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Distribution of Energy Eigenvalues in the Irregular Spectrum

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The distribution of energy eigenvalues in the irregular spectrum is derived in the semiclassical limit $\hbar \to 0$ by use of a plausible assumption on the spatial distribution of the corresponding eigenfunctions.

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Percival[1,2] used the terms "regular" and "irregular" to distinguish between near-classical quantum systems whose classical motion is respectively quasiperiodic and ergodic. The distribution of energy eigenvalues in the regular spectrum has been obtained by Berry and Tabor[3]; it is random, with spacing between adjacent levels distributed à la Poisson. Here I determine the eigenvalue distribution in the irregular spectrum.

Berry and Tabor studied the regular spectrum in the semiclassical limit $\hbar \to 0$, using the formulas of semiclassical quantization. There are no such formulas for the irregular spectrum, and so a different approach is necessary. The energy-level pattern in the irregular spectrum is obtained by combining a natural assumption on the *spatial* pattern of "irregular" eigenfunctions—that all eigenfunctions of roughly the same energy look roughly the same—with the "equations of motion" governing the eigenvalues as $\hbar$ varies. One is led, as $\hbar \to 0$, to a statistical mechanics of energy eigenvalues.

Not all classically ergodic systems will have irregular eigenfunctions, even in the semiclassical limit; it is now well-known that classical chaos does not imply quantum chaos,[4-6] whatever the latter may be. For the rest of this paper the term "irregular" will be reserved for quantum systems having irregular eigenfunctions, without reference to the classical mechanics of such systems.

Let the Hamiltonian be $H = -\hbar^2 D + V$, where D is a real differential operator in $d > 1$ dimensions, V is the potential, and the spectrum of H is discrete. We may think, for example, of a single particle confined to a d-dimensional potential well. Let $\hbar^2 = \exp(-\lambda)$, so that $\hbar \to 0$ is $\lambda \to \infty$, and let $\{\varphi_n(\lambda)\}$ be orthonormal real eigenfunctions of H, with energies $\{E_n(\lambda)\}$. We may assume that the energy spectrum is nondegenerate; accidental degeneracies will be broken as λ varies, while symmetry-enforced degeneracies imply that the quantum system cannot be considered ergodic. Then the equations of motion for $E_n(\lambda)$ and the various matrix elements $V_{mn}(\lambda) = (\varphi_m(\lambda), V\varphi_n(\lambda))$ are

$$dE_n/d\lambda = V_{nn} - E_n, \tag{1}$$

$$dV_{nn}/d\lambda = 2\sum_{m \neq n} V_{mn}{}^2/(E_n - E_m), \tag{2}$$

$$\frac{dV_{mn}}{d\lambda} = \sum_{l \neq m,n} V_{ml} V_{ln}[(E_m - E_l)^{-1} + (E_n - E_l)^{-1}] + \frac{V_{mn}(V_{mm} - V_{nn})}{(E_n - E_m)}. \tag{3}$$

To see how the spatial pattern of the eigenfunctions can determine the spectral pattern of the eigenvalues, consider first the regular regime. Here two eigenfunctions of roughly the same energy typically look very different: They differ greatly in the division of energy among the vibrational modes in potential V. Where these functions overlap in space, they beat violently against each other, and the matrix element V_{mn} of the smooth potential V is very small—typically, exponentially small with $\hbar$, $V_{mn} = O(\exp[-(\cdots)/\hbar])$. Compared to the energy level spacings, which are $O(\hbar^d)$, such a matrix element is zero. Further, the diagonal elements V_{nn} and V_{mm} are typically very different, because states n and m, with very different spatial distributions, sample very different regions of the potential; the order of magnitude of the difference $V_{nn} - V_{mm}$ is independent of $\hbar$.

Consider N consecutive levels centered around E_0. Each state will couple strongly only to states that do not differ greatly from it in the assignment of vibrational quantum numbers; these states will differ in energy by $O(\hbar)$ from E_0; therefore for small $\hbar$ we expect all V matrix elements among the N states to be effectively zero. As λ varies, each energy $E_n(\lambda)$ moves with a different "velocity" $dE_n/d\lambda$, according to Eq. (1), the velocities being $O(1)$ as $\hbar \to 0$. The "acceleration" $d^2E_n/d\lambda^2$ is no greater than $O(\hbar^{-1})$, according to Eq. (2), and so if we follow these energies for $\Delta\lambda = O(\hbar^{1+\epsilon})$, $\epsilon > 0$, we may consider the velocities constant. Think of the energies as positions in one dimension, and λ as the time: We have a very dense gas—"mean free path" $= O(\hbar^d)$—of one-dimensional free particles making vast numbers of free-particle collisions during the interval for which we follow them. At any instant—that is, at any particular value of $\hbar$—we expect the energy levels to distribute themselves along the energy axis as one-dimensional free particles distribute themselves along the line: at random, with a Poisson distribution of nearest-neighbor spacings.

Obviously this argument is no substitute for the beautiful analysis of Berry and Tabor,[3] but it conveys the essence of the situation.

In the irregular regime the assumption is that all eigenfunctions of roughly the same energy look roughly the same: Each is spread over the entire classically allowed region of configuration space appropriate to its energy, with coarse-grained probability density that agrees well at each point in space with the classical microcanonical density at that energy. This is the standard hypothesis for the irregular regime[7-10] and is usually expressed as the expectation that the Wigner phase-space densities associated with irregular eigenfunctions of energy E will in some sense converge, as $\hbar \to 0$, to the classical microcanonical density at energy E. Support for this hypothesis has been published by Hutchinson and Wyatt,[11] who computed the Wigner distribution associated with eigenstates in the Henon-Heiles potential, finding reasonable agreement with microcanonical distributions at high energy, where the classical motion is irregular.

The irregular-eigenfunction hypothesis has two important implications for the eigenvalue equations of motion. First, there are no strong selection rules in the irregular regime[1,2]: We cannot throw away off-diagonal V matrix elements, because all these elements are of the same order of magnitude in $\hbar$. Second, the diagonal V matrix elements are roughly the same for states of roughly the same energy, so that the energy eigenvalue curves $E_n(\lambda)$ run roughly parallel to each other. It is fluctuations about the mean drift of the energy levels that determine the distribution of eigenvalues in the irregular spectrum.

Let us estimate orders of magnitude. As in the regular regime, a given state n couples mainly to states that lie within $O(\hbar)$ in energy from E_n; outside this range, the mismatch in local wavelength kills the V_{mn} integral. Since the mean level spacing is $O(\hbar^d)$, state n couples to $O(\hbar^{1-d})$ others, as Percival first observed.[1] From the sum rule $\sum_{m\neq n} V_{mn}^2 = (\varphi_n, \{V^2 - V_{nn}^2\}\varphi_n) = O(1)$, we see that $V_{mn}^2 = O(\hbar^{d-1})$. The fluctuations in diagonal matrix elements should be of the same order of magnitude, $V_{nn}^2 - \langle V_{nn}\rangle^2 = O(\hbar^{d-1})$.

In the regular regime, with strong selection rules, V matrix elements between nearby states are small compared to the mean level spacing; in the irregular regime, with no selection rules, they are large.

Let us now follow a number $N \gg 1$ of consecutive levels, centered around E_0 at λ_0, for a short interval $\Delta\lambda$ centered on λ_0. We shall imagine doing this many times, holding N and E_0 fixed while $\lambda_0 \to \infty$; by a "short" interval $\Delta\lambda$ we mean $\Delta\lambda = O(\hbar_0^{\epsilon})$, $\epsilon > 0$, where $\hbar_0^2 = \exp(-\lambda_0)$. We remove the mean level drift by defining $e_n(\lambda) = E_n(\lambda) - E(\lambda)$, where $E(\lambda) = E_0 + (\lambda - \lambda_0)(\langle V\rangle_0 - E_0)$ and $\langle V\rangle_0$ is the classical microcanonical average of V at E_0,

$$\langle V\rangle_0 = \int d\Gamma\, V\delta(E_0 - H)/\int d\Gamma\, \delta(E_0 - H).$$

Then $v_{nn} = V_{nn} - \langle V\rangle_0$ is the fluctuation in the diagonal matrix element, and, with the notation $v_{mn} \equiv V_{mn}$ for the off-diagonal elements, Eqs. (1)–(3) still hold when all E's and V's are replaced by e's and v's.

These equations are now modified in the following three ways: (1) e_n is dropped from the right-hand side of Eq. (1). Since e_n is $O(\hbar_0{}^d)$ and we shall follow the levels for an interval $\Delta\lambda = O(\hbar_0{}^\epsilon)$, this approximation is inconsequential in the limit $\hbar_0 \to 0$. (2) We allow each level to interact only with its N' nearest neighbors; i.e., we set $v_{mn} = 0$ for $|m-n| > N'$, where $1 \ll N' \ll N$. Consider Eq. (2). The terms we keep are $O(\hbar_0{}^{-1})$. So are all the terms in the sum we drop; but in this sum interactions of state n with higher-energy states almost cancel interactions with lower-energy states, because of the energy denominator. In fact, in the sum we may replace $v_{mn}{}^2$ by its average over a number N'' of states m, where $1 \ll N'' \ll N'$, and this average should be a smooth function of e_m and e_n, concentrated on the range $|e_m - e_n| = O(\hbar_0)$ and smoothly dependent on the mean energy $(e_m + e_n)$: $\langle v_{mn}{}^2\rangle = \hbar_0{}^{d-1} f((e_m - e_n)/\hbar_0, (e_m + e_n))$, where $f(x, y)$ is independent of $\hbar_0$ and even in x because the v matrix is symmetric. With the notation $\langle \Delta E\rangle_0$ for the mean level spacing at λ_0, the sum over m that we neglect is, to terms of order $\hbar_0{}^{-1}$,

$$\sum_{|m-n|>N'} \frac{v_{mn}{}^2}{(e_n - e_m)} \cong \hbar_0{}^{d-1} \sum_{|m-n|>N'} \frac{f((e_m - e_n)/\hbar_0, (e_m + e_n))}{e_n - e_m}$$

$$\cong \hbar_0{}^{d-1} \sum_{|m-n|>N'} \frac{f((e_m - e_n)/\hbar_0, 0)}{e_n - e_m}$$

$$\cong \hbar_0{}^{-1} \left(\frac{\hbar_0{}^d}{\langle \Delta E\rangle_0}\right) \int_{|e_m - e_n|>N'\langle \Delta E\rangle_0} de_m \frac{f((e_m - e_n)/\hbar_0, 0)}{e_n - e_m} = 0,$$

and therefore negligible beside the $O(\hbar_0{}^{-1})$ terms that we keep. Similar considerations justify the same approximation in Eq. (3). (3) To make the problem finite, we adopt "periodic boundary conditions"; i.e., we imagine N energy levels $e_1 < \ldots < e_N$ arranged on a circle of length $N\langle \Delta E\rangle_0$, each level interacting with its N' nearest neighbors according to Eqs. (1)–(3), under the convention that $e_{N+j} = e_j + N\langle \Delta E\rangle_0$.

Equations (1)–(3), with the modifications noted above, scale nicely with $\hbar_0$. Let $\tau = \lambda/\hbar_0{}^{(d+1)/2}$ and define new variables $x_n(\tau)$ and $u_{mn}(\tau)$, which are $O(1)$ in magnitude, by

$$e_n(\lambda) = x_n(\tau)\langle \Delta E\rangle_0, \quad v_{mn}(\lambda) = u_{mn}(\tau)\langle \Delta E\rangle_0/\hbar_0{}^{(d+1)/2}.$$

Then

$$dx_n/d\tau = u_{nn}, \tag{4}$$

$$du_{nn}/d\tau = 2\sum u_{mn}{}^2/(x_n - x_m), \tag{5}$$

$$du_{mn}/d\tau = \sum u_{ml}u_{ln}[(x_m - x_l)^{-1} + (x_n - x_l)^{-1}] + u_{mn}(u_{mm} - u_{nn})/(x_n - x_m). \tag{6}$$

We are now dealing with N points $x_1 < \ldots < x_N$ on a circle of length N. The interval $\Delta\lambda$ over which we follow these points shrinks to zero as $\hbar_0 \to 0$, but the scaled interval $\Delta\tau$ goes to infinity. To find the distribution of energy levels in the irregular spectrum—to find the distribution of the N points $\{x_n\}$ on the circle of length N—we must integrate Eqs. (4)–(6) for an arbitrarily long "time" τ. We should therefore apply the methods of classical statistical mechanics.

The "dynamical variables" are the N $\{x_n\}$, the N diagonal elements $\{u_{nn}\}$, and the NN' off-diagonal elements $\{u_{mn}\}$. Consider the continuity equation $\partial\rho/\partial\tau + \mathrm{div}(\rho v) = 0$ for a probability density in the space of these variables. We look for an "equilibrium" solution, $\partial\rho/\partial\tau = 0$. The flow according to Eqs. (4)–(6) is not divergence-free, so that an equilibrium ρ will not be a constant of the motion; but notice that

$$\mathrm{div} v = \sum \frac{\partial \dot{u}_{mn}}{\partial u_{mn}} = \sum \frac{u_{mm} - u_{nn}}{x_n - x_m}$$

$$= \sum \frac{\dot{x}_m - \dot{x}_n}{x_n - x_m} = -\frac{d}{d\tau} \ln \prod |x_n - x_m|,$$

where the sum and the product are over interacting pairs of levels, each pair counted once. This implies that the continuity equation can be written as $(d/d\tau)(\rho/\prod|x_n - x_m|) = 0$ and therefore that any ρ of the form $c\prod|x_n - x_m|$, where c is a properly normalized constant of the motion, will be an equilibrium density. There are many constants of the motion: motion according to Eqs. (4)–(6)

generates a real orthogonal transformation of the u matrix; all the orthogonal invariants—tr$u$, tru^2, etc.—are constants of the motion. Let us assume there are no others. Then any equilibrium ρ is a product of a function of u matrix elements and the factor $\prod|x_n - x_m|$. The eigenvalue distribution is therefore independent of the constant of the motion c, and the joint distribution of N eigenvalue positions x_n on the circle of length N is

$$p(x_1, \ldots, x_N) \propto \prod|x_n - x_m|. \quad (7)$$

Equation (7) is the principal result of this paper.

What is the level-spacing distribution predicted by Eq. (7)? In the proper limit—$N \to \infty$, then $N' \to \infty$—it must be the same as in Dyson's "circular ensemble,"[12] which involves particles on a circle with logarithmic potential of interaction, the distance between particles being Cartesian distance in two dimensions rather than distance around the circle. Dyson's level-spacing distribution in turn is equal[13] to the limiting distribution in the "real Gaussian ensemble" which has been beautifully analyzed by Mehta[14] and by Gaudin[15] and found to be very close to the Wigner distribution $p(S) = (\pi/2)S \exp(-\pi S^2/4)$, where $S = \Delta E/\langle \Delta E \rangle$. There is some evidence for the Wigner distribution from recent numerical work on the quantum mechanics of classically ergodic two-dimensional "billiard" problems: McDonald and Kaufman[16] and Casati, Valz-Gris, and Guarneri[17] calculated eigenvalues for the stadium, while Berry[18] studied the Sinai billiard, and in all cases the computed $p(S)$ agrees with the Wigner distribution to within the statistical uncertainty in the computed distribution. On the other hand, Buch, Gerber, and Ratner[19] computed $p(S)$ for a two-dimensional model of Morse oscillators with strong kinetic coupling and found that the data were fitted significantly better by a Brody distribution[20] differing somewhat from the Wigner form; the authors speculate that this means that their coupled oscillator model is not "fully chaotic."

More extensive numerical work on eigenvalue distributions in the irregular spectrum would clearly be helpful; for one thing, it would be nice to have numerical evidence that the Mehta-Gaudin spacing distribution is to be preferred to the Wigner distribution, although a simple estimate of the size of the calculation needed is discouraging.[21] There are also a number of interesting formal questions left. Here are two: (1) In the regular spectrum, successive level spacings are uncorrelated; this is not so in the irregular spectrum. What is the correlation predicted by Eq. (7)? (2) Equations (4)–(6) have an equilibrium solution, $u_{nn} = 0$, $u_{mn} = c$, $x_n = n$; i.e., equal-strength interactions and equally spaced energy levels. This is, of course, the spectral pattern in any narrow energy range for a class of familiar ergodic systems: one-dimensional vibrations in a simple potential well. Is this solution stable? If so, how does that affect the statistical mechanics leading to Eq. (7)?

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[21]Let us determine the level-spacing distribution by diagonalizing an $N \times N$ "irregular matrix" and presenting the data in a histogram. Except in the tail of the distribution, the Mehta-Gaudin and Wigner distributions differ by only (4–5)%, so that in a given bar of the histogram, containing a fraction f of the distribution, we will want to be sure—at, say, the 95% confidence level—that we are within 2% of the correct value. An elementary calculation [see, e.g., W. Feller, *An Introduction to Probability Theory and Its Application* (Wiley, New York, 1957), 2nd ed., Vol. 1] gives the estimate $N \cong 4(1-f)/(0.02)^2 f$. For a histogram with 20 bars, $f \cong 0.05$ per bar and $N \cong 200\,000$. In the tail, the Mehta-Gaudin and Wigner distributions differ by circa 20%, and so a calculation accurate to 10% will suffice, but only circa 1% of the distribution is in the tail ($f = 0.01$), so that $N \cong 4/(0.01)^2 f \cong 40\,000$. In either case, it is not a small calculation.