

New Conserved Quantities and Test for Regular Spectra

Asher Peres

Department of Physics, Technion-Israel Institute of Technology, 32000 Haifa, Israel

(Received 24 May 1984)

When Einstein-Brillouin-Keller quantization is possible, it applies to *all* conserved dynamical variables (not only to the Hamiltonian) and in particular to the time average of *any* dynamical variable. Thus, for an integrable system of n degrees of freedom, the eigenvalues of n independent constants of motion form a locally regular n -dimensional lattice, in the limit $\hbar \rightarrow 0$. Failure of doing that may be an indication of quantum chaos.

PACS numbers: 03.65.-w, 03.20.+i

Energy spectra often become very complicated for highly excited systems and it is difficult to ascribe quantum numbers to the various levels. Yet, these quantum numbers ought to exist if the system is "regular" (i.e., if its classical analog is *integrable*) because Einstein-Brillouin-Keller (EBK) quantization¹⁻³ is a very good approximation for large quantum numbers (or, equivalently, in the semiclassical limit $\hbar \rightarrow 0$). On the other hand, a classically *nonintegrable* system is "irregular" and its energy levels cannot be labeled in a natural way by quantum numbers related to constants of motion.⁴ It would thus be very helpful to have a simple criterion to distinguish regular from irregular quantum systems (i.e., to decide whether there are "good" quantum numbers other than the energy).

If a classical system with n degrees of freedom is integrable (i.e., if it has n independent constants of motion in involution) its orbits in phase space lie on n -dimensional surfaces, conventionally called "tori." On each one of these tori, one can draw n topologically independent closed curves C_k and thereby define n action variables⁵

$$J_k = \oint_{C_k} \sum_i p_i dq^i. \quad (1)$$

The values of these J_k can then serve to label the tori. Any constant of motion A therefore is a function $A(J_1, \dots, J_n)$.

EBK quantization, which is a refinement of the old Bohr-Sommerfeld quantization, states that $J_k = a_k + m_k \hbar$, where the a_k are constants and the m_k are integers. If we expand A in powers of Planck's constant \hbar , we thus obtain

$$A = A(0) + \hbar \sum m_k v_k + O(\hbar^2), \quad (2)$$

where $v_k = \partial A / \partial J_k$ is a function of the J_i . Therefore, the eigenvalues of A differ by $\hbar \sum m_k v_k$. This property is well known for energy spectra but it is actually valid for the spectrum of *any* constant of motion, *if* the system is integrable (so that there are tori and EBK quantization can proceed).

It is trivial (in principle) to test numerically whether or not a given spectrum satisfies Eq. (2).⁶ Unfortunately, this simple test becomes impractical when there are hundreds of levels belonging to overlapping "ladders." It is then much more efficient to consider n independent constants of motion and to plot the corresponding eigenvalues in an n -dimensional diagram, as shown below.

How can we get n constants of motion? If a system is not integrable (or not *known* to be integrable) we cannot find functions of the canonical variables $A(p, q)$ having vanishing Poisson brackets with the Hamiltonian. However, the *time-average* of any bounded $A(p, q)$ is, trivially, a constant of motion. If the tori exist, it has a fixed value on each torus, so that it is a function of the J_i and therefore obeys Eq. (2).

In quantum mechanics, it is very simple to construct these time averages and to find their eigenvalues. Any dynamical variable, in the energy representation, has matrix elements $A_{jk}(t) = A_{jk}(0) \times \exp[2\pi i(E_j - E_k)t/\hbar]$. If the Hamiltonian is not degenerate, the time average is simply obtained by crossing out all the off-diagonal elements of A (in the energy representation). If H is degenerate, one first removes all matrix elements of A connecting different energies, and then one diagonalizes the resulting matrix. Once this is done, it only remains to plot the resulting eigenvalues versus those of the Hamiltonian and to see whether the result looks like a regular lattice. The lattice spacing and orientation may smoothly vary from one place to another, because the v_k in Eq. (2) depend on the J_i .

This method will now be illustrated by two numerical examples. First, consider the classical Hamiltonian

$$H = p_1 + p_2 + (L^2 - p_1^2)^{1/2} (M^2 - p_2^2)^{1/2} \cos q_1 \cos q_2, \quad (3)$$

where p_j and q_j are two pairs of canonical variables, and L and M are constants. It is convenient to de-

fine new variables $L_x = (L^2 - p_1^2)^{1/2} \cos q_1$, $L_y = (L^2 - p_1^2)^{1/2} \sin q_1$, and $L_z = p_1$, which satisfy the same Poisson brackets as components of angular momentum. Likewise, we define $M_x = (M^2 - p_2^2)^{1/2} \cos q_2$, etc. The Hamiltonian (3) thus becomes

$$H = L_z + M_z + L_x M_x, \quad (4)$$

and can be interpreted as representing a pair of nonlinearly coupled rotators. The classical orbits of (4) have been discussed in detail elsewhere⁷: For some values of L , M , and H , most orbits are regular, and for other values most are chaotic. These properties are reflected in the quantum mechanical energy spectrum⁶ and matrix elements.⁸

In quantum theory, the constants L and M must satisfy $L^2 = \hbar^2 l(l+1)$ and $M^2 = \hbar^2 m(m+1)$ and the Hamiltonian (4) is a *finite* matrix of order $(2l+1)(2m+1)$. In this first numerical example, I have taken $l=m=20$ and $\hbar=0.1707825$. This corresponds to $L=M=3.5$, giving a maximum classical energy⁷ $L^2+1=13.25$. From Fig. 2 of Ref. 8, the classical regular domain is $|E| \geq 9.1$ and the classical chaotic one is $|E| \leq 6.6$. However, for *finite* \hbar , there may still be a regular spectrum in a domain which is classically chaotic, because of the existence of "tori remnants" in the chaotic part of the classical phase space.^{9,10} As long as the missing parts of these "vague tori" are small compared to \hbar^n , EBK quantization is nearly valid and the quantum system behaves as if it were regular.

In order to find the energy spectrum, it is convenient to use a basis labeled by $j_z = (p_1 + p_2)/\hbar$ and $k_z = (p_1 - p_2)/\hbar$. The Hilbert space then splits into four disjoint subspaces, with j_z even or odd,

and with states even or odd with respect to $k_z \rightarrow -k_z$. The Hamiltonian (4) has no matrix elements connecting these subspaces. The discussion will henceforth be restricted to the even-even subspace, having dimension $21^2=441$. The energy spectrum is nondegenerate and symmetric with respect to $E=0$.

As a second constant of motion, I took the time average of $p_1 + p_2$, which I call P . The 441 eigenvalues of P are $\langle E|P|E \rangle$. Figure 1 is a scatter plot of these eigenvalues versus E , for $E > 0$ (the figure is symmetric with respect to the origin). As expected, one sees a regular pattern for $E \geq 9$, which gradually melts away for lower values of E . There are, however, remnants of regularity (strings of roughly aligned and equidistant points) in the disordered region. These are apparently due to the tori remnants mentioned above.

On the other hand, some deviations from regularity appear in the regular zone, especially when energy levels are nearly degenerate. This too was expected, because degeneracy is related by Eq. (2) to overlapping classical resonances¹¹ which generate classical chaos.

The second numerical example is based on the Hamiltonian¹²

$$H = \frac{1}{2}(p_x^2 + p_y^2 + x^2 + y^2) + 0.05x^2y^2, \quad (5)$$

which, in the classical case, has mostly regular orbits for low E and becomes gradually chaotic for $E > 10$. These properties are reflected in the quantized energy spectrum.¹³

While the Hamiltonian (5) is more easy to

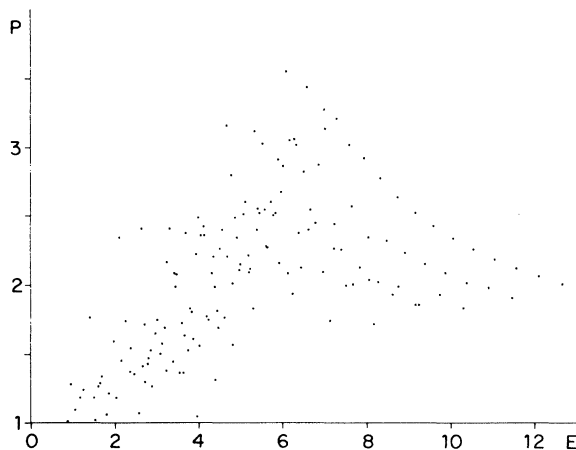


FIG. 1. The energy levels E vs the diagonal matrix elements $P = \langle E|(p_1 + p_2)|E \rangle$, for $E \geq 0$.

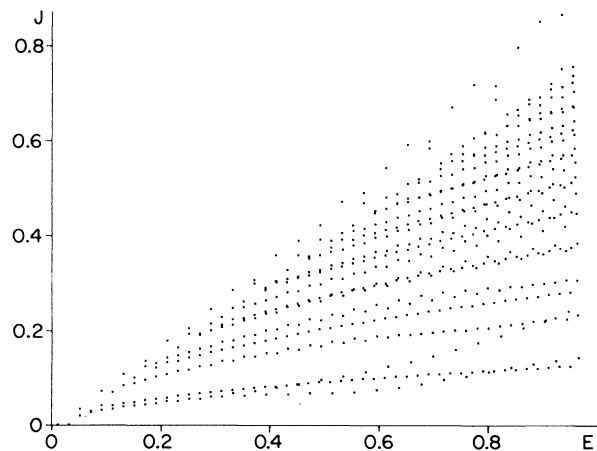


FIG. 2. The energy levels E vs $J^2 = \langle E|(xp_y - yp_x)^2|E \rangle$ for $E < 0.966$. (I plotted J , rather than J^2 , because the result is visually nicer.)

comprehend than (4), it has an *infinite* number of energy levels and some approximations are needed. I took as the basis functions $u_m(x)u_n(y) + u_m(y)u_n(x)$, where the u_m are one-dimensional oscillator wave functions. I considered only one symmetry class (m and n even) and obtained 600 well converged levels.

The square of the angular momentum $(xp_y - yp_x)^2$ is not a constant of motion, but has no matrix elements connecting this basis with others belonging to different symmetry classes. Figure 2 is a plot of

$$J^2 = \langle E | (xp_y - yp_x)^2 | E \rangle \quad (6)$$

versus E , for $\hbar = 0.01$. A regular pattern is apparent, showing that the energy levels fall in sets which can be labeled by a second quantum number. (The situation for higher E will be discussed in a separate paper.)

The method illustrated above is readily generalized to more than two degrees of freedom. Three-dimensional patterns can be visually inspected with the help of computer graphics. Higher-dimensional ones would require a suitable pattern-recognition algorithm. In summary, these regular or chaotic patterns of quantum levels play a role similar to that of Poincaré surfaces of section in classical mechanics.

I am grateful to Mario Feingold for supplying the numerical data for Fig. 1. This work was supported by the Gerard Swope Fund, the Lawrence Deutsch Research Fund, and the Fund for Encouragement of Research of Technion.

¹A. Einstein, Verh. Dtsch. Phys. Ges. **19**, 82 (1917).

²L. Brillouin, J. Phys. Radium **7**, 353 (1926).

³J. B. Keller, Ann. Phys. (N.Y.) **4**, 180 (1958).

⁴I. C. Percival, J. Phys. B **6**, L229 (1973).

⁵M. Born, *The Mechanics of the Atom* (Bell, London, 1927; reprinted by Ungar, New York, 1960).

⁶A. Peres, in *Quantum Chaos*, edited by G. Casati and J. Ford (Plenum, New York, 1984).

⁷M. Feingold and A. Peres, Physica (Utrecht) D **9**, 433 (1983).

⁸M. Feingold, N. Moiseyev, and A. Peres, Phys. Rev. A **30**, 509 (1984).

⁹C. Jaffé and W. P. Reinhardt, J. Chem. Phys. **77**, 5191 (1982).

¹⁰R. B. Shirts and W. P. Reinhardt, J. Chem. Phys. **77**, 5204 (1982).

¹¹G. H. Walker and J. Ford, Phys. Rev. **188**, 416 (1969).

¹²R. A. Pullen and A. R. Edmonds, J. Phys. A **14**, L477 (1981).

¹³E. Haller, H. Köppel, and L. S. Cederbaum, Phys. Rev. Lett. **52**, 1665 (1984).