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Contour splitting as a criterion for surface roughness in irregular wavefunctions

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Abstract. A measure of irregularity in a quantum state lies in the surface roughness of the corresponding eigenfunction and shows up as a splitting of contours at successive heights. This phenomenon seems to be absent in integrable systems where the states are regular. We carry out an analysis based on the semiclassical theory and extend it by a detailed numerical investigation which reveals that (i) a Gaussian amplitude distribution and the splitting of contours occur together, and (ii) the percentage increase in the number of contours with height is a measure of the degree of surface irregularity. Regular, localized states in chaotic systems for which good quantum numbers can be assigned do, however, show 'contour splitting'.

1. *Introduction*

Recent advances in the understanding of classical Hamiltonian dynamics have led to a reinvestigation of the nature of semiclassical eigenstates in generic quantum systems with non-integrable classical analogues. It is now clear that the classification scheme conceived by Percival [1] in the early 1970s does work. The quantum energy levels in systems with a mixed phase space (containing Kolmogorov-Arnold-Moser tori and chaotic regions) belong either to a regular or an irregular class. Using ideas of dynamical quasidegeneracy, Bohigas *et al* [2, 3] have corroborated the above proposition, though their studies also reveal the existence of a small percentage of levels with an intermediate nature. This, of course, gives rise to an important question: *how irregular is an eigenstate*? Methods based on eigenvalues such as the one used by Bohigas *et al* [2] are no doubt helpful, but the complexity of an eigenstate really lies in the nature of its eigenfunction since we expect the invariant structures of classical mechanics to be reflected in these stationary states of the quantum system. In this paper, we provide a visual picture of the degree of surface roughness in irregular wavefunctions, an area which is largely unexplored to the best of our knowledge. Before proceeding with our investigations, however, we take a brief look at some of the commonly used criteria for recognizing the nature of an eigenstate.

Nodal patterns and contour plots are some of the most important tools for distinguishing regular and irregular wavefunctions. In the former case, the patterns are quasiperiodic and the regularity is quite evident in sharp contrast to the complex structures and avoided crossings that characterize the latter. An irregular pattern, however, does not necessarily imply that the underlying classical dynamics is chaotic. This issue, initially discussed by Heller [4], has been elaborated by Biswas and Jain

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[5] for eigenfunctions belonging to pseudointegrable systems which are non-chaotic in the Lyapunov sense.

The amplitude distribution, $P(\psi)$, is increasingly being recognized as another important criterion and provides a more quantitative picture [5, 6]. Recently Biswas *et al* [7] used the periodic orbit theory approach to show that $P(\psi)$ does have a limiting form which closely approximates a Gaussian when the underlying classical dynamics is chaotic. The earlier arguments were based on the representation of the eigenfunction as an infinite superposition of plane waves with random phases [8], an idea which is essentially an extension of the integrable case. Incidentally, such a picture also leads to a spatial correlation function which is isotropic and has a Bessel function dependence [8]. The prediction, however, has been subjected to a test with reasonable success only for the Bunimovich stadium billiard [6]. The path correlation function of Shapiro and Goelman [9] has also been used to distinguish regular and irregular states but has found limited usage.

The above criterion together with the degree of 'surface roughness' that we seek to investigate in this paper, provides a more or less complete picture of the nature of irregular eigenfunctions. A rough surface in this context is characterized by the presence of one or more local extrema between successive crossings through zero (nodal curves). In other words, there are minor humps and valleys which manifest themselves as a splitting of contours when sections through successive heights are taken (a closed contour at a lower height, $|\psi|$, splits into two or more at a larger value of $|\psi|$). Some of the questions that we shall address are:

(i) Do quantum mechanical eigenfunctions possess surface roughness?

(ii) If so, is it peculiar only to eigenfunctions irregular in the usual sense?

(iii) Can the degree of contour splitting be used as a measure of irregularity?

The paper is organized along the following lines. Section 2 deals with the semi-classical representation of eigenfunctions for the integrable and chaotic cases, using which we shall rule out the possibility of surface roughness in separable integrable systems and argue in favour of such a possibility when the underlying classical dynamics is chaotic. Section 3 is devoted to numerical investigations and helps us to establish some of the predictions of the earlier section. Discussions and a summary form the concluding section.

2. Surface roughness and contour splitting—a semiclassical analysis

2.1. Integrable systems

We shall confine ourselves mostly to separable integrable systems with two degrees of freedom in this subsection and provide a proof for the absence of surface roughness in such cases. The ideas can easily be extended to higher degrees of freedom as well. As an example of a non-separable system, we shall consider the equilateral triangle billiard.

The eigenfunction for a separable integrable system characterized by the Hamiltonian

$$\begin{aligned} H &= p_1^2/2m + p_2^2/2m + V_1(x_1) + V_2(x_2) \\ &= H_1 + H_2 \end{aligned} \tag{1}$$

can be expressed in the form

$$\psi_{m,n} = \phi_m^1(x_1)\phi_n^2(x_2) \tag{2}$$

where $\phi^i(x_i)$ is an eigenfunction of H_i. In the semiclassical case where eigenstates correspond to classical motion on a torus, the global solution can be expressed as

$$\phi^i(x_i) = c_i|\partial^2 S_i/\partial x_i \partial I_i| \sin\{S_i(x_i)/\hbar\} \tag{3}$$

where

$$S_i(x_i) = \int_{x_i^0}^{x_i} p_i \, \mathrm{d}x_i \tag{4}$$

and I_i is the action on the irreducible circuit characterized by the turning points of the potential $V_i(x_i)$.

It is easy to verify that the amplitude $\partial^2 S_i/\partial x_i \partial I_i$ has no zero as a function of x_i. Thus an extremum of $\psi_{m,n}(x_1, x_2)$ occurs at points (x_1, x_2) for which

$$S_1(x_1)/\hbar = (2p+1)\pi/2 \tag{5a}$$

$$S_2(x_2)/\hbar = (2q+1)\pi/2. \tag{5b}$$

It is clear from the quantization conditions

$$\oint p_i \, \mathrm{d}x_i = 2\pi n_i \hbar \qquad i = 1, 2 \tag{6}$$

(and by considering the points x_i^0 on the turning points) that the maximum number of possible extrema are $(n_1) \cdot (n_2)$. The number of nodal curves ($\psi = 0$) on the other hand are $(n_1+1) \cdot (n_2+1)$ and hence *eigenfunctions of separable integrable systems do not possess surface roughness.*

The proof outlined above can easily be generalized to higher dimensions but cannot be extended to non-separable integrable systems. We give here an alternate proof for separable systems which is purely quantum mechanical. In such cases, it is sufficient to show that an eigenfunction of the 1D Schrödinger equation cannot have undulations or humps and valleys. If it does, the second derivative ought to change sign or pass through a zero at a point x_0 where ψ is non-zero. It follows from the Schrödinger equation, however, that in the classically allowed region, $\mathrm{d}^2\psi/\mathrm{d}x^2$ cannot be zero unless ψ itself vanishes while in the region outside, ψ rapidly decays. Thus in a separable integrable system, the quantum eigenfunctions do not possess surface roughness.

Non-separable integrable systems are not as easily tractable, however. Of course the semiclassical eigenfunction can still be expressed as a finite sum,

$$\psi = \sum c_i|\partial^2 S_i/\partial x_i \partial I_i| \exp\{\mathrm{i}S_i(x_i)/\hbar\} \tag{7}$$

due to the existence of the torus. The equilateral triangle billiard is one such system for which we shall carry out a numerical investigation in the following section.

2.2. Chaotic systems

The representation of an eigenfunction when the classical dynamics is chaotic is still a basic open problem. A lot of progress has, however, been achieved in the last few years and a reasonable understanding now exists.

Among the important developments has been the theory of scars initiated by Heller [4] and subsequently followed up by Bogomolny [10] and Berry [11] to arrive at an expression for the averaged intensity, $\langle\psi^*\psi\rangle$ in terms of the periodic orbits of the underlying classical system. Scarred states in most systems are an exception, however, and most wavefunctions are rather complicated and must be interpreted as a superposition of several contributions from both periodic and recurrent (those which return to the same point but with different momentum) trajectories. An important clue about their nature is provided by the semiclassical expansion of the Green function

$$G(\boldsymbol{q}', \boldsymbol{q}; E) = \sum_n \psi_n(\boldsymbol{q}')\psi_n(\boldsymbol{q})/(E - E_n) \tag{8}$$

in terms of classical trajectories [12]. The intensity and hence the wavefunction thus solely depend on those trajectories which are closed. Unlike the density of states where only periodic orbits contribute, recurrent trajectories play an important role in eigenfunctions. Most of these with comparable actions reside in the neighbourhood of periodic orbits. There are others, however, which explore the entire domain of the potential but have arbitrarily large lengths.

A study of the map on a Poincaré surface of section is more revealing. The periodic orbit now appears as a fixed point or a k-cycle of the map. For a system with two degrees of freedom, an unstable periodic orbit gives rise to a stable manifold, W_s and an unstable manifold, W_u, the points of which tend to the periodic orbit (fixed point) for $t \to \infty$ in the former case and $t \to -\infty$ in the latter. For a surface of section defined by (say) the (q_1, p_1) plane, a closed non-periodic orbit corresponds to the $q_1 = \text{constant}$ line. It is easy to see now that in the neighbourhood of the fixed point there exists closed non-periodic orbits of almost the same action. However, there are others as well with arbitrarily large lengths.

It is thus possible to represent an individual eigenstate as

$$\psi_n(q) = \sum \Phi_i(\boldsymbol{q}, E_n) \tag{9}$$

where Φ_i is the contribution of the ith periodic orbit taking appreciable non-zero values in a narrow tube around it (arising from the contributions of the recurrent orbits in the neighbourhood which have almost the same action). Its contribution decays rapidly thereafter and in the rest of the domain the long recurrent orbits merely provide a background fluctuating around zero. In other words, the support of Φ_i lies in a narrow tube around the ith periodic orbit.

Using the representation given by equation (11) and a couple of limiting theorems for non-uniform distributions, Biswas *et al* [7] have been able to show that $P(\psi)$ does have a limiting form which closely approximates a Gaussian.

This information does indeed have relevance in our study of surface roughness as we shall now see. The distribution $P(\psi)$ is evaluated numerically [5–6, 9] by sampling points (say 10 000) in configuration space and the fraction taking values in small intervals $[\psi - \Delta\psi, \psi + \Delta\psi]$ is determined. The distribution is then normalized.

In a sense, therefore, $P(\psi)$ contains information about the lengths of contours (which is proportional to the number of points on it) at a given value of ψ. At $\psi = 0$, the length is thus maximum as expected since there are crossings (through the section at $\psi = 0$) from both positive and negative values. At a small non-zero value, however, the length (or the fraction of points) instead of reducing sharply registers only a marginal decrease, thus suggesting an increase in the number of contours. In other words, *the surface would be rough and manifests itself as contour splitting.* If the numerically obtained amplitude distribution has spikes at other values of ψ as well, a similar conclusion can be arrived at.

We have thus used ideas of the semiclassical periodic orbit theory to show that a quantum mechanical eigenfunction having a Gaussian amplitude distribution does possess surface roughness.

Plausibility arguments based on the expressions for averaged intensity, $\langle|\psi|^2\rangle$ in terms of periodic orbits [10, 11] also lead to a similar conclusion. Since the orbits are isolated and have an irregular spatial distribution, the variation of $\langle|\psi(\boldsymbol{q})|^2\rangle$, over a small element of area would depend sensitively on the lengths and stability properties of the periodic orbits passing through it as well as the energy, E_n. Under favourable conditions, the Gaussian decay of a contribution transverse to a periodic orbit could be arrested such that neighbouring contributions take over. This would result in minor humps and valleys, characteristic of a rough surface.

We substantiate the arguments outlined above with numerical studies in the following section.

3. Numerical studies

The chief thrust of this section is to provide a visual picture of surface roughness in irregular eigenfunctions belonging to chaotic systems and propose a quantitative measure as well. First, however, we shall take up the case of equilateral triangle discussed in the previous section.

In order to facilitate the plotting of contours, we choose the origin as a $\pi/3$ vertex of the 60°-120° rhombus. Half the eigenstates of this system are identical to those of the equilateral triangle billiard [13, 14] and are characterized by the eigenvalues

$$E_{m,n} = 16\pi^2(m^2+n^2+mn)/9L^2 \tag{10}$$

and eigenfunctions

$$\begin{aligned}\psi_{m,n} = {} & \sin[2\pi(m+2n)x/3L]\sin[2\pi my/\sqrt{3}L] \\ & +\sin[-2\pi(2m+n)x/3L]\sin[2\pi ny/\sqrt{3}L] \\ & -\sin[2\pi(m-n)x/3L]\sin[2\pi(m+n)y/\sqrt{3}L].\end{aligned} \tag{11}$$

We shall consider the state labelled by the quantum numbers (13, 14). Figure 1 shows a contour plot at $\psi=0.4$ and 0.8. The regularity and lack of surface roughness seem

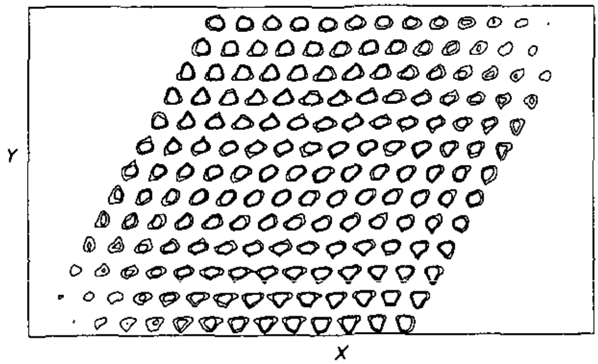

Figure 1. Contour plots of an equilateral triangle eigenfunction at $\psi=0.4$ and 0.8 shown in the $\pi/3$ rhombus enclosure. Distortions at the 60° vertices are due to discretization errors in the data set.

evident. At the 60° vertices, however, there are certain distortions due to interpolation errors arising from the lack of an adequate number of points. A magnification of the data set reveals that there are regular curves even at these corners. We have taken sections at various other heights (values of ψ) as well but have observed no contour splitting.

A note of caution, however, seems to be in order. Apart from corner distortions, spurious effects can occur even in separable integrable systems at values of ψ near zero due to the discretization process. Thus closed disconnected curves start appearing as a single closed loop with pseudo-avoided crossings. The extent to which this can be eliminated depends on the efficiency of the contour-plotting routine used but in general it is safer to restrict oneself to larger values of $|\psi|$. We shall return to this point again later.

Other equilateral triangle eigenfunctions behave in much the same way and the number of extrema (measured by taking a section at the lowest possible value of $|\psi|$) on the average is $(m)(n)$. We are currently carrying out further studies to explore the possibility of extending this result for general non-separable integrable systems.

As examples of chaotic systems, we shall consider the Bunimovich stadium billiard and a point particle moving freely on a compact 2D surface of constant negative curvature. Both these have been studied in great detail [4, 6, 9, 15] and plots of typical eigenfunctions are thus readily available. Figure 2 shows a contour plot of an irregular eigenfunction in the stadium. A close inspection in any quadrant reveals the existence of several 'split contours' indicating the presence of surface roughness. A similar phenomenon occurs in other eigenfunctions of this system as well. Figure 3 is a contour plot of the 100th wavefunction with positive parity in the hyperbola billiard [15]. The presence of surface roughness is quite evident. It also serves to confirm our prediction that contour splitting and a Gaussian amplitude distribution occur together (see figure 9 of [15] for a plot of $P(\psi)$).

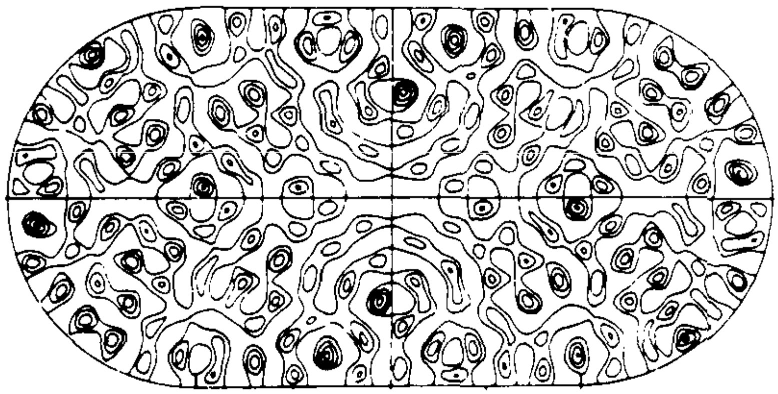

Figure 2. Contour plot of a typical irregular eigenfunction of the Bunimovich stadium billiard (taken from [16]). Several 'split contours' are visible.

Thus irregular eigenstates in chaotic systems do indeed possess surface roughness as well a Gaussian amplitude distribution. The phenomenon, however, seems to occur in other non-integrable systems as well. The study of Biswas and Jain [5] on the even parity eigenfunctions of the $\pi/3$ rhombus billiard (a pseudointegrable system) clearly shows that irregular states do occur in these non-chaotic systems as well. Figure 4 shows contour plots of a typical eigenfunction belonging to this system (see caption

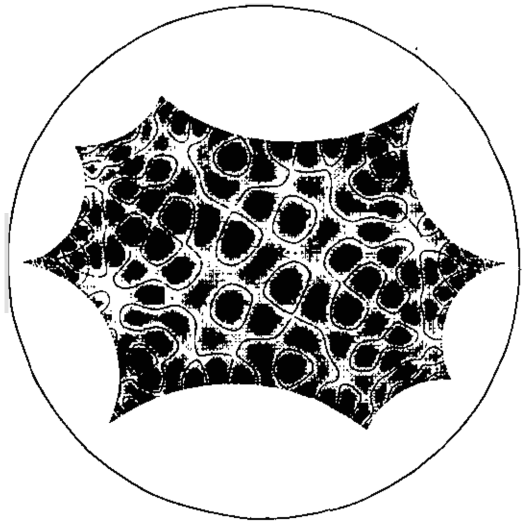

Figure 3. A similar plot for an eigenfunction of a point particle moving on a compact surface of constant negative curvature (taken from [15]). The presence of surface roughness is evident. The corresponding amplitude distribution is Gaussian (see [15]).

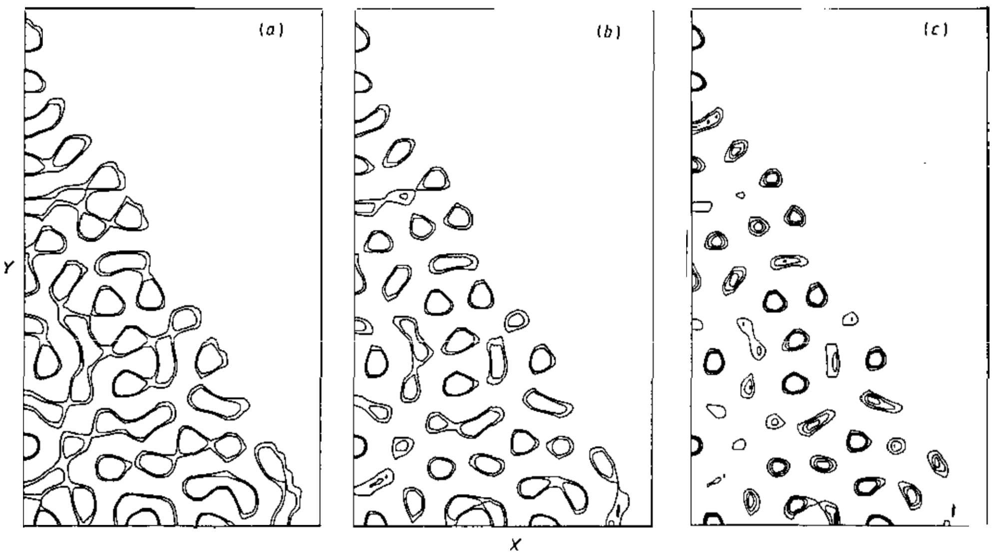

Figure 4. Contour plots of an irregular eigenfunction belonging to the $\pi/3$ rhombus billiard at $\psi = (a)$ 0.1 and 0.5, (b) 0.5 and 0.9, (c) 0.9, 1.3 and 1.6. A contour at a lower height splits into several at a larger height.

for more details). Only one quadrant is displayed here since the others are related by symmetry. Sections at various heights have been considered and the splitting seems to persist even at larger values of ψ. Moreover the inhomogeneity of the heights of individual peaks is also clearly visible. A similar effect can be seen even in certain localized (regular) states belonging to chaotic systems (see [4] for a plot).

An attempt to quantify these observations so as to get an indicator of the degree of irregularity is in general difficult, since a lot of local information which the plots provide gets washed out. Nevertheless we shall take a look at variation of the number of contours, $N(z)$, with height z $(=\psi)$. For separable integrable systems, the number should either remain constant or decrease monotonically with $|\psi|$ till the maximum value is encountered where it drops to zero. Figure 5 shows a plot of $N(2)$ for the equilateral triangle billiard eigenfunction considered earlier. For smaller values of ψ, there is an increase in the value of $N(z)$ but thereafter it decreases monotonically and smoothly as expected even for this non-separable system. The initial increase is due to the spurious phenomenon discussed earlier. Several closed disconnected curves start appearing as a single closed loop due to which the number of contours at lower heights turns out be smaller than expected. With the increase in height, $N(z)$ quickly attains its maxima (when all closed curves remain distinct) and thereafter steadily decreases. Figure 6 shows a similar plot for the even parity eigenfunction of the $\pi/3$ rhombus

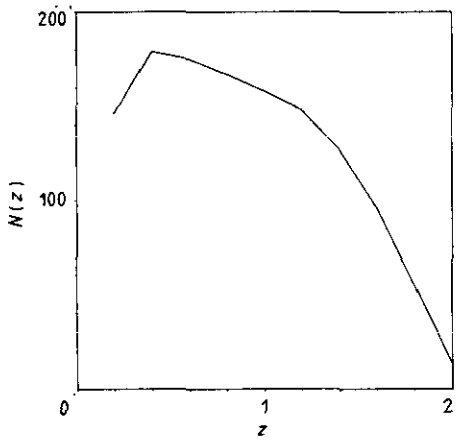

Figure 5. The number of contours, $N(z)$, plotted as a function of the height z $(=\psi)$ for the equilateral triangle eigenfunction considered in figure 1. The initial increase is due to interpolation errors. The fall is smooth even for this non-separable integrable system.

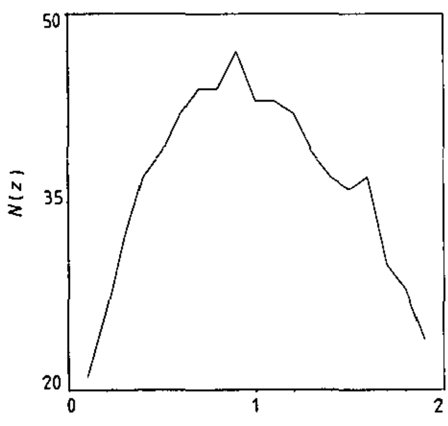

Figure 6. As in figure 5 for the $\pi/3$ rhombus eigenfunction of figure 4. The initial increase is sharper and the fall has spikes indicating a rapid splitting of contours.

considered earlier. The contours have been counted only in the first quadrant. The number increases initially as before, but at a faster rate possibly due to genuine contour splittings. At larger values, there is a competition between the disappearance of peaks and the splitting of contours both of which seem to have a certain random nature. This is manifested by the presence of spikes in the plot of $N(z)$.

4. Discussions

The concept of surface roughness provides information complementary to that obtained from nodal patterns, amplitude distributions and certain correlation functions. This phenomenon is certainly absent in separable integrable systems but needs to be conclusively investigated in non-separable integrable systems. For chaotic systems on the other hand, contour splitting and a Gaussian amplitude distribution seem to occur together. Thus surface roughness is yet another manifestation of the underlying classical dynamics. The variation of the number of contours with $|\psi|$ does provide a measure of irregularity in quantum states and could be exploited in future studies.

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