Catastrophe and Stochasticity in Semiclassical Quantum Mechanics

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1. Introduction

The symposium talk was an account of material already published [1,2,3,4]. Therefore this contribution will be an extended summary, in the form of a series of assertions for which justification will be found in the papers cited.

As the classical limit (Planck's constant $\hbar \to 0$) is approached, quantum bound states bifurcate into two universality classes distinguished by the morphologies of their wave functions $\psi(\underline{q})$. PERCIVAL [5] calls these 'regular' and 'irregular' states; they are associated with different sorts of classical motion as foreseen by EINSTEIN [6]. In what follows, the classical motion is Hamiltonian, with N degrees of freedom and hence a 2N-dimensional phase space.

Regular states are associated with integrable motion [7,8,9], that is motion restricted by the existence of N constants of motion to N-dimensional tori in phase space. The projections of these tori onto the coordinate space $\underline{q}$ are singular on caustics that generically take the form of the catastrophes classified by Professor THOM [10].

Irregular states are associated with ergodic classical motion, that is motion where only the Hamiltonian is conserved, so that the system explores the whole 2N-1-dimensional energy surface in phase space. Neighbouring trajectories separate exponentially fast (if $N > 1$) and this implies that ergodic motion is stochastic. The projections of stochastic regions onto $\underline{q}$ are bounded by 'anti-caustics' [1] whose strength is not infinite and which need not be catastrophes. The distinction between caustics and anticaustics is analogous to the distinction between the boundaries of projections from 3 space to 2 space of surfaces and volumes respectively.

These classical motions are connected with quantum mechanics via the Wigner function $W(\underline{q}, \underline{p})$, defined for a state $\psi(\underline{q})$ by

$$W(\underline{q}, \underline{p}) \equiv \left(\frac{2\pi}{\hbar}\right)^N \int d^N X \, e^{-i\underline{p}\cdot\underline{X}/\hbar} \quad \psi(\underline{q} - \tfrac{1}{2}\underline{X}) \quad \psi^*(\underline{q} + \tfrac{1}{2}\underline{X}). \tag{1}$$

Its projection 'down' $\underline{p}$ onto $\underline{q}$ gives the coordinate probability density:

$$\int d^N p \, W(\underline{q}, \underline{p}) = |\psi(\underline{q})|^2, \tag{2}$$

and its projection 'along' q gives the momentum probability density.

The assumption is made that for typical semiclassical quantum energy eigenstates $W(\underline{q}, \underline{p})$ is localised on the manifolds in phase space that are explored by typical classical orbits, that is tori for integrable systems and whole energy surfaces for ergodic systems. Each quantum state has its own manifold, selected by a quantum condition. For tori the quantum condition [11,12,8] is that the action $\oint \underline{p} \cdot d\underline{q}$ round each irreducible cycle must be a half-integer multiple of $2\pi\hbar$. For energy surfaces the quantum condition is unknown. (Conjecture: the phase space volume enclosed by the energy surface E_n is quantised by

$$\int_{E_n > \text{Hamiltonian}} d^N q \int d^N p = (n + \mu)\, h^N, \tag{3}$$

where n is an integer and μ a constant. This would lead for these ergodic systems to an asymptotically regular sequence of levels in sharp contrast to the clustering [13] generic in integrable systems.)

The status of the assumption that $W(\underline{q}, \underline{p})$ is localised on the typical classical orbits is as follows: for integrable systems W is known to condense onto a delta function on a torus when $\hbar = 0$,[2,14]. Moreover, when $\hbar$ is small but not zero more refined asymptotic results [2,3,15] show W to take the form of 'Airy' fringes decorating the torus. For ergodic systems it is still a conjecture that the W corresponding to an eigenstate condenses onto the energy surface [1,16]. (An alternative conjecture, due to GUTZWILLER [17,18], is that quantum states in ergodic systems correspond to the exceptional (but dense) unstable closed orbits. My opinion is that it is implausible for quantum conditions to select orbits that are both untypical and unstable, and indeed GUTZWILLER's own analysis yields not delta-function energy levels, but a spectrum of Lorentzian resonances of width $\hbar$, strongly suggesting that what he has found are not true bound states but 'quasi-modes' [19,20] which decay after times of order $\hbar^{-1}$.)

Making the assumption about W leads easily [1,16] to strikingly different predictions about the morphology of regular and irregular states. The probability density $|\psi(\underline{q})|^2$, smoothed over the (semiclassically very rapid) oscillations near $\underline{q}$, is given by (2) simply by projecting the classical torus or energy surface onto $\underline{q}$. The pattern of oscillations of ψ near $\underline{q}$, as embodied in the autocorrelation function [1] of ψ, is obtained from the momenta $\underline{p}$ of intersections of the fibre through $\underline{q}$ with the classical manifold W (by de Broglie's rule, each $\underline{p}$ gives an oscillatory contribution to ψ, with wave vector $\underline{k} = \underline{p}/\hbar$). The predictions are:

Regular states have probability densities rising to high values on caustics at classical boundaries, and are decorated with vivid patterns of highly anisotropic interference oscillations with a discrete spectrum of wave vectors.

Irregular states have probability densities falling to zero (or, when $N = 2$, remaining constant) on anticaustics at classical boundaries, and are decorated with more moderate oscillations (like those of a Gaussian random function) which for ergodic systems are statistically isotropic and which have a continuous spectrum of wave vectors.

A generic Hamiltonian classical system with $N > 1$ is neither fully integrable nor fully ergodic [7,8,9]. Some orbits lie on N-tori while others explore 2N-1-dimensional stochastic regions of the energy surface. In the corresponding quantum systems this should lead to a mixed spectrum, with some states regular and some irregular. If the system is quasi-integrable, that is if its departure from integrability depends on a perturbation parameter ε, then I have speculated [2,8] that there should be three semiclassical régimes depending on the value of $\hbar$ in comparison with ε (both quantities being small).

It is not easy to test these predictions by actual or numerical experiment. In nature, irregular states (of, say, vibrating asymmetric molecules) would be vulnerable to perturbation [5]. In the computer, the small value of $\hbar$ means that ψ oscillates rapidly and is vulnerable to numerical noise. The regular and irregular states are emergent morphologies; they appear as $\hbar \to 0$ and for finite $\hbar$ are encoded in the Schrödinger equation in a form too economical to be easily reconstructed.

To get over this computational problem we have invented quantum maps [4, see also 21]. Instead of quantising the simplest stationary Hamiltonian system with generic properties, which has $N = 2$, we have directly quantised a class of area-preserving maps of the plane. These are obtained by taking a system with $N = 1$ but with Hamiltonian periodic in time with period T, and taking snapshots of the phase plane q,p at times nT where n is an integer. Such maps can be made to exhibit both integrable and stochastic behaviour. The corresponding quantum systems evolve under the action of a unitary operator and the mapping of wave functions ψ is described by an integral equation.

To see a continuous transition from a regular to an irregular ψ, an initial state (not an eigenfunction of the map) was chosen to correspond to a curve C in qp whose points map stochastically. Under the classical map, C soon develops complication by throwing off 'tendrils' snaking violently back and forth. In the projection of C onto q, caustics proliferate rapidly and when they are closer together than the de Broglie wavelength they no longer contribute individually to ψ. In the computer-generated pictures [4] it is easy to see the transition from regular states, with intense caustics and spectrally pure oscillations, to irregular states, with anti-caustics and oscillations with multiple scales. Fig. 1 shows one example taken from several presented in [4], where a detailed discussion is given of the relation between C and ψ. (Actually, the tendril is one of two morphological elements in C's developing complication. The other is the 'whorl,' a wrapping of C around itself, associated not with stochasticity but with the smooth invariant curves (tori) associated with stable regions of the map. Again details are given in [4].)

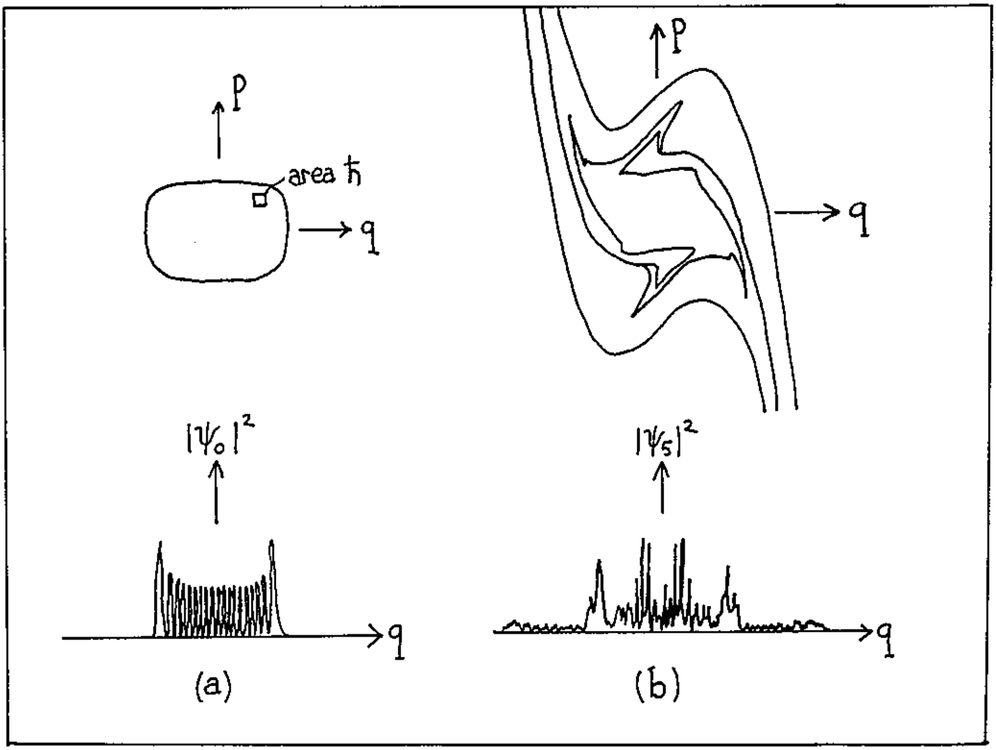

Fig. 1 Transition of state ψ from regular (a) to irregular (b) after five iterations of a quantum map, as computed by Dr. M. Tabor. The state is represented by the classical curve C shown above, which develops 'tendrils' under iteration.

In an extension of the quantum map formalism to phase spaces with the topology of a 2-torus, we [22] have succeeded in quantising 'Arnol'd's cat' [7,8,9], a map that is completely ergodic. To achieve this it is necessary to quantise Planck's constant by h = area of torus/M, where M is an integer. The quantum cat map has M eigenstates and in the semiclassical limit $M \to \infty$ neither the distribution of eigenvalues nor the eigenfunctions $\psi(q)$ themselves can be described by smooth function but instead seem to have a 'number-theoretic' dependence on M.

The two sorts of quantum state discussed here show how Planck's constant plays a much more subtle role than previously supposed. For regular states, $\hbar$ imposes extra detail, in the form of quantum oscillations, on a classical background that is smooth apart from isolated caustic singularities. For irregular states, however, $\hbar$ acts as a quantum smoothing parameter on a classical orbit structure which because of stochasticity has detail down to arbitrarily fine scales.

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