limit was formulated clearly by Chirikov *et al.*² Casati *et al.*³ had in an earlier paper studied the simplest example known, that of the periodically kicked quantum rotator. Although some early numerical results claimed the opposite,³ it is now believed² that for nearly all the values of the parameters the quantum motion

will resemble the classical motion only during a finite interval of time after which quantum effects become important. These quantum effects generally prevent stochasticity.² This is at first surprising since even the simplest quantum problem has a probabilistic interpretation. Reference 2 gives an instructive but heuristic discussion of the fundamental difference between the classical and quantum-mechanical motions. More recently, Hogg and Huberman⁴ noted that if a certain condition is met [namely that the local density of quasienergy states is discrete (see below)] the motion is quasiperiodic in time. Their numerical studies indicated that this condition is satisfied at least for certain parameter values. As a consequence of quasiperiodicity the quantum system recurs to almost the same state repeatedly whereas the classical system grows more and more complicated in time.

A second problem of great interest is that of electrical conduction in systems with random scattering potentials. A classical particle in such a potential makes a random walk, and eventually diffuses a distance whose square is proportional

to the time. It was first realized by Anderson^{5,6} that a quantum particle does not necessarily behave in this way, but, depending on dimension and energy, may eternally remain in the vicinity of its initial position. In particular, in one dimension, it is known⁷ that *any* degree of randomness localizes *all* the electronic states.

To show the connection, we consider the problem of a quantum rotator periodically kicked,^{2,3} and produce a mapping in which the (integer) angular momentum of the rotator corresponds to a lattice site in the conduction problem. The pseudorandom number generator in the classical rotator problem reappears in the Anderson problem as a pseudorandom potential. The solution of the quantum problem is, however, dramatically different from the classical solution, since according to Anderson the random walk is cut off and the wave functions are localized. In this way we give a physical understanding of the results obtained in the context of the quantum rotator model. Conversely, from the rotator results we can conclude that the time-dependent wave function of an electron in an Anderson lattice is almost periodic, implying a time-persistent probability of finding an electron in the vicinity of its initial position.

The Schrödinger equation of the rotator is

$$i\hbar \partial \psi(\theta, t) / \partial t = \{H + \hat{k}V(\theta)\Delta(t)\} \psi(\theta, t). \quad (1)$$

Here $H = -(\hbar^2/2I)\partial^2/\partial\theta^2$ and $\Delta(t) = \sum_n \delta(t - nT_0)$. We take T_0 as the unit of time and \hbar/T_0 as the unit of energy, and define dimensionless parameters $\tau = \hbar T_0/I$, $k = \hat{k}/\hbar$, and $K = k\tau$, the last of which is classical. We consider a general potential, $V(\theta)$, satisfying $V(\theta) = V(-\theta) = V(\theta + 2\pi)$. The equations for p_n and θ_n , the classical angular momentum and angle just after the n th kick, are $p_{n+1} - p_n = -\hat{k}V'(\theta_{n+1})$, $\theta_{n+1} - \theta_n = Kp_n/k$, with $V' = dV/d\theta$. If K is large enough, for many¹ functions V , e.g., $V = \cos\theta$, V' generates random numbers for successive n values. The momentum then makes a random walk and the energy increases as $p_n^2 \approx \hat{k}^2 \langle V'^2 \rangle n$.

We reformulate (1) to make contact with Anderson theory. Since (1) is invariant under $t \rightarrow t+1$, the quasienergy ω characterizes the eigenstates, which are orthogonal⁸ for distinct ω 's. The states then have the form $\psi_\omega = e^{-i\omega t} u(\theta, t)$ where $u(t) = u(t+1)$. It suffices to study u_\pm , the values of u just after (before) a jump. The relationship $u_+ = e^{-ikV(\theta)} u_-$ holds. We denote $\bar{u} = (u_+ + u_-)/2$. Then $\bar{u} = u_-/(1-iU) = u_+/(1+iU)$, where $U(\theta) = -\tan[k \times V(\theta)/2]$. Another relation may be obtained by

integrating between kicks to find

$$u_-(\theta) = \int d\varphi \sum \exp[im(\theta - \varphi)] \exp(iE_m) u_+(\varphi) / 2\pi \quad (2)$$

with $E_m = \omega - \tau m^2/2$. We eliminate u_\pm in favor of \bar{u} , introduce the Fourier coefficients u_n of \bar{u} , and find the m th Fourier coefficient of (2). The result may be written

$$T_m u_m + \sum_{r \neq 0} U_r u_{m+r} = \epsilon u_m, \quad (3)$$

where $U_r = U_{-r}$ is the Fourier coefficient of $U(\theta)$, $T_m = \tan(E_m/2)$, and $\epsilon = -U_0$. This is the equation for a one-dimensional Anderson model, a tight-binding model with hopping elements U_r to the r th neighbor.

In the Anderson model, T_m is an externally given random number so that there is "diagonal" disorder. Then we know that the eigenstates of (3) are localized about some site and decay exponentially away from that site with a characteristic length $\gamma^{-1}(\epsilon)$. Eigenstates with nearly identical energies are, however, generally localized at centers which are far apart. Conversely, two eigenstates localized at centers close compared with γ^{-1} will typically have eigenenergies separated by a finite-energy spacing ΔE which is roughly γ times the bandwidth in the absence of disorder. It is also well established^{5,9} that, because of these properties, the *local* density of states (i.e., as weighted by the absolute square of the wave function, and defined explicitly below) is discrete and, at a given site n , it consists of about γ^{-1} δ -function peaks at certain energies ϵ_n . The main assumption of the present paper, supported by numerical evidence given below, is that the sequence T_m of relevance for the quantum dynamical problem, although not satisfying the most stringent mathematical tests of randomness,¹⁰ is nevertheless sufficiently so that the above statements apply. The eigenvalues $\epsilon_n(\omega)$ are monotonic functions of ω which determine the quasienergy spectrum by $\epsilon_n(\omega) = -U_0$. This spectrum has the same properties as the energy spectrum. In particular, the *local* density of quasienergy states is discrete. It is the local rather than the total density of states that determines much of the behavior of the system, including that discussed here.

To study the time evolution of the system we integrate (1) in time.² We denote the s th wave function in the angular momentum representation

by $a_n^s(t)$, which satisfies

$$a_n^s(t+1) = \sum J_{m-n}(k) \exp(-im^2\tau/2) a_n^s(t), \quad (4)$$

where $J_r(k) = (2\pi)^{-1} \int d\theta \exp[ir\theta - ikV(\theta)]$. Any initial condition, specified by s , may be used, but it is convenient to require $a_n^s(0+) = \delta_{ns}$. We define $\bar{a}_n^s(t) = [a_n^s(t+) + a_n^s(t-)]/2$. It is found $\bar{a}_n^s(\omega) = \sum_\alpha A_n^s(\alpha) \delta(\omega - \omega_\alpha)$, where $A_n^s(\alpha) = u_n(\alpha) \times u_s^*(\alpha)$. The local density of quasienergy states at n is \bar{a}_n^n . The discreteness follows from the localized character of the u 's; i.e., because of the exponential decay of the u 's, A_n^s is large for only a few values of α . It then follows that $\bar{a}_n^s(t)$ is almost periodic.¹¹

We have numerically solved Eq. (4) for $\bar{a}(t)$ and taken its time Fourier transform, to obtain the A 's and the ω_α 's. In Fig. 1 we show the transform of $\text{Re}\bar{a}_n^0(t)$ for several n 's in the nearest-neighbor ($U = \kappa \cos\theta - \epsilon$) case. It can be seen that ω_α is independent of n and that the amplitude depends strongly on n . We have chosen κ fairly small so that γ is quite large and ω_n is approximately known. In Fig. 2 we show $\ln|\text{Re}A_n^0(0)|$ and compare it with $-\gamma n$, where γ is the value determined from localization theory and given below. There is qualitative agreement.

An issue raised in Refs. 2 and 3 is whether there are distinct types of quantum behavior depending on the values of k and τ . Clearly, there is localization (and thus near periodicity) for *all* k if T_m is random. The transient and recurrence time scales do depend on k , of course, since γ does. The randomness of T_m depends only on τ .

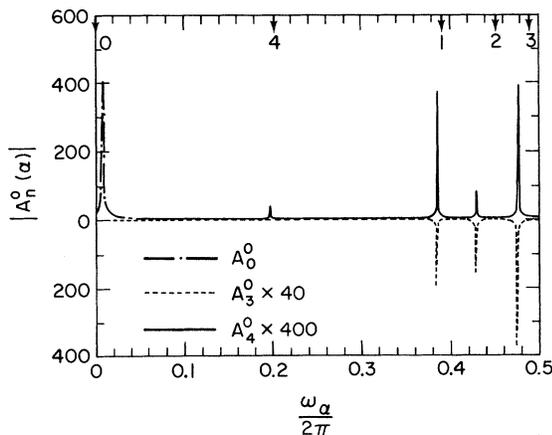


FIG. 1. The Fourier transform of \bar{a}_n^s for $s=0$ and $n=0, 3, 4$, for $\kappa=0.25$, $\tau=30$, and $\epsilon=0$. The arrows indicate the expected quasienergy spectrum in the limit of $\kappa \rightarrow 0$.

We do not attempt a discussion of the interesting question of the characterization of the randomness as a function of the value and number theoretic character of τ , as it is unknown how random the sequence T_m has to be for Anderson localization to take place. We mention only two cases, $\tau/4\pi$ rational or irrational (excluding the Liouville numbers).

For $\tau/4\pi$ irrational, T_m is apparently pseudorandom. $E_m \bmod 2\pi$ is uniformly distributed and its power spectrum is numerically broadband ruling out pair correlations. Then, T_m has a Cauchy distribution, $1/(T^2+1)\pi$. This distribution defines a well studied and simple case known as the Lloyd model.¹² In the nearest-neighbor case, several exact results are known, e.g., the inverse localization length $\gamma(\epsilon, \kappa)$ is^{7,13}

$$2\kappa \cosh\gamma = [(\epsilon - \kappa)^2 + 1]^{1/2} + [(\epsilon + \kappa)^2 + 1]^{1/2}. \quad (5)$$

The potential in the rotator model corresponding to this U is $V(\theta) = (2/\kappa) \arctan(\kappa \cos\theta - \epsilon)$. This has a rather unpleasant appearance but is analytically simpler than the choice $V = \cos\theta$ studied previously in the rotator model. Note, too, that for $\epsilon=0$ and κ small, $V(\theta) \approx \cos\theta$. The numerical results are qualitatively similar for either choice of V . We have checked that the Lyapunov exponent of the classical map associated with this potential is positive for appropriate values of the parameters, i.e., the map is chaotic.

The agreement between the value of γ given by Eq. (5) and the one obtained from the numerical solution of Eq. (4) supports our conjecture that the sequence T_m is sufficiently random for Anderson localization to occur.

In the rotator, γ enters through the kernel J .

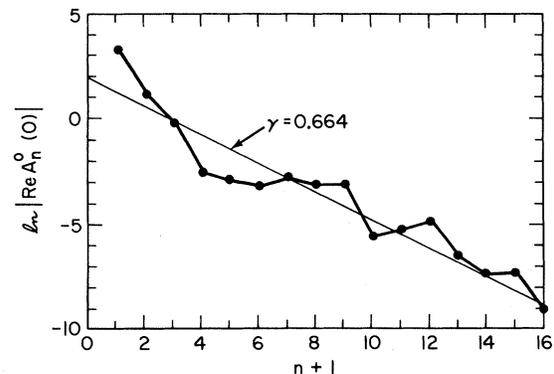


FIG. 2. The real part of $A_n^0(\alpha)$ for $\omega_\alpha/2\pi=0.059$, for $\kappa=1.4$ and $\tau=30$. The straight line is the envelope calculated from Eq. (5).

For the nearest-neighbor case we find $J_r \propto e^{-\gamma|r|}$, where γ is given by (5). That the range of J gives the localization length is not transparent, but it numerically works in the cases we have studied. This allows the conjecture that the localization length for more complicated Anderson-Lloyd models can be determined analytically by studying J . It can in any case be studied numerically by this method.

If $\tau/4\pi$ is a rational p/q , then $T_m = T_{m+q}$ is periodic and the eigenstates of (3) are band states. This is called a quantum resonance² in the rotator context. For example, take $\tau = 4\pi$. Then $T_m = \tan(E_\alpha/2) = -U(\alpha)$, $u_m = u_0 e^{-i\alpha m}$, and α is any real number. The eigenstates are

$$u(\theta, t) \propto \sum_m \exp[im(\theta - \alpha) - i2\pi m^2 t + iE_\alpha t]$$

for $0 < t < 1$. Note that u is not normalizable. Indeed, for $t \rightarrow 0$ u becomes proportional to $\delta(\theta - \alpha)$. Thus, although the eigenstates of the quantum rotator are bounded in θ , they are unbounded in momentum, and possess a continuous spectrum. However, if q is very large, the single band which would exist for T_m constant is split into q bands each of exceedingly small width, which can be estimated to vanish exponentially for large q , and as a practical matter, the states might as well be localized.

There are many related problems of interest. One is the generalization of Eq. (1) to d dimensions. Another is the choice $H = (\tau/i)\partial/\partial\theta$, which gives (3) with $T_m = \tilde{T}_m = \tan[(E - m\tau)/2]$. This appears to be a case of a periodic potential incommensurate (or commensurate) with the lattice. If so, a theorem¹⁴ would indicate that all states are extended, in disagreement with previous studies.¹⁵ Certainly, \tilde{T}_m is not a good random number generator as in this case its power spectrum has many discrete peaks. However, we succeeded in solving this model exactly¹⁶ and found that, if $\tau/4\pi$ is irrational, all the states are localized consistent with the Anderson-Lloyd model. Thus, \tilde{T}_m produces the same effects as a truly random sequence as far as localization is concerned. As T_m is surely not less random than \tilde{T}_m , this strongly suggests that the latter sequence leads to localization as well.

In summary, there is a connection between a quantum problem whose classical limit is chaotic and the problem of conduction in a random potential. We have shown that one may apply the known results of one of these problems to the elucidation of the other. In particular, that the energy is bounded in the rotator and that there is no dif-

fusion on the disordered lattice have a common explanation, namely, for fixed energy or quasi-energy, Anderson localization (in space or angular momentum, respectively), or equivalently, near periodicity in the time representation. It may be quite general that problems with external randomness can be studied by introducing a pseudorandom number generator which depends on a convenient parameter.

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