

INTENSITY MOMENTS OF SEMICLASSICAL WAVEFUNCTIONS

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For normalized wavefunctions $\psi(q)$ of N coordinates q , we obtain semiclassical approximations to the moments $I_m \equiv \int dq |\psi(q)|^{2m}$, as a measure of the intensity variations of ψ . If ψ is a regular state, associated with an N -dimensional phase-space torus T , I_m diverges as $\hbar \rightarrow 0$ because of strong and rapidly-varying intensities at caustic singularities C , as follows: if C is a fold catastrophe, $I_m \sim F_m/\hbar^{(m-2)/3}$ if $m \geq 3$ and $I_2 \sim F_2 \ln(B/\hbar)$; if C is a cusp point, $I_m \sim C_m/\hbar^{(3m/2-1/2)}$; if C is a hyperbolic umbilic 'corner' point, $I_m \sim H_m/\hbar^{2(m-2)/3}$ if $m \geq 3$ and $I_2 \sim H_2 [\ln(B/\hbar)]^2$, the constants F_m , C_m and H_m are evaluated explicitly in terms of diffraction catastrophe integrals and the geometry of T . If ψ is a chaotic state, associated with a phase-space region of dimensionality $> N$ (e.g. the energy surface of an ergodic system), $I_m \rightarrow \text{constant}$ as $\hbar \rightarrow 0$ because the (moderate) intensity fluctuations arise not from caustics but from incoherent interference of many de Broglie waves.

1. Introduction

Evidence is accumulating to support Percival's conjecture [1] that in the semiclassical limit (i.e. as Planck's constant $\hbar \rightarrow 0$) the forms of quantum-mechanical wavefunctions ψ are very different for states associated with regular and irregular classical motion. By analytical reasoning, Berry [2, 3] and Voros [4] predicted that for regular states, i.e. those associated with classical phase-space tori, ψ would have an anisotropic pattern of oscillations and $|\psi|^2$ would rise to large values on caustics; for irregular (chaotic) states, i.e. those associated with phase-space regions larger than tori (for example the whole energy surface in the case of an energy eigenstate of an ergodic system), ψ would have a random pattern of oscillations and be bounded by anticaustics. Computations of ψ show these differences vividly: compare, for example, fig. 8 of Davis and Heller [5] with fig. 1 of McDonald and Kaufman [6].

Our purpose here is to study one aspect of these two asymptotically emergent universality

classes of wavefunction, namely the *variations* in probability density $|\psi(q)|^2$ across the N -dimensional configuration space $q = (q_1 \dots q_N)$; in what follows, N will often be 1 or 2. The variations are embodied in the behaviour as $\hbar \rightarrow 0$ of the *moments* I_m , defined by

$$I_m \equiv \int dq |\psi(q)|^{2m}, \quad (1)$$

where, of course, normalization gives $I_1 = 1$.

Where classical phase-space trajectories fill tori, the q -space trajectories envelop caustics, which are the singularities of the projections of the tori (Ozorio de Almeida and Hannay [7] give a detailed study of these for $N = 2$). On the caustics, $|\psi|^2$ is large and when this effect is magnified by raising to the m th power the caustics dominate the integrals (1) for I_m . The analysis of sections 2–6 will show how as $\hbar \rightarrow 0$ I_m varies according to a power law or logarithmically, in universal ways which depend only on m and the nature (diffeotype) of the caustic singularities when classified as catastrophes [7, 8]; these \hbar -dependences are multiplied by factors involving the geometry of the torus. This way of thinking about quantum waves was inspired by similar 'singularity-dominated strong

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fluctuations' in short-wave optical propagation in a random medium, i.e. twinkling [8–10, 19].

For chaotic classical motion these singularities, and the associated strong fluctuations in $|\psi|^2$, do not occur, and the I_m do not diverge as $\hbar \rightarrow 0$. This case will be studied in section 7.

Thus we hope to show how the moments reflect in a dramatic way the differences between the two sorts of quantum state

2. Torus states: caustic dominance and Maslov's representation

Consider an N -torus T in the $2N$ -dimensional phase space q, p (fig. 1). T is labelled by its N actions $I = (I_1 \dots I_N)$ defined as

$$I_j \equiv \frac{1}{2\pi} \oint_{\gamma_j} p \cdot dq \quad (1 \leq j \leq N), \tag{2}$$

where γ_j is the j th irreducible cycle of T . For each q , T is intersected at momenta $p^\mu(q; I)$, which define a multibranched generating function

$$S^\mu(q; I) \equiv \int_{q_0}^q p^\mu \cdot dq, \tag{3}$$

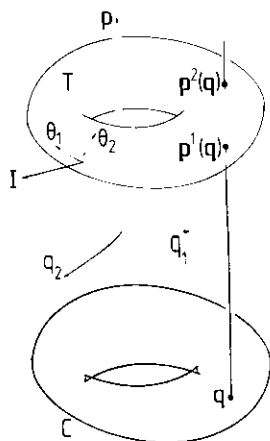


Fig. 1. Geometry of torus T and caustic C .

where the lower limit q_0 is arbitrary. Conjugate to I in a canonical transformation from q, p are angle variables θ on T at q , $p^\mu(q; I)$ the angles are

$$\theta^\mu(q; I) = \nabla_I S^\mu(q; I). \tag{4}$$

Provided the I satisfy quantization conditions (unimportant here), T can be associated with a quantum state whose normalized wavefunction, in simplest semiclassical approximation, is [3]

$$\psi(q) \approx \frac{1}{(2\pi)^{N/2}} \sum_\mu \left| \det_{ij} \left\{ \frac{\partial^2 S^\mu}{\partial q_i \partial I_j} \right\} \right|^{1/2} \times \exp \left\{ \frac{i S^\mu(q; I)}{\hbar} + \chi^\mu \right\}, \tag{5}$$

where here and hereinafter χ^μ denotes phases whose precise value we do not need to specify. Squaring, and ignoring as incoherent the interference between different branches μ , we obtain the probability density

$$|\psi(q)|^2 \approx \frac{1}{(2\pi)^N} \sum_\mu \left| \det \left\{ \frac{\partial^2 S^\mu}{\partial q_i \partial I_j} \right\} \right| = \frac{1}{(2\pi)^N} \sum_\mu \left| \frac{d\theta^\mu}{dq} \right|, \tag{6}$$

corresponding to the projection onto q of a (purely classical) distribution on T that is uniform in θ .

On the caustic C (fig. 1), formed by the singularity of the projection of T onto q , two or more branches θ^μ or p^μ coalesce, causing (6) to diverge. To see how this affects the moments I_m , we make a preliminary study of the typical case, where C is a fold catastrophe. First we show in a simple way that (6) has a square-root divergence. Let q_1 be a local coordinate perpendicular to C and let the local shape of T (which is smooth) be (fig. 2)

$$q_1 = \frac{K}{2} (p_1 - p_c)^2. \tag{7}$$

For $q_1 > 0$ there are two branches, namely $p_1^\pm =$

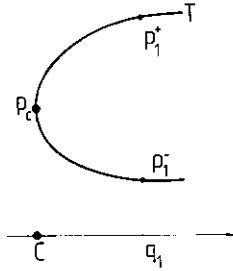


Fig. 2. Section of torus perpendicular to fold caustic.

$p_c \pm \sqrt{(2q_1/K)}$, and for each branch

$$\left| \frac{d\theta}{dq} \right| = \left| \frac{d\theta}{dp} \right| \left| \frac{dp}{dq} \right| \approx q_1^{-1/2}. \tag{8}$$

It is obvious from (1) that such a divergence would make the moments I_m infinite if $m \geq 2$. The true moments are, however, finite (provided $\hbar > 0$) and the infinities are artefacts of the approximations (5) and (6), which fail precisely at the most important places, i.e. on caustics.

The correct semiclassical behaviour of I_m must depend on the nature of the caustics arising by projection of T in each particular case. We shall consider only caustics which are stable under perturbation (in the sense that their diffeotype [8, 14] does not change) and hence classifiable as catastrophes. In one dimension ($N = 1$), T is a curve in the phase plane and its stable caustics on the q -axis are fold points. If $N = 2$ the stable caustics in the q plane are fold curves and cusp points. In the special but important case where $N = 2$ and the Hamiltonian is quadratic and isotropic in momentum, Ozorio de Almeida and Hannay [7] show that it is also stable for two caustic curves to meet at a finite angle in a hyperbolic umbilic ‘corner’ (these corners are enveloped by the ‘box orbits’ of Noid and Marcus [15, 16]).

For each singularity we shall in later sections calculate the contribution to I_m . A preliminary estimate of these contributions can be obtained from the scaling laws of catastrophe wave theory [8, 14]: as $\hbar \rightarrow 0$, $|\psi|$ diverges as $\hbar^{-\beta}$ and

the measure of the fringes shrinks as \hbar^γ , where β and γ are universal exponents characterising each catastrophe. Thus

$$I_m \approx \text{‘size’ of } |\psi|^{2m} \times \text{‘size’ of } q \\ \sim A_m \hbar^{-2m\beta} \hbar^\gamma = \frac{A_m}{\hbar^{2m\beta-\gamma}}. \tag{9}$$

We shall confirm these power-law dependences and calculate the factors A_m in all except certain delicate cases with $m = 2$, for which $2m\beta - \gamma = 0$ and I_m diverges logarithmically with \hbar^{-1} . Where several sorts of singularity are present, I_m is dominated [9] by the one for which $2m\beta - \gamma$ is greatest.

We shall employ a representation of ψ which gives the correct semiclassical behaviour across caustics. This was devised by Maslov [11, 12 see also 3 and 13], and begins by writing ψ as a Fourier integral, over one or more momenta, of the wave $\bar{\psi}$ in a mixed coordinate–momentum representation. Next, the fact is used that $\bar{\psi}$ can be validly approximated in a form analogous to (5), because the smoothness of T implies that caustics cannot simultaneously occur in q and p from a given phase-space point. The integral representation, to be written explicitly in sections to follow, enables us to calculate the semiclassical limit of I_m in full detail.

3. One-dimensional tori

Here T is a closed curve in the phase plane q, p (fig. 3) with caustics at positions q_c . I_m can be calculated from a wave approximated in the ‘Maslov’ form which near any q_c can be written

$$\psi_c(q) \approx \frac{e^{ix_c}}{2\pi\sqrt{\hbar}} \int dp \left| \frac{d\theta}{dp} \right|^{1/2} \exp\left\{ \frac{i}{\hbar} [S(p) + qp] \right\}, \tag{10}$$

where

$$S(p) = - \int_{p_c}^p q(p) dp \tag{11}$$

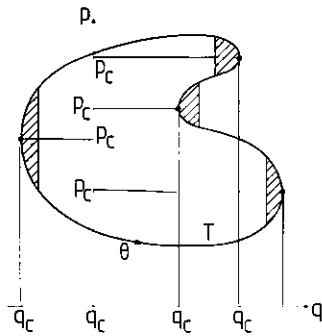


Fig. 3. One-dimensional torus T with caustic points q_c . The shaded areas correspond to the q -regions excluded in integrating to give I_2 .

and $q(p)$ is the local (singlevalued) equation for T . It is not hard to confirm by stationary-phase evaluation that away from q_c (10) reduces to the simple semiclassical form (5).

Near q_c , T is parabolic and so we can write

$$q(p) = q_c + \frac{K_c}{2} (p - p_c)^2, \tag{12}$$

where K_c is the curvature of T at the caustic. Therefore

$$S(p) = -\frac{K_c}{6} (p - p_c)^3. \tag{13}$$

Substituting in (10) and replacing $d\theta/dp$ by its (nonsingular) value at C gives

$$\psi_c \approx \frac{e^{i\chi_c}}{\hbar^{1/6}} \left| \frac{d\theta_c}{dp} \right|^{1/2} \frac{2^{1/3}}{K_c^{1/3}} \text{Ai} \left\{ -\frac{(q - q_c) 2^{1/3} \text{sign } K_c}{\hbar^{2/3} |K_c|^{1/3}} \right\}, \tag{14}$$

where Ai denotes the Airy function (fold diffraction catastrophe [8, 14]) defined by

$$\text{Ai}(x) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i(t^3/3 + xt)}. \tag{15}$$

The final step is to integrate over q to get I_m , using the fact that when $m > 2$ the contributions

$|\psi_c|^{2m}$ from separate caustics are so strongly localised near q_c that they are independent and simply add. This gives, after a simple scaling of the Airy function,

$$I_m \approx \frac{1}{\hbar^{(m-2)/3}} \times 2^{(2m-1)/3} A_m \times \sum_c \left| \frac{d\theta_c}{dp} \right|^m / |K_c|^{(2m-1)/3} \tag{16}$$

$(m > 2),$

whose three factors will now be discussed.

The first factor gives the \hbar -divergence anticipated in (9), with $\beta = 1/6$ and $\gamma = 2/3$ – the known fold diffraction exponents. The second factor involves

$$A_m = \int_{-\infty}^{\infty} dx [\text{Ai}(x)]^{2m} \tag{17}$$

which are numbers, given in table 1 for $3 < m < 6$, characteristic of the fold diffraction catastrophe integral. The third factor involves the torus geometry at the caustics, via $d\theta_c/dp$ relating the global variables θ and p at C , and the local curvature K_c .

Now we discuss the case $m = 2$. This is delicate because the integral for A_2 in (17) diverges as a result of $\text{Ai}(x)$ not falling quickly enough as $x \rightarrow -\infty$, implying that $|\psi|^4$ is not strongly localised near caustics and (16) is invalid. Moreover the exponent $(m - 2)/3$ vanishes when $m = 2$. Nevertheless, the validity of the representation (5) away from caustics and (14) close to caustics enables I_2 to be determined, as follows.

Table I
Integrals A_m and P_m
of the Airy and
Pearcey functions
(eqs. (17) and (48))

m	A_m	P_m
3	0.0366	—
4	0.00704	78
5	0.001654	82
6	0.000417	—

Write (5) as the complex superposition

$$\psi = \sum_{\mu} a_{\mu} e^{iS^{\mu}/\hbar} \quad (18)$$

and assume first that the fast semiclassical oscillations for each branch μ are independent of the oscillations for the other branches: essentially this means that T has no symmetry. We shall later consider a case where this assumption is false. Then, if $\langle \rangle$ denotes local averaging over q to wash out these oscillations,

$$\begin{aligned} \langle |\psi|^4 \rangle &= \left\langle \sum_{\mu\nu\lambda\sigma} a_{\mu} a_{\nu} a_{\lambda}^* a_{\sigma}^* \exp \frac{i}{\hbar} (S^{\mu} + S^{\nu} - S^{\lambda} - S^{\sigma}) \right\rangle \\ &= \sum_{\mu} |a_{\mu}|^4 + 4 \sum_{\mu < \nu} |a_{\mu}|^2 |a_{\nu}|^2. \end{aligned} \quad (19)$$

The first term corresponds to $\mu\nu\lambda\sigma$ all equal and the second term to μ, ν and λ, σ being equal in (different) pairs. Note that $\langle |\psi|^4 \rangle \neq \langle |\psi|^2 \rangle^2$; the difference reflects the weak trigonometric intensity fluctuations caused by interference, which are different from the strong caustic fluctuations we are concerned with here (but see section 7).

Near a caustic C and on the 'lit' side, the amplitudes for two branches become equal and large, and (19), (6) and (12) give

$$\begin{aligned} \langle |\psi|^4 \rangle &\approx 6|a_{\mu}|^4 = \frac{6}{4\pi^2} \left| \frac{d\theta_c}{dp} \frac{dp}{dq} \right|^2 \\ &= \frac{3}{4\pi^2} \left(\frac{d\theta_c}{dp} \right)^2 \frac{1}{K_c |q - q_c|}. \end{aligned} \quad (20)$$

If we attempt to integrate this over q to get I_2 , the result diverges, which of course reflects the fact that close to the caustic we should really be integrating the correct asymptotic expression (14).

The remedy is to integrate $\langle |\psi|^4 \rangle$ only up to a point q^* which is chosen such that the integral of (20) up to q^* from infinitely far on the 'lit' side equals the integral of (14) over all q . Thus q^* must satisfy the following equation, which is

written for the case where T curves away to the left of q_c (fig. 4) and where Θ denotes the unit step function:

$$\begin{aligned} \left(\frac{d\theta_c}{dp} \right)^2 \int_{-\infty}^{\infty} dq \left[\frac{2^{4/3}}{\hbar^{2/3} |K_c|^{4/3}} \text{Ai}^4 \left\{ \frac{(q - q_c) 2^{1/3}}{\hbar^{2/3} |K_c|^{1/3}} \right\} \right. \\ \left. - \frac{3\Theta(q^* - q)}{4\pi^2 |K_c| (q_c - q)} \right] = 0 \end{aligned} \quad (21)$$

q^* is related to a critical (negative) argument x^* of the Airy function by

$$x^* = \frac{(q^* - q_c) 2^{1/3}}{\hbar^{2/3} |K_c|^{1/3}} \quad (22)$$

and x^* is determined by

$$\int_{-\infty}^{\infty} dx \left[\text{Ai}^4(x) + \frac{3\Theta(x^* - x)}{8\pi^2 x} \right] = 0. \quad (23)$$

Computation gives

$$\begin{aligned} x^* = -\exp \left\{ -\frac{8\pi^2}{3} \lim_{A \rightarrow \infty} \left[\int_{-A}^{\infty} dx \text{Ai}^4(x) - \frac{3}{8\pi^2} \ln A \right] \right\} \\ - 0.17025. \end{aligned} \quad (24)$$

To interpret this result in physical terms, note

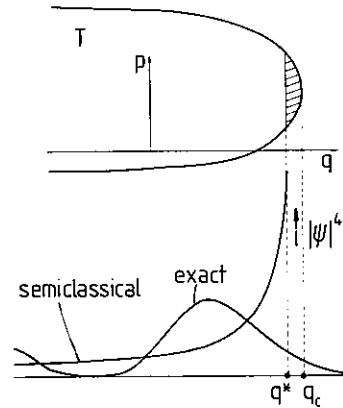


Fig. 4. To obtain I_2 , the semiclassical approximation to $|\psi|^4$ is integrated only up to q^* .

that the argument of the Airy function at q^* is

$$x^* = -\left(\frac{3S_c^*}{4\hbar}\right)^{2/3}, \quad (25)$$

where S_c^* is the phase-space area (shaded in fig. 4) enclosed by T between q^* and q_c . Eq. (24) gives

$$S_c = 0.09366\hbar, \quad (26)$$

and it is this area that must be excluded from the region near each caustic in integrating $\langle |\psi|^4 \rangle$ to get I_2 . Thus the second moment is

$$I_2 \approx \frac{1}{(2\pi)^2} \int_{\mathcal{R}} dq \left[\sum_{\mu} \left| \frac{d\theta^{\mu}}{dq} \right|^2 + 4 \sum_{\mu < \nu} \left| \frac{d\theta^{\mu}}{dq} \frac{d\theta^{\nu}}{dq} \right| \right], \quad (27)$$

where \mathcal{R} denotes the unexcluded segments of the q -axis. Note that the excluded areas may lie outside T ; this occurs for example near one of the caustics in fig. 3.

The semiclassical divergence of I_2 can be extracted explicitly by integrating (20) up to q^* . This gives

$$I_2 \approx \frac{1}{2\pi^2} \sum_c \left| \frac{d\theta_c}{dp} \right|^2 \frac{1}{|K_c|} \ln\left(\frac{B_c}{\hbar}\right), \quad (28)$$

where the sum is over all caustics c and B_c is a phase-space area globally determined by (27) (if T is a circle, B_c is 1.133 times the area enclosed by T). This formula exhibits the expected logarithmic singularity.

Finally we consider a special but important case which can arise when the system's Hamiltonian is an even function of p , namely tori T which are symmetric under reflection in the q -axis. Then the branches μ occur in pairs whose momenta p^{μ} have equal amplitude and opposite sign and whose contributions to (18) are complex conjugates and so do not oscillate independently. To deal with this case we write (18) as the real

superposition

$$\psi = \sum_k (a_k e^{iS^k/\hbar} + a_k^* e^{-iS^k/\hbar}), \quad (29)$$

where each k denotes a symmetric pair of branches. Averaging over independent oscillations now gives, instead of (19),

$$\begin{aligned} \langle |\psi|^4 \rangle &= 6 \left\langle \sum_{klmn} a_k a_l a_m^* a_n^* \right. \\ &\quad \left. \times \exp[(i/\hbar)(S^k + S^l - S^m - S^n)] \right\rangle \\ &= 6 \sum_k |a_k|^4 + 24 \sum_{k < l} |a_k|^2 |a_l|^2. \end{aligned} \quad (30)$$

(If there is a single pair of branches this gives the same as (19), but for more pairs the results are different.) For I_2 we obtain a modified formula in which (27) is multiplied by 6 and μ reinterpreted as denoting symmetric pairs of branches rather than individual ones.

4. Fold diffraction catastrophe moments

Now let $N = 2$, so that T is a 2-torus, and concentrate on the smooth fold caustic C produced in the q plane by projection (cusp and hyperbolic umbilic points will be studied in later sections). Let s be a curvilinear coordinate denoting arc length round C (fig. 5) and at each point of C set up local Cartesian axes q_1 (perpendicularly outwards from C) and q_2 (along the tangent to C).

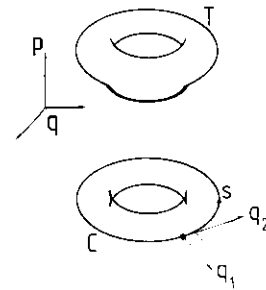


Fig. 5. Arc length s and local Cartesian q_1 , q_2 for fold caustic C projected from torus T .

For $m > 2$ the moments will be dominated by the concentration of ψ near C , i.e. by small q_1 . The Maslov procedure can be applied to give ψ as a Fourier integral over p_1 , namely

$$\psi(q_1, q_2) \approx \frac{1}{(2\pi)^{3/2} \hbar^{1/2}} \int dp_1 |D(q_2, p_1)|^{1/2} \times \exp\left\{\frac{i}{\hbar}[S(q_2, p_1) + p_1 q_1]\right\}, \quad (31)$$

where

$$S(q_2, p_1) \equiv \int_{q_0}^{q_2} p_2 dq_2 - \int_{p_0}^p q_1 dp_1 \quad (32)$$

and

$$D(q_2, p_1) \equiv \det \begin{pmatrix} \frac{\partial^2 S}{\partial I_1 \partial p_1} & \frac{\partial^2 S}{\partial I_1 \partial q_2} \\ \frac{\partial^2 S}{\partial I_2 \partial p_1} & \frac{\partial^2 S}{\partial I_2 \partial q_2} \end{pmatrix}. \quad (33)$$

This representation ‘tames’ the multivaluedness associated with the variable q_1 by expressing T in terms of singlevalued functions q_1 and p_2 of variables p_1 and q_2 . It is not necessary to Fourier-transform over p_2 as well, and indeed such a representation is degenerate in important special cases (for instance when p_2 is the angular momentum of a system with circular symmetry).

Away from C , (31) can be reduced to the simple semiclassical form (5) by applying the method of stationary phase and using the identity

$$\left| \det \left\{ \frac{\partial^2 S(q_1, q_2)}{\partial q_i \partial I_j} \right\} \right| = \left| D / \frac{\partial^2 S(q_2, p_1)}{\partial p_1^2} \right| = \left| D / \frac{\partial q_1}{\partial p_1} \right|. \quad (34)$$

Close to a given point s on C , T will be parabolic in p_1 , q_1 with equation

$$q_1 = -K(s)p_1^2/2, \quad (35)$$

where $K(s)$ is the local curvature of a cut through T by a plane perpendicular to C . The action with $q_2 = 0$ is therefore

$$S(q_2 = 0, p_1) = -K(s)p_1^3/6. \quad (36)$$

and in the integral (31) D may be set equal to its (nonsingular) value $D(s)$ on C . Then the wave can be considered as a function of q_1 and s , which on using the definition (15) can be expressed in terms of the Airy function:

$$\psi(q_1, s) \approx \frac{e^{ix_c} 2^{1/3} |D(s)|^{1/2}}{\hbar^{1/6} [K(s)]^{1/3}} \text{Ai} \left\{ \frac{q_1 2^{1/3}}{\hbar^{2/3} [K(s)]^{1/3}} \right\}. \quad (37)$$

This is the two-dimensional version of (14).

It is now straightforward to integrate over q_1 and s to get I_m , and the result is

$$I_m \approx \frac{1}{\hbar^{(m-2)/3}} \frac{A_m}{\pi^m 2^{(m+1)/3}} \oint ds \frac{|D(s)|^m}{[K(s)]^{(2m-1)/3}} \quad (m > 2), \quad (38)$$

where A_m are the numbers (17) (table 1). Just as in the one-dimensional version (16), the first factor gives the universal \hbar -dependence, the second factor involves the universal fold diffraction catastrophe, and the third factor depends on the torus geometry around the caustic.

An interesting special case for which (38) can be evaluated explicitly (and also checked independently – albeit laboriously – because the wave functions are known exactly) is the moments of the energy eigenstates of a non-relativistic particle with mass M moving freely within a circle of radius R (‘circular billiard’). Orbits consist of repeated chords making an angle θ with the tangent to the circle (fig. 6) and envelop a circular caustic with radius $R \cos \theta$. Tori are labelled by the conserved energy E and angular momentum J , or alternatively by θ and the wavenumber k :

$$E = \hbar^2 k^2 / 2M, \quad J = \hbar k R \cos \theta. \quad (39)$$

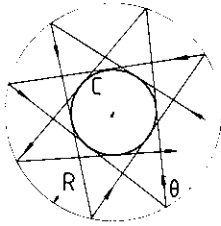


Fig. 6. Trajectory in a circular billiard.

The moments of the probability density of the wave supported by a k, θ torus are

$$I_m \approx \frac{(kR)^{(m-2)/3} A_m}{\pi^{m-1} 2^{(m-2)/3} \sin^m \theta (\cos \theta)^{(2m-4)/3} R^{2m-2}} \quad (m > 2) \quad (40)$$

Just as in one dimension the case $m = 2$ is delicate, but exactly the same arguments as used in section 3 and leading to (27) can be applied and give, for the 'non-symmetric' case where the oscillations associated with different branches μ are independent.

$$I_2 \approx \frac{1}{(2\pi)^4} \iint_{\mathcal{R}} dq \left[\sum_{\mu} \left| \frac{d\theta^{\mu}}{dq} \right|^2 + 4 \sum_{\mu < \nu} \left| \frac{d\theta^{\mu}}{dq} \frac{d\theta^{\nu}}{dq} \right| \right], \quad (41)$$

where \mathcal{R} is the region of the q plane covered by the projection of T , excluding a thin strip whose local width is (cf. 22)

$$q^*(s) = 2^{-1/3} \times 0.17025 \hbar^{2/3} [K(s)]^{1/3}. \quad (42)$$

Extracting the semiclassical divergence we obtain

$$I_2 \approx \frac{1}{8\pi^4} \oint ds \frac{D^2(s)}{K(s)} \ln \left\{ \frac{B(s)}{\hbar} \right\}, \quad (43)$$

where (cf. (28)) $B(s)$ is globally determined by (41).

5. Cusp diffraction catastrophe moments

Now let C denote a cusp point on the caustic produced by projecting T onto the q plane (fig. 7) and employ Cartesian coordinates with C as

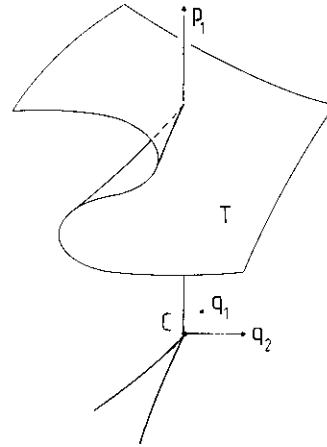


Fig. 7. Coordinates for torus T near a cusp caustic C .

origin, oriented as in fig. 5, i.e. with q_1 perpendicular to the caustic curve at C .

The wave near C can be represented by the Maslov procedure as in (31)–(33) involving a Fourier integral over p_1 alone, because although the cusp is a higher singularity than a fold it also has corank unity (there is only one 'bad' direction). However when $q_2 = 0$, T is not locally parabolic as in (35), but cubic, and unfolds with two extrema (caustics) when $q_2 < 0$ and none when $q_2 > 0$. This behaviour is represented by the action conveniently written as

$$S(q_2, p_1) = \frac{A_c p_1^4}{24} + \frac{3^{2/3} A_c^{1/3} B_c q_2 p_1^2}{4} + F(q_2), \quad (44)$$

where F is an arbitrary smooth function. T then has the local form (cf. (32))

$$\begin{aligned} q_1 &= -\frac{A_c p_1^3}{6} + \frac{3^{2/3} A_c^{1/3} B_c q_2 p_1}{2}, \\ p_2 &= \frac{3^{2/3} B_c p_1^2}{4} + \frac{dF(q_2)}{dq_2}. \end{aligned} \quad (45)$$

The caustic in q is given by

$$\frac{\partial q_1}{\partial p_1} = -\frac{A_c p_1^2}{2} + \frac{3^{2/3} A_c^{1/3} B_c q_2}{2} = 0, \quad (46)$$

which on eliminating p_1 and using the first of (45) becomes

$$q_1 = \pm (-B_c q_2)^{3/2}. \tag{47}$$

Thus B_c has a simple geometric interpretation as the ‘splay’ of the fold curves as they leave C . A_c also has a simple interpretation, as the rate of change of curvature of T at C :

$$A_c = -\frac{\partial^3 q_1}{\partial p_1^3}. \tag{48}$$

Inserting (44) into (31) and setting D equal to its (nonsingular) value D_c at C , and scaling the integration variable p_1 , we obtain, for the cusp wavefunction,

$$\begin{aligned} \psi_c(q_1, p_2) \approx & \frac{e^{i\chi_c} 6^{1/4} |D_c|^{1/2}}{\hbar^{1/4} |A_c|^{1/4} 2\pi} \\ & \times \text{Pe} \left\{ \frac{q_1 6^{1/4}}{\hbar^{3/4} |A_c|^{1/4}}, \frac{q_2 3^{7/6} |B_c|}{\hbar^{1/2} 2^{1/2} |A_c|^{1/6}} \right\}, \end{aligned} \tag{49}$$

where Pe is the Pearcey function (cusp diffraction catastrophe) defined [8, 14] by

$$\text{Pe}(x, t) \equiv \frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{\infty} dt e^{i(t^{4/4} + yt^2/2 + xt)}. \tag{50}$$

It is now straightforward to integrate over q_1 and q_2 to get I_m , with the result

$$I_m \approx \frac{1}{\hbar^{m/2-5/4}} \times \frac{P_m 3^{m/2-17/12}}{2^{3m/2-1/4} \pi^{2m}} \times \sum_c \frac{|D_c|^m}{|B_c| |A_c|^{m/2-5/12}}, \tag{51}$$

whose three factors will now be discussed.

The first factor gives the \hbar -divergence anticipated in (9) with $\beta = 1/4$, $\gamma = 5/4$ – the known cusp diffraction exponents. For $m = 2$ the exponent $m/2 - 5/4$ is negative, so that cusps do not cause I_2 to diverge. On the other hand we recall from the previous section (eq. (43)) that folds cause a logarithmic divergence. Thus folds

dominate cusps in the second moment. Consistent with this is the fact that the fold integral in (43) converges if the caustic contains a cusp point, even though $K(s)$ vanishes there (as $(s - s_c)^{1/2}$). For $m = 3$ the exponent is $m/2 - 5/4 = 1/4$, so that cusps do contribute a diverging term to I_3 . But the corresponding fold exponent is $(m - 2)/3 = 1/3$, so that folds dominate cusps in the third moment as well. However for $m \geq 4$ the cusp exponent exceeds the fold exponent and so cusps dominate folds (consistent with the fold geometry integral (38) diverging for $m \geq 4$ if there is a cusp).

The second factor involves integrals over the Pearcey function, namely

$$P_m \equiv \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy |\text{Pe}(x, y)|^{2m}, \tag{52}$$

and these are tabulated in table 1 for $m = 4$ and $m = 5$.

The third factor involves the torus geometry in the form of a sum over all cusps C .

6. Hyperbolic umbilic diffraction catastrophe moments

Now let H denote a hyperbolic umbilic point where two caustic curves in the q plane meet at a finite angle (fig. 8). Such a singularity has codimension three, i.e. it usually lives stably in a three-dimensional space [8, 14], but can be stable in two dimensions [7] when generated by projecting an invariant torus T of a Hamiltonian isotropic and quadratic in p . Umbilics have corank two and so require the Maslov procedure to be applied in both directions, leading to a double Fourier integral for $\psi(q)$. This is

$$\psi(q) \approx \frac{e^{i\chi_c}}{4\pi^2 \hbar} \iint dp |\Delta(p)|^{1/2} \exp\left\{ \frac{i}{\hbar} [S(p) + q \cdot p] \right\}, \tag{53}$$

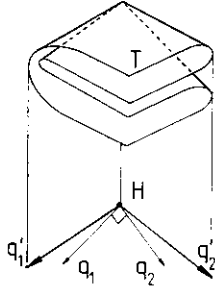


Fig. 8. Coordinates near hyperbolic umbilic singularity H from torus T .

where

$$S(\mathbf{p}) = - \int_{\mathbf{p}_0}^{\mathbf{p}} \mathbf{q}(\mathbf{p}) \cdot d\mathbf{p} \quad (54)$$

and

$$|\Delta(\mathbf{p})| = \left| \det \frac{\partial^2 S}{\partial I_i \partial p_j} \right| = \left| \frac{d\boldsymbol{\theta}}{d\mathbf{q}} \right|. \quad (55)$$

This representation ‘tames’ the multivaluedness associated with \mathbf{q} by representing T as a single-valued function $\mathbf{q}(\mathbf{p})$.

Away from H and the caustics leading to it, (53) can be reduced to the simple semiclassical form (5) by applying the method of stationary phase and using the identity

$$\left| \frac{\Delta}{\det \frac{\partial^2 S}{\partial p_i \partial p_j}} \right| = \left| \frac{d\boldsymbol{\theta}/d\mathbf{p}}{d\mathbf{q}/d\mathbf{p}} \right| = \left| \frac{d\boldsymbol{\theta}}{d\mathbf{q}} \right|. \quad (56)$$

Close to H , $S(\mathbf{p})$ is cubic in \mathbf{p} and will be written in the general form studied by Berry and Hannay [17], namely

$$S(\mathbf{p}) = \frac{\alpha p_1^3}{6} + \frac{\beta p_1^2 p_2}{2} + \frac{\gamma p_1 p_2^2}{2} + \frac{\delta p_2^3}{6}. \quad (57)$$

To evaluate ψ , we introduce a linear canonical transformation to new variables \mathbf{q}' , \mathbf{p}' in which the exponent of (53) takes the standard hyper-

bolic umbilic form [8, 14]

$$S(\mathbf{p}) + \mathbf{q} \cdot \mathbf{p} = \frac{p_1^3}{3} + \frac{p_2^3}{3} + \mathbf{q}' \cdot \mathbf{p}' \quad (58)$$

This is induced by a 2×2 matrix \mathbf{M}_H according to

$$\mathbf{p} = \mathbf{M}_H \mathbf{p}', \quad \mathbf{q} = \tilde{\mathbf{M}}_H^{-1} \mathbf{q}', \quad (59)$$

where the tilde denotes transposition. The \mathbf{q}' coordinates axes so defined lie on the fold caustics (fig. 8). \mathbf{M}_H depends on the constants α , β , γ , δ in a manner soon to be established.

On substituting (58) into (53) and replacing Δ by its nonsingular value Δ_H at the caustic corner, ψ can be written as a product of Airy functions:

$$\psi(\mathbf{q}) \approx \frac{e^{i\kappa_c |\Delta_H|^{1/2}} \det \mathbf{M}_H}{\hbar^{1/3}} \text{Ai} \left\{ \frac{q'_1(\mathbf{q})}{\hbar^{2/3}} \right\} \text{Ai} \left\{ \frac{q'_2(\mathbf{q})}{\hbar^{2/3}} \right\}. \quad (60)$$

To get I_m we must integrate over \mathbf{q} , and this is easily accomplished by changing variables using (59) giving the surprisingly simple result that for $m > 2$

$$I_m \approx \frac{1}{\hbar^{2(m-2/3)}} \times A_m^2 \times \sum_H |\Delta_H|^m |\det \mathbf{M}_H|^{2m-1}, \quad (61)$$

whose three factors will now be discussed.

Firstly, there is the \hbar -divergence, whose exponent is twice that of (38) for fold caustics. In terms of (9), the index γ is $4/3$, which differs from the corresponding optical index [8, 9, 14], because the control space here is not the full three-dimensional umbilic control space but a two-dimensional section of it (i.e. the \mathbf{q} plane). For $m > 2$ the moments diverge semiclassically and dominate both folds and cusps. The delicate situation $m = 2$ will be discussed at the end of this section.

Secondly, there is the diffraction catastrophe factor involving the square of the numbers A_m defined by (17) (table 1).

Thirdly, there is the torus geometry factor which is a sum over all corners H . This involves $\det \mathbf{M}_H$ which is invariant under rotation and shear of \mathbf{p} space and so must be expressible in terms of the umbilic catastrophe invariant [17]

$$C \equiv 4(\alpha\gamma - \beta^2)(\beta\delta - \gamma^2) - (\alpha\delta - \beta\gamma)^2, \quad (62)$$

which has the same invariances and which is negative for hyperbolic umbilics. To discover the exact relation we compare the behaviour of $\det \mathbf{M}_H$ and C under isotropic dilation $\mathbf{p} \rightarrow T\mathbf{p}$. It is easily shown that $C \rightarrow T^{12}C$ and $\det \mathbf{M}_H \rightarrow T^{-2} \det \mathbf{M}_H$. Moreover if S already has the form (58) then $C = -16$ while $\det \mathbf{M}_H = 1$. It follows that

$$|\det \mathbf{M}_H| = |16/C|^{1/6}. \quad (63)$$

C has a simple geometric interpretation. To see what it is, denote by $G(f)$ the Gaussian curvature of any function $f(p_1, p_2)$ when considered as the infinitesimal deviation of a surface from the \mathbf{p} plane. Denoting derivatives by subscripts, we have

$$G(f) = f_{11}f_{22} - f_{12}^2. \quad (64)$$

If f is the action S given by (57), its curvature is

$$G(S) = (\alpha\gamma - \beta^2)p_1^2 + (\alpha\delta - \gamma\beta)p_1p_2 + (\beta\delta - \gamma^2)p_2^2. \quad (65)$$

From (54) we also have

$$G(S) = \left| \frac{dq}{dp} \right|, \quad (66)$$

which is of course the Jacobian whose vanishing is central to the whole discussion. Now take the Gaussian curvature again, i.e. form

$$G(G(S)) = G\left(\left| \frac{dq}{dp} \right|\right). \quad (67)$$

A short calculation based on (65) shows that this is precisely the invariant C of eq. (62) (and

moreover the *total* curvature of $G(S)$ is precisely the different invariant [17] giving the Poincare index of the singularity of the net of lines of curvature of S at H). Therefore

$$|\det \mathbf{M}_H| = \left| 16/G\left(\left| \frac{dq}{dp} \right|\right) \right|^{1/6} \quad (68)$$

and the geometric part of the moment formula (61) is completely interpreted.

For $m = 2$ the formula (61) does not apply, because of the divergence of A_2 which reflects the fact that I_2 is not determined solely by the neighbourhood of H . The procedure described in one dimension at the end of section 3 can be applied and leads to a result closely analogous to the 'fold' formula (41), but for the case where all branches come in pairs (denoted k or l) with equal and opposite \mathbf{p} , rather than being independent. On using (30) for the average of $|\psi|^4$ we obtain

$$I_2 \approx \frac{6}{(2\pi)^4} \iint_{\mathcal{R}} dq \left[\sum_k \left| \frac{d\theta^k}{dq} \right|^2 + 4 \sum_{k < l} \left| \frac{d\theta^k}{dq} \frac{d\theta^l}{dq} \right| \right], \quad (69)$$

where \mathcal{R} is as before the region excluding the strip of width q_1^* given by (42).

To extract the semiclassical divergence of I_2 associated with a corner H , we realise that two pairs of branches coalesce there (T has the topology of a four-folded handkerchief as shown in fig. 8), so that

$$I_2 \approx \frac{36}{(2\pi)^4} \iint_{\mathcal{R}} dq \left| \frac{d\theta}{dq} \right|^2. \quad (70)$$

For $|d\theta/dq|$ we use (56) and replace $|d\theta/dp|$ by its nonsingular value $|\Delta_H|$ at H , and transform to p' and q' using (59). Thus

$$I_2 \approx \frac{36}{(2\pi)^4} |\Delta_H|^2 \iint_{\mathcal{R}} dq \left| \frac{dp}{dq} \right|^2 \approx \frac{36}{(2\pi)^4} |\Delta_H|^2 |\det \mathbf{M}_H|^3 \iint_{\mathcal{R}} dq'_1 \int dq'_2 \left| \frac{dp'}{dq'} \right|^2. \quad (71)$$

But in the primed variables T separates in the form (cf. (58) and (54))

$$q'_1 = -p'^2_1, \quad q'_2 = -p'^2_2, \quad (72)$$

so that

$$I_2 \approx \frac{36}{(2\pi)^4} |\Delta_H|^2 |\det \mathbf{M}_H|^3 \frac{1}{16} \int^{q^*} \frac{dq'_1}{|q'_1|} \int^{q^*} \frac{dq'_2}{|q'_2|}. \quad (73)$$

For q^* we have (42) with the sectional curvatures $K(s)$ both equal to 2, giving, finally, after summing over all H ,

$$I_2 \approx \frac{1}{16\pi^4} \sum_H |\Delta_H|^2 |\det \mathbf{M}_H|^3 \left\{ \ln \left(\frac{B_H}{\hbar} \right) \right\}^2. \quad (74)$$

where, as previously, B_H is globally determined. Exactly this result can be obtained directly from (60) on employing asymptotic forms for the Airy functions and integrating up to $-q^*$. Evidently the singularity, while still logarithmic, is stronger than that at a fold, which is not unexpected in view of the fact that the singular section of the hyperbolic umbilic is simply the product of two folds.

7. Chaotic states

Now we consider the moments of states associated with classical phase-space-densities $\rho(q, p)$ whose support has dimensionality exceeding the value N corresponding to tori. An important example is the energy surface E of a time-independent Hamiltonian H with classically ergodic motion, for which

$$\rho = \delta(E - H(q, p)). \quad (75)$$

E has dimensionality $2N - 1$ which exceeds N if $N \geq 2$; in this case it is likely [2–4] that semiclassical eigenstates of H are associated with E .

The important feature of such densities ρ is that to each q there correspond infinitely many p for which ρ is nonzero, in contrast to tori where there are finitely many branches $p^\mu(q)$. Consideration of the two-point correlation of the wavefunction [2–4] gives reason to believe that $\psi(q)$ is the infinite super-position of complex contributions (de Broglie waves) from all these p with amplitudes proportional to $\rho^{1/2}$ and phases that are either totally independent, as in the complex sum (18) or, for p -symmetric Hamiltonians, correlated as in the real sum (29). By the central limit theorem, ψ as given by such an incoherent sum fluctuates randomly with q with either a complex or real Gaussian distribution.

When integrating over q to get I_m , it is permissible to replace $|\psi(q)|^{2m}$ by its local average $\langle |\psi(q)|^{2m} \rangle$ calculated according to the appropriate Gaussian distribution. Both distributions depend on the average probability density which when normalised is

$$\langle |\psi(q)|^2 \rangle = \int dp \rho(q, p) / \iint dq dp \rho(q, p). \quad (76)$$

For the complex Gaussian, the distribution is

$$P(\text{Re } \psi, \text{Im } \psi) = \frac{\exp\{-[(\text{Re } \psi)^2 + (\text{Im } \psi)^2]/\langle |\psi|^2 \rangle\}}{\pi \langle |\psi|^2 \rangle}, \quad (77)$$

and for the real Gaussian the distribution is

$$P(\psi) = \frac{\exp\{-\psi^2/2\langle \psi^2 \rangle\}}{\sqrt{2\pi\langle \psi^2 \rangle}}. \quad (78)$$

It follows that

$$\langle |\psi|^{2m} \rangle = C_m \{\langle |\psi|^2 \rangle\}^m, \quad (79)$$

where

$$\begin{aligned} C_m &= m! \quad (\text{complex } \psi) \\ &= 1.3.5 \dots (2m-1) \quad (\text{real } \psi) \end{aligned} \quad (80)$$

The semiclassical m th moment is therefore

$$I_m = \frac{C_m \int dq \left[\int dp \rho(q, p) \right]^m}{\left[\int \int dq dp \rho(q, p) \right]^m}. \quad (81)$$

In sharp contrast to the moments of torus states, this does not diverge as $\hbar \rightarrow 0$ (because the probability density (76) does not possess caustic singularities). Indeed I_m does not involve \hbar at all – although the fact that $C_m > 1$ is a consequence of ψ being an incoherent superposition of waves, and causes I_m to increase with m .

We emphasize that (81) is not restricted to ergodic systems; for example in a quasi-integrable system ρ could represent the density with which a chaotically moving particle explores a phase-space region between Kolmogorov–Arnold–Moser tori [18]. Nevertheless it is interesting to evaluate I_m explicitly when ρ is supported by the whole energy surface (eq. (75)), corresponding to an eigenstate of an ergodic Hamiltonian (or to an appropriate superposition of eigenstates of a nonergodic Hamiltonian) and where, moreover, H has the form

$$H = p^2/2M + V(q). \quad (82)$$

Then (81) can easily be shown to give

$$I_m = \frac{C_m \int dq [E - V(q)]^{mN/2 - m} \Theta(E - V(q))}{\left\{ \int \int dq [E - V(q)]^{N/2 - 1} \Theta(E - V(q)) \right\}^m}, \quad (83)$$

where the step functions Θ restrict the integrations to the classically allowed region. The case where $N = 2$ is particularly simple: in terms of the area $\mathcal{A}(E)$ of the classically allowed region of the q plane at energy E ,

$$I_m = C_m / \mathcal{A}^{m-1}(E). \quad (84)$$

(For planar billiards [3], \mathcal{A} is independent of E .)

Finally, we point out that (81) predicts larger fluctuations, the more ρ is concentrated in a small region. To illustrate this, let ρ be constant within, and zero outside, a hypercube with sides $\Delta q, \Delta p$. Then

$$I_m = C_m / (\Delta q)^{N(m-1)}, \quad (85)$$

which increases as Δq diminishes.

8. Conclusions

We have shown that the spatial variations in the probability density $|\psi|^2$, as embodied in the moments I_m , are very different for regular and chaotic states. For regular states the variations are intense and rapid because of the presence of caustic singularities (catastrophes) in q space which make I_m diverge as $\hbar \rightarrow 0$, in a manner depending on the caustic's diffeotype. In two dimensions, cusp points (if present) dominate fold curves for $m \geq 4$, and hyperbolic umbilic corners (if present) dominate folds and cusps for all m . In higher dimensions N it would be easy to work out the \hbar -exponents (cf. (9)) and the caustic dominance relations, using techniques from twinkling theory [9] (although the exponents generally differ from those in twinkling problems); however, the torus geometry factors would be hard to calculate. For chaotic states there are no caustics and the fluctuations, which arise from incoherent interference, are not large and $I_m \rightarrow \text{constant}$ as $\hbar \rightarrow 0$.

It is important to appreciate that although our results describe the semiclassical behaviour of eigenstates associated with a given classical phase-space region, they do not solve the 'inverse' problem of determining the type of classical region associated with a given eigenstate. Suppose, for example, that for given \hbar a particular eigenstate $\psi(q)$ with energy E is obtained 'exactly' (e.g. by numerical matrix diagonalization based on Schrödinger's equation) and I_m is computed and found to be large. Does this mean

that ψ is associated (a) with a torus, or (b) with a concentrated higher-dimensional region in phase space (cf. the last paragraph of section 7)? To choose between these alternatives, it would be necessary to diminish \hbar and see whether I_m increased (alternative (a)) or remained constant (alternative (b)). But the spectrum is discrete, so that it is not possible to vary \hbar continuously whilst keeping E constant, and when the next smaller \hbar -value is found for which an eigenstate exists with energy E , there is no guarantee that it is associated with the same classical region as ψ , rather than with a quite different region on the same energy surface.

Of course our calculations have been based on semiclassical approximations to ψ , rather than exact solutions of Schrödinger's equation. Therefore our formulae for I_m are the first terms of asymptotic series involving higher powers of \hbar . For regular states the higher terms come from corrections to the diffraction catastrophes representing ψ near caustics. For chaotic states the higher terms may reflect the division of phase space into 'cells' of volume h^N , which will cause the number of de Broglie waves contributing to ψ at q to be not infinite but large (e.g. $\mathcal{O}(\hbar^{-1})$). This effect should reduce the values of I_m found in section 7.

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