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Classical Chaos and Quantum Eigenvalues

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The connection between classical and quantum mechanics (i.e., the semiclassical limiting asymptotics as $\hbar \to 0$) must be subtle and complicated, because classical mechanics itself (i.e., the classical limit $\hbar = 0$) is subtle and complicated: the orbits of systems governed by Hamilton's equations of motion may be predictable (regular) or unpredictable (irregular) depending on subtle details of the form of the Hamiltonian $H(\{q_i\}, \{p_i\})$.[1-3] A natural question is: how does the "chaology" of classical orbits reflect itself in the corresponding quantum system? Sometimes this question is put in the form: what is quantum chaos?

There are many approaches to this question. One is to study the *dynamics* of quantum systems which are classically chaotic, that is, to study nonstationary states. There have been many studies of mathematical models of such quantum evolution[4-10] which have found important recent application in interpreting experiments on the microwave ionization of hydrogen atoms.[11-13] Another approach is to look at *stationary states* and concentrate on the form of the wave functions: these are remarkably different for eigenstates corresponding to regular and chaotic systems.[14-19]

Here, however, we concentrate on the *energies* of stationary states, and ask how the *distribution of eigenvalues* $\{E_n\} = E_1, E_2, \ldots$ of a quantum Hamiltonian $\hat{H} = H(\{\hat{q}_i\}, \{\hat{p}_i\})$ reflects the chaology of the classical trajectories generated by the classical H, in which $\{q_i\}$ and $\{p_i\}$ are variables rather than operators. Of course the energies $\{E_n\}$ depend on $\hbar$. We consider only the nontrivial case where the number of freedoms N exceeds unity.

Ideally one would like an explicit asymptotic expression giving $\{E_n(\hbar)\}$ with an error that decreases as $\hbar \to 0$ faster than the mean level spacing. Such

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an expression has been found only for classically integrable (i.e., nonchaotic systems[20-22] and is a generalization of the familiar WKB theory for one dimension. For integrable systems with N freedoms, there are N constants of motion (including the energy) which confine motion to N-dimensional tori in the $2N$-dimensional phase space.[23] In lowest order, quantization selects the energies E of those tori whose N actions are separated by multiples of $\hbar$, i.e.,

$$E_{\{n_i\}} = H\{[I_i = (n_i + \alpha_i/4)\hbar]\} \tag{11.1}$$

where $\{n_i\} = n_1, \ldots, n_N$ are the quantum numbers, $\{I_i\}$ are the actions

$$I_i \equiv \oint_{\gamma_i} p_j \, dq_j \tag{11.2}$$

round the irreducible cycle γ_i of the torus, and the α_i are constants (Maslov indices[20]). Obviously equation (11.1) works only when tori exist. In the chaotic extreme, motion is ergodic and there are no constants of motion apart from E; therefore there are no tori and the semiclassical rule (11.1) cannot be applied: so far nobody has found a semiclassical quantization rule for chaotic systems.

In these circumstances one must seek less precise information, in the form of *average* properties of the distribution of energies. These spectral averages can be defined semiclassically, because as $\hbar \to 0$ infinitely many levels crowd into any fixed energy interval however small. The simplest spectral average is the mean *spectral density* $\langle d(E)\rangle$. This is the average of

$$d(E) \equiv \sum_n \delta(E - E_n) = \operatorname{Tr} \delta(E - \hat{H}) \tag{11.3}$$

and is given semiclassically by the "Weyl rule"[21]

$$\langle d(E)\rangle = \frac{d\Omega(E)/dE}{h^N} \tag{11.4}$$

where Ω is the phase volume given by

$$\Omega(E) = \int_{(H<E)} d^N q \int d^N p, \qquad \text{i.e.,}$$

$$d\Omega/dE = \int d^N q \int d^N p \delta[E - H(\{q_i\}, \{p_i\})] \tag{11.5}$$

The Weyl rule formalizes the old idea of "one quantum state per volume h^N of phase space."

The result (11.4) tells us nothing about quantum chaos, because the classical volume $\Omega(E)$ is insensitive to the regularity or chaos of the orbits. This is disappointing, but nevertheless two useful pieces of information can be obtained. First, the mean level spacing $\langle d\rangle^{-1}$ is of order $\hbar^N$, thus, for example, in a classically small energy range of size h there are many levels (of order $\hbar^{-(N-1)}$); this will be important later. And second, a rough quantization rule can be found by realizing that the integral of $d(E)$ is the *spectral staircase*

$$\mathcal{N}(E) \equiv \sum_n \theta(E - E_n) = \int_{-\infty}^{E} dE'\, d(E') \tag{11.6}$$

where θ is the unit step; the rule, expressing the idea that the smooth curve of the average staircase might intersect the steps halfway, on average, is then

$$(n + \tfrac{1}{2}) = \langle \mathcal{N}(E_n)\rangle = \Omega(E_n)/h^N \tag{11.7}$$

The above rule is rough because it fails to describe the fine-scale *fluctuations* in the levels (in graphs of the E_n as a function of a parameter on which H depends, these fluctuations appear as avoided crossings[24-26]). To describe these fluctuations it is necessary to employ statistics which (unlike $\langle d\rangle$ and $\langle \mathcal{N}\rangle$) involve correlations between nearby levels, that is, on scales $\hbar^N$. Such fluctuation measures have been devised in *random-matrix theory*[27] and applied to sequences of excited resonance levels of atomic nuclei. The fluctuation statistics depend not on the raw spectrum levels $\{E_n\}$ but on the "unfolded" spectrum of levels $\{x_n\}$ which have been scaled so as to have unit mean spacing. Thus

$$x_n + \tfrac{1}{2} \equiv \langle \mathcal{N}(E_n)\rangle \tag{11.8}$$

[without the fluctuations, equation (11.7) shows that x_n would be simply n]. Two particularly useful statistics are the probability distribution $P(S)$ of the *level spacings* $\{S_n \equiv x_{n+1} - x_n\}$, and the *spectral rigidity*[28-30]

$$\Delta(L) \equiv \left\langle \min \frac{1}{L} \int_{x-L/2}^{x+L/2} d\zeta [\mathcal{N}(\zeta) - A - B\zeta]^2 \right\rangle \tag{11.9}$$

(this is the least-squares deviation of the staircase from a straight line, over a range of L mean spacings, averaged over an interval of energies x that includes many levels). $P(S)$ is useful in describing spectral correlations on the finest scales—i.e., between neighboring levels—and $\Delta(L)$ is useful for describing how spectral correlations depend on range—i.e., large or small L.

When spectral statistics are computed for sequences of levels of Hamiltonian systems with classical limits, a remarkable "experimental" fact emerges: the statistics display *universality* and the spectral universality class depends on the chaology of the classical orbits. The universality classes are:

(a) *Classically integrable systems.* Here the spectral statistics are those of a *Poisson*—i.e., uncorrelated random—distribution of levels.[30,31] At first sight it is surprising that the quantum conditions (11.1) can give rise to a random sequence, but the surprise dissipates with the realization that neighboring levels E_n, E_{n+1} can have very different sets of quantum numbers $\{n_i\}$. For Poisson statistics,

$$P(S) = \exp(-S) \qquad \text{and} \qquad \Delta(L) = L/15 \tag{11.10}$$

(b) *Classically chaotic spinless (or integral-spin) systems with time-reversal symmetry.* Here the spectral statistics are those of the *Gaussian orthogonal ensemble* (GOE), which consists[27] of real symmetric matrices whose elements are Gauss-distributed so as to make the statistics of the ensemble invariant under orthogonal rotations. Only real symmetric matrices are involved because time-reversal symmetry implies that the wave functions are real. For the GOE, to a close approximation,

$$P(S) \approx \frac{\pi}{2} S \exp(-\pi S^2/4) \tag{11.11}$$

and

$$\begin{aligned} \Delta(L) & L/15 \qquad (L \ll 1) \\ & \to \frac{\ln L}{\pi^2} - 0.00695 \qquad (L \gg 1) \end{aligned} \tag{11.12}$$

(c) *Classically chaotic systems without time-reversal symmetry.* This is in a sense the generic case which best justifies the label "quantum chaos." Time-reversal symmetry (T) can be broken most simply by magnetic fields, either smoothly-varying[32] or consisting of a single (Aharonov-Bohm) flux line.[33] Here the spectral statistics are those of the Gaussian unitary ensemble (GUE),[27] of complex Hermitian matrices whose elements are Gauss-distributed so as to make the statistics of the ensemble invariant under unitary transformations. For the GUE, to a close approximation,

$$P(S) \approx \frac{32 S^2}{\pi^2} \exp(-4S^2/\pi) \tag{11.13}$$

and

$$\Delta L \to L/15 \qquad (L \gg 1)$$
$$\to \frac{\ln L}{2\pi^2} + 0.05902 \qquad (L \gg 1) \tag{11.14}$$

Before anticipating that a system without T will have GUE statistics, care must be taken to determine whether it has any geometric symmetries, because these can act so as to mimic T-symmetry and generate levels with GOE statistics; in the theory of this "false time-reversal symmetry-breaking"[34] it is shown that for GUE the system must possess no antiunitary symmetry operator $\hat{A}$ [27,35] (commuting with H) and satisfying $\hat{A}^2 = 1$ or $\hat{A}\hat{A}^* = 1$ (T is represented in position representation by the operator A = complex conjugation). A set of numbers recently discovered to have GUE statistics is the imaginary parts of zeros of Riemann's zeta function[36]; this is surprising and suggestive.[37]

(d) *Classically chaotic systems with half-integer spin and with T* (or, more generally, chaotic systems with an antiunitary symmetry satisfying $\hat{A}^2 = -1$). Here there are so far no numerical experiments (I am planning one now) but the spectral statistics are expected to be those of the *Gaussian symplectic ensemble* (GSE),[27] of quaternion real Hermitian matrices whose elements are Gauss-distributed so as to make the ensemble invariant under symplectic transformations. For the GSE, to a close approximation,

$$P(S) \approx \frac{2^{18} S^4}{3^6 \pi^3} \exp(-64S^2/9\pi) \tag{11.15}$$

and

$$\Delta(L) \to L/15 \qquad (L \ll 1)$$
$$\to \frac{\ln L}{4\pi^2} + 0.07832 \qquad (L \gg 1) \tag{11.16}$$

That completes the list of universality classes. But I now reveal that life is really not so simple, and describe two ways in which universality is compromised. First, most classical systems are neither purely regular nor purely chaotic,[1] but exhibit mixed (or, in the jargon, "KAM") behavior in which some orbits are regular and some predictable, depending on initial conditions. Such cases are important in quantum mechanics because they correspond to the anharmonically coupled oscillators describing vibrating molecules and to atoms in strong magnetic fields occurring astrophysically. It is natural to expect that in lowest approximation the spectral statistics will interpolate between those of the Poisson and the appropriate random-matrix universality classes, to a degree which depends on the relative phase-space volumes of regions of regular and chaotic motion; a theory along these lines[38] is supported by numerical experiments.[39] Second, even for purely regular or purely chaotic systems the domain of universal behavior is limited to energy ranges not exceeding a quantity of order $\hbar$; for the rigidity $\Delta(L)$, this means that universality holds when $L < L_{max} \sim \hbar^{-(N-1)}$, so that in the semiclassical limit the domain of universality shrinks to zero in energy but nevertheless extends over infinitely many levels. When $L > L_{max}$ numerical experiments[40] (so far restricted to integrable systems) show, and a theory[30] (for both integrable and chaotic systems) explains, that $\Delta(L)$ does not continue to increase as in equations (11.10), (11.12), (11.14), and (11.16), but saturates at nonuniversal values characteristic of the particular system.

In spite of these caveats, the universality of semiclassical spectra is a remarkable phenomenon that demands explanation. One class of theories[41,42] considers the energies to depend on a parameter t which is regarded as akin to a time variable, and the "motion" of the eigenvalues $\{E_n(t)\}$ on the E axis is put into correspondence with the statistical mechanics of particles on a line. These theories can be made to generate random-matrix behavior but the derivations rest on statistical assumptions about the matrix elements of the t derivatives of $\hat{H}$ between different eigenstates. It is desirable to understand spectral statistics directly, without introducing parameters or extra statistical assumptions. Some progress has been made, as will now be described.

The behavior of $P(S)$ as $S \to 0$ can be related to the codimension K of degeneracies when the system is embedded in an ensemble of similar ones,[43,21-24] where K is the number of parameters that must be varied to produce a degeneracy: for separable systems $K = 1$, for real symmetric matrices $K = 2$, for complex Hermitian matrices $K = 3$, and for quaternion real matrices $K = 5$. The result is

$$P(S) \sim S^{K-1} \qquad \text{As } S \to 0 \tag{11.17}$$

and this agrees with equations (11.10), (11.11), (11.13), and (11.15). But K is only roughly related to the classical symmetries (subtleties arise from barrier penetration[44]) and a semiclassical understanding of $P(S)$ is still lacking.

The behavior of $\Delta(L)$, on the other hand, is rather well understood[30] in terms of a semiclassical theory. According to equation (11.9), $\Delta(L)$ is a quadratic functional of the spectral staircase (11.6). This can be expressed as its average $\langle \mathcal{N} \rangle$ [equation (11.7)] plus a series of correction terms which are oscillatory functions of E. Each such correction comes from a *closed orbit* of the classical system,[45-47] and gives an oscillation with energy period $\hbar/T$, where T is the time period of the orbit. So values of $L \ll L_{max}$, corresponding to energy scales $\ll \hbar$, correspond to *very long orbits*. In particular, any fixed L corresponds as $\hbar \to 0$ to periods of order $\hbar^{-(N-1)}$. But for these very long orbits there exist *universal sum rules*[48] which depend on the classical chaology, and it is these that enable the theory[30] to reproduce the random-matrix results (11.10), (11.12), and (11.14) [but not yet relation (11.16)]. When $L \gg L_{\max}$, the previously-mentioned breakdown of universality occurs and is explained by $\Delta(L)$ depending only on short closed orbits which, or course, differ from system to system.

Much work remains to be done in understanding semiclassical spectra. The most pressing and also fundamental problem is to discover whether the semiclassical sum over the closed orbits or a chaotic system can be extended (or interpreted, or analytically continued[37]) so as to describe the finest spectral scales such as those embodied in $P(S)$ (or even—we are entitled to hope—a complete quantization formula). Then there are "crossover" phenomena associated with the breakdown of universality when $L \sim L_{\max}$. Finally, higher spectral statistics, depending more than quadratically on $\mathcal{N}(E)$, should be studied semiclassically. It is likely that from the program outlined in the last two sentences there might emerge a statistic which, for chaotic systems, depends on the Kolmogorov-Sinai[1] entropy which is so important in classical chaology.

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