PHYSICAL REVIEW LETTERS

VOLUME 49 6 SEPTEMBER 1982 NUMBER 10

Chaotic States of Almost Periodic Schrödinger Operators

J. Bellissard
Université de Provence et Centre de Physique Théorique, Centre National de la Recherche Scientifique, Luminy, F-13288 Marseille Cédex 9, France

and

D. Bessis and P. Moussa
Service de Physique Théorique, Centre d'Etudes Nucléaires de Saclay, F-91191 Gif-sur-Yvette Cédex, France
(Received 16 June 1982)

A one-dimensional quantum mechanical model defined by the "quadratic mapping Hamiltonian" which is almost periodic is presented. The model admits a Cantor spectrum of Lebesgue measure zero with a singular continuous measure and produces extended states displaying an unexpected chaotic behavior at large distances.

PACS numbers: 02.50.+s, 63.10.+a, 71.10.+x

Many physical systems can be described via a Schrödinger equation with an almost periodic potential. This is the case for linear organic conducting chains,[1] electronic properties of crystals in a uniform magnetic field,[2] and the Ginzburg-Landau theory of filamentary superconductors.[3] In all these systems, the problem is reduced to a one-dimensional Schrödinger equation, in which the potential $V(x)$ is an almost periodic function; namely, $V(x)$ can be expanded in a Fourier series:

$$V(x)=\sum_{\omega\in\Omega} v_\omega \exp(2i\pi\omega x)\,, \qquad (1)$$

where Ω is a countable subset of the real numbers. Of particular interest for physical applications are the nature of the spectral measure (pure point, absolutely continuous, and singular continuous), the behavior of the wave function (localized or extended, chaotic or nonchaotic), and finally the topological feature of the spectrum (connected, band spectrum, Cantor spectrum).

A discretized version of the Schrödinger equation is provided by the popular "almost Mathieu" equation:

$$\psi(n+1)+\psi(n-1)+2\mu\cos 2\pi(x-n\alpha)\,\psi(n) = E\psi(n), \qquad (2)$$

where now $\psi(n)$ is a sequence indexed by positive or negative integers, α being irrational. Equation (2) has been studied by several authors, using both heuristic or numerical methods[4] and rigorous arguments.[5,6] Aubrey and André[4] have conjectured that states have to be localized (exponentially decreasing) or extended (Bloch waves) according to whether μ is greater or smaller than 1. The conjecture has been proved to be valid under restrictive conditions[7]; in particular α is required to be far from any rational p/q, according to

$$|\alpha-p/q|\geq C/q^{(2+\epsilon)}, \quad C>0, \quad \epsilon>0. \qquad (3)$$

On the other hand Avron and Simon,[8] following Gordon,[9] have considered the case where α is close to rational numbers, namely, when there exists a sequence of rationals p_n/q_n such that

$$|\alpha-p_n/q_n|\leq 1/n^{q_n}, \quad n\geq 1. \qquad (4)$$

In this case, for any μ there are no localized states. Therefore the Aubry-André conjecture is not valid for $\mu > 1$ and according to Pastur[10] the spectrum has no absolutely continuous part. In this case, as well as in the case $\mu = 1$, we have a singular continuous spectrum and we expect a strange behavior of the wave functions.

A similar situation occurs in the Kronig-Penney equation[11,12]:

$$\left(-\frac{d^2}{dx^2} + \sum_{n=-\infty}^{n=+\infty} g(u - n\alpha)\,\delta(x - x_n(u))\right)\psi(x) = E\psi(x), \quad (5)$$

where

$$x_{n+1}(u) - x_n(u) = f(u - n\alpha). \quad (6)$$

Here f and g are assumed to be continuous periodic functions with period one. Perturbation arguments show that for g small enough, the solutions of (5) are extended Bloch waves provided α fulfills condition (3). The localization region is reached when g is large enough; however, the spectrum remains singular continuous when α obeys condition (4) and no solution vanishes at infinity even for g large.

However, in the singular-spectrum case, it still remains to understand the behavior of the wave functions at large distances. Here we propose a solvable almost periodic model, the solutions of which display a chaotic behavior. This model is derived from the observation[13,14] that quadratic iterated polynomials appear to belong to a family of polynomials that are orthogonal with respect to a measure with support on a Cantor set. The related operator is nothing but the Jacobi tridiagonal matrix associated with the linear recursion relation. We use here a different starting point, and define the Hamiltonian as the solution of a quadratic polynomial renormalization-group equation, and therefore we will call this model the quadratic mapping Hamiltonian H_{QM}. More precisely if $\psi = (\psi(n),\ n \geq 0)$ is a square integrable sequence, we define the (doubling) dilation operator D as

$$D\psi(n) = \psi(2n). \quad (7)$$

The renormalization-group equation satisfied by H_{QM} can be written as

$$H_{\mathrm{QM}} D = D(H_{\mathrm{QM}}^2 - \lambda). \quad (8)$$

The quadratic mapping Hamiltonian is given in a Schrödinger-type discrete form as

$$(H_{\mathrm{QM}}\psi)(n) = (R_{n+1})^{1/2}\psi(n+1) + (R_n)^{1/2}\psi(n-1), \quad (9)$$

where the coefficients R_n are recursively defined[13,14] by

$$\text{(i) } R_0 = 0, \quad \text{(ii) } R_{2n} + R_{2n+1} = \lambda, \quad \text{(iii) } R_{2n}R_{2n-1} = R_n. \quad (10)$$

When $\lambda = 2$, the solution is $R_0 = 0$, $R_1 = 2$, and $R_n = 1$, $n \geq 2$, and the corresponding H_{QM} is a discrete Laplace operator with a special boundary condition at $n = 0$. The spectrum is the interval $[-2, +2]$. The Hermiticity condition is fulfilled if and only if $\lambda \geq 2$. The corresponding H_{QM} is a generalized Schrödinger-like operator which also describes a chain of inhomogeneous harmonic oscillators, each coupled with its nearest neighbors.[15]

We have the following results for $\lambda \geq 2$.

Result 1.—The spectrum of H_{QM} is invariant under the map F and its inverse $\varphi_\pm$ defined by

$$F(z) = z^2 - \lambda, \quad \varphi_\pm(z) = \pm(\lambda + z)^{1/2}. \quad (11)$$

Result 2.—Let μ be the spectral measure relative to the vector $e_0(n) = \delta_{0,n}$:

$$\langle e_0 | (z - H)^{-1} | e_0 \rangle = \int (z - E)^{-1} d\mu(E); \quad (12)$$

then μ is invariant under F and $\varphi_\pm$, namely,

$$\int d\mu(E) f(E) = \int d\mu(E) f(E^2 - \lambda),$$
$$\int d\mu(E) f(E) = \tfrac{1}{2}\int d\mu(E)\{f((\lambda + E)^{1/2}) + f(-(\lambda + E)^{1/2})\}. \quad (13)$$

From the classical results on iteration of polynomials (see Brolin[16] for a review), when $\lambda > 2$, we get the spectrum of H_{QM} as the set $\mathcal{K}$ of points $E(\underline{\sigma})$:

$$\underline{\sigma} = (\sigma_0, \sigma_1, \ldots, \sigma_n, \ldots), \quad \sigma_i = \pm 1, \quad (14)$$

$$E(\underline{\sigma}) = \lim_{n\to\infty} \varphi_{\sigma_0} \circ \varphi_{\sigma_1} \circ \cdots \circ \varphi_{\sigma_{n-1}}(0) = \sigma_0\sqrt{\lambda + \sigma_1\sqrt{\lambda + \sigma_2 \cdots}}\,. \quad (15)$$

$\mathcal{K}$ is a Cantor set of Lebesgue measure zero,[14,16] obtained as follows. We start from $[-\xi, +\xi]$ where ξ is the positive fixed point of F: $F(\xi) = \xi$, $\varphi_+(\xi) = \xi$. We remove the segment $]\varphi_-(-\xi), \varphi_+(-\xi)[$; then in each remaining interval we remove $]\varphi_\pm \circ \varphi_-(-\xi), \varphi_\pm \circ \varphi_+(-\xi)[$ and so on. The end points of the removed segments have the form $\varphi_{\sigma_0} \circ \varphi_{\sigma_1} \circ \cdots \circ \varphi_{\sigma_{n-1}}(-\xi)$, with $\sigma_i = \pm 1$, and they are mapped onto ξ when transformed $(n+1)$ times by F. The representation (15) of the points of $\mathcal{K}$ is a well-adapted coding satisfying

$$F(E(\underline{\sigma})) = E(T\underline{\sigma}), \quad \varphi_{\pm}(E(\underline{\sigma})) = E(\pm, \underline{\sigma}), \tag{16}$$

where T denotes the one-sided shift

$$T(\sigma_0, \sigma_1, \sigma_2, \ldots) = (\sigma_1, \sigma_2, \sigma_3, \ldots) \tag{17}$$

and

$$(\pm, \underline{\sigma}) = (\pm, \sigma_0, \sigma_1, \sigma_2, \ldots). \tag{18}$$

However, (16) expresses that there is only one measure μ satisfying (13), which in terms of $\underline{\sigma}$ is nothing else than the "coin-tossing" probability distribution giving a probability one-half for each σ_n to be either $+1$ or -1:

$$\int d\mu\, f = \int \prod_{n=0}^{\infty} d\sigma_n\, \tfrac{1}{2}[\delta(\sigma_n - 1) + \delta(\sigma_n + 1)] f(E(\sigma_0, \sigma_1, \ldots)). \tag{19}$$

From (19) it is easily seen that the support of μ is the set $\mathcal{K}$ which has Lebesgue measure zero,[16] and that μ has no atomic part. μ is thus a singular continuous measure. The shift T (or equivalently F) is ergodic and even a Bernoulli shift, which is the most chaotic example of a dynamical system.

We shall now analyze the properties of the coefficients R_n occurring in the Hamiltonian. We have the following.

Result 3.—For $\lambda \geqslant 2$, the sequence $\underline{R} = (R_n)$, $n \geqslant 0$, satisfies

$$\lim_{k\to\infty} |R_{2^k n+s} - R_s| = 0, \quad s \geqslant 0, \quad n \geqslant 1; \tag{20}$$

the limit holds uniformly in s and n. This result can be found in Ref. 13 in a weaker form which does not insure uniformity. In fact a recursive argument on s similar to the method used in Ref. 13 allows one to get a better estimate:

$$|R_{2^k n+s} - R_s| \leqslant \lambda/(\lambda - 2)^k. \tag{21}$$

The uniformity property is therefore achieved for $\lambda > 3$. An analyticity argument allows us to extend the result toward $\lambda \geqslant 2$. From the uniformity property we can deduce that $\underline{R}$ is almost periodic. More precisely, $\underline{R}$ is a limit-periodic sequence[17] and from the general theory of almost periodic functions, we conclude that $\underline{R}$ admits a Fourier expansion:

$$R_n = \sum_{q=0}^{\infty} \sum_{p=0}^{2^{q-1}-1} r_{p,q} \exp 2i\pi \frac{n}{2^q}(2p+1). \tag{22}$$

The last step of our analysis is devoted to the eigenfunctions which can be written as [see Eq. (26) below]

$$\psi_n(E) = P_n(E)/(R_1 \cdots R_n)^{1/2}. \tag{23}$$

The long-distance behavior of the eigenfunctions is described by the Lyapunov exponent $\gamma(E)$ defined as

$$\gamma(E) = \lim_{n\to\infty} \ln\left(\frac{\psi^2(n) + \psi^2(n+1)}{\psi^2(1) + \psi^2(0)}\right). \tag{24}$$

From the Thouless formula[18] we can prove by using (13)

$$2\gamma(E) = \gamma(F(E)), \tag{25}$$

so that $\gamma(E)$ vanishes on the spectrum, indicating that the states are extended.

The most significant property of the states is their chaotic behavior, which is seen from the following argument: $P_n(E)$ is the sequence of polynomials defined by the usual three-term recursion relation:

$$P_0 = 1, \quad P_1(E) = E,$$

$$P_{n+1}(E) = EP_n(E) - R_n P_{n-1}(E). \tag{26}$$

They are the orthogonal polynomials with respect to the measure μ:

$$\int \psi_n(E)\psi_m(E)\, d\mu(E) = \delta_{m,n}. \tag{27}$$

Then using Result 2 and Eq. (9), we get,[13,14] for any $E \in \mathfrak{K}$,

$$P_{2^k n}(E) = P_n(F^{(k)}(E)), \tag{28}$$

where $F^{(k)}$ is the nth iterate of the quadratic polynomial F. Thanks to (10) and (16), we have

$$\psi_{n2^k}(E(\underline{\sigma})) = \frac{P_n(E(T^k\underline{\sigma}))}{(R_1R_2 \cdots R_n)^{1/2}}. \tag{29}$$

For almost every $E(\underline{\sigma})$ in $\mathcal{K}$ the sequence $\underline{\sigma}$ is really chaotic, which implies as $k\to\infty$ that the spatial behavior of $\psi_{2^k n}(E(\underline{\sigma}))$ is itself chaotic with probability one. Exceptional sequences $\underline{\sigma}$ can be periodic in such a way that $k \to \psi_{2^k n}(E(\underline{\sigma}))$ is periodic, but this happens with probability zero with respect to μ.

Besides its solvability, the most interesting property of the model is its chaotic behavior: *At large distances the states, which are all extended, retain no memory of the near periodicity and fluctuate at random.* It is tempting to conjecture that a chaotic behavior occurs also in the almost Mathieu equation (2) when α fulfills condition (4).

The question is then how to characterize the randomness property involved here, and its connection with the tunneling effect between narrow resonances which creates the extended states.

The situation is reminiscent of properties of dynamical systems. Discretized equations can be considered as Poincaré maps of dynamical systems with infinite degrees of freedom, an analogy which has been often pointed out, and recently used in the study of the Frenkel-Kontorova model for incommensurate structures.[19] Bloch waves in the almost Mathieu equation correspond to invariant tori observed under perturbation in completely integrable systems, according to the so-called Kalmogorov-Arnold-Moser theorem.[5,7] Similarly we conjecture that chaotic waves appear in the vicinity of hyperbolic points, i.e., near the edges of the bands in the spectrum. Along this line, the quadratic mapping Hamiltonian looks similar to that of completely chaotic systems, for example, the so-called standard map, where it has been shown that chaotic behavior is associated with the absence of invariant tori.[20]

Our model looks promising in many other respects, for example, the electrical conductivity, diffusion constant, stability properties under small perturbation, and scattering experiments if such a system allows the scattered particle to be trapped during a very long time.[6]

We think of a possible generalization to higher-degree polynomials of the quadratic mapping Hamiltonian, and we leave open the question of what happens for λ smaller than 2, where Hermiticity is lost.

We wish to thank M. Aizenman and E. Lieb from Princeton University, where part of this work was initiated, and one of us (J.B.) wishes to thank J. Avron and B. Simon at Caltech, P. Deift and P. Perry at the Courant Institute, and C. Soukoulis and L. M. Turkevitch at Exxon Research and Engineering Company for valuable discussions and facilities provided at the corresponding insitutions.

[1]See, for instance, A. N. Bloch, in *Organic Conductors and Semiconductors*, edited by L. Pal *et al.*, Lectures Notes in Physics Vol. 65 (Springer-Verlag, Berlin, 1977), p. 317, and references therein; D. Jerome, A. Mazaud, M. Ribault, and K. Bechgaard, J. Phys. (Paris), Lett. 41, L95 (1980).

[2]P. G. Harper, Proc. Phys. Soc., London, Sect. A 68, 874 (1955).

[3]L. A. Turkevitch and R. A. Klemm, Phys. Rev. B 19, 2520 (1979), and references therein.

[4]D. R. Hofstadter, Phys. Rev. B 14, 2239 (1967); S. Aubry and G. André, Ann. Israel Phys. Soc. 3, 111 (1980); J. B. Sokoloff, Phys. Rev. B 22, 5823 (1980), and 23, 6422 (1980).

[5]E. I. Dinaburg and Ya. G. Sinai, Funct. Anal. Appl. 9, 279 (1976); E. D. Belokolos, Theor. Math. Phys. 25, 1176 (1976); H. Rüssmann, Ann. N. Y. Acad. Sci. 357, 90 (1980).

[6]B. Simon, to be published; J. Bellissard, in *Mathematical Problems in Theoretical Physics*, edited by R. Schrader, Lectures Notes in Physics Vol. 153 (Springer-Verlag, Berlin, 1982), p. 356.

[7]J. Bellissard, R. Lima, and D. Testard, to be published.

[8]J. Avron and B. Simon, Bull. Am. Math. Soc. 6, 81 (1982).

[9]A. Ya. Gordon, Usp. Mat. Nauk 31, 257 (1976).

[10]L. Pastur, Usp. Mat. Nauk 28, 3 (1973), and Commun. Math. Phys. 75, 179 (1980).

[11]M. Y. Azbel, Phys. Rev. Lett. 43, 1954 (1979).

[12]J. Bellissard, A. Formoso, R. Lima, and D. Testard, Phys. Rev. B 25, 2073 (1982).

[13]D. Bessis, M. L. Metha, and P. Moussa, Lett. Math. Phys. 6, 123 (1982).

[14]M. F. Barnsley, J. Geronimo, and A. N. Harrington, to be published.

[15]F. J. Dyson, Phys. Rev. 92, 1331 (1953).

[16]A review including the classical results of G. Julia and P. Fatou can be found in H. Brolin, Ark. Mat. 6, 103 (1965).

[17]H. Bohr, *Almost Periodic Function* (Chelsea, New York, 1951).

[18]D. J. Thouless, J. Phys. C 5, 77 (1972).

[19]S. Aubry and P. Y. Le Daeron, "The Discrete Frenkel-Kontorova Model and Its Extension" (to be published).

[20]J. M. Greene, J. Math. Phys. 20, 1183 (1979).