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# Eigenvalue dependence on small pseudointegrable perturbation of a two-dimensional box 

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#### Abstract

The eigenvalues of a hard-walled parallelogram-shaped enclosure were investigated using quantum perturbation theory, the perturbation being a small angle distortion of a pair of parallel sides of the rectangle. A comparison of perturbation theory results and exact computations for low-lying states showed good agreement. The distribution of eigenvalues grossly disturbed from their value in the nearby regular system was studied and found to be systematic.


## 1. Introduction

A class of dynamical systems with $2 N$ degrees of freedom and $N$ constants of the motion which are nevertheless not integrable was first discussed in detail by Richens and Berry (1981), who coined the name 'pseudointegrable'. Such systems produce motion which, although largely regular, does also display some unpredictability, characteristic of chaotic motion. All trajectories of integrable systems lie on $N$-dimensional surfaces in phase space which are topologically equivalent to tori (Arnol'd 1978). Trajectories of pseudointegrable systems also lie on $N$-dimensional surfaces of the phase space, but these have the topology of multiply handled spheres. The phase flow on an $N$-torus is described by $N$ smooth independent vector fields; such vector fields on a multiply handled sphere, however, have singular points which split beams of trajectories. Thus it is not always possible to correlate initially nearby trajectories over long times for pseudointegrable systems, and this degree of unpredictability, which distinguishes them from integrable systems, is akin to chaotic behaviour where neighbouring trajectories separate exponentially with time.

Therefore, in some sense, pseudointegrable motion can be said to lie between integrable and chaotic motion, but it is not the generic case of such non-integrable behaviour. A generic perturbation of an integrable system:

$$
\begin{equation*}
H^{\prime}=H_{\mathrm{int}}+\varepsilon H_{1}, \tag{1}
\end{equation*}
$$

results in most of the motion still being confined to tori, with number-theoretically determined areas of chaos in regions centred on those unperturbed 'rational' tori that supported closed orbits.

[^0]This result, known as KAM theorem, (Lichtenberg and Lieberman 1983) has been proved to hold in the general case for only extremely gentle perturbations where $\varepsilon$ is very small and all derivatives of $H_{1}$ exist (Arnol'd 1978). It is nevertheless widely believed that these conditions are more stringent than necessary, and efforts to reduce them are an active field of research (Lichtenberg and Lieberman 1983).

It is impossible to obtain a pseudointegrable system by such a generic perturbation of an integrable system. However, in that their behaviour is largely similar it is possible to conceive of a 'pseudointegrable perturbation' which, by a small change in some parameter, would convert an integrable system into a pseudointegrable one.

As in previous studies, (Richens and Berry 1981, Henyey and Pomphrey 1982), we consider a 'billiard' problem, concerning motion within a two-dimensional hardwalled container. Such an enclosure in the shape of a rectangle is integrable because the absolute values of the velocities in the two directions parallel to the walls are both conserved, and together constitute the two constants of the motion required. A generic, non-integrable perturbation, such as a small potential variation within the rectangle, would give a typical non-integrable system with a mixture of regular and irregular motion as described by the KAM theorem. We can perturb the rectangle in a non-generic way by slightly altering the boundary conditions: We can consider a parallelogram of the same height (and hence same area) with one pair of parallel sides very close to the vertical. The perturbation in this case is the small angle they make with the vertical, which measures the deviation of the parallelogram from the rectangle.

In § 2 a quantum mechanical perturbation theory is presented with which we calculate the eigenvalues of the parallelogram for some small angle $\varepsilon$.

The justification for the term 'pseudointegrable perturbation' is that any parallelogram with angles which are rational fractions of $\pi$ is pseudointegrable. Richens and Berry (1981), have shown that any polygon with rational angles which tesselates the plane under a translation rule but not under a reflection rule is pseudointegrable. They hypothesise further, that irrational angles result in ergodic motion. However, there exists as yet no proof for the latter suggestion, although it is also implied by Hobson (1975). In that we are studying a small angle perturbation theory there is of course no possibility of distinguishing between rational and irrational values, although rational numbers being of zero measure amongst real numbers suggest it would be sensible to assume irrationality. It is also true, however, that any real number is always infinitely close to a rational number so that although the system may be ergodic it is always infinitely close to a nearby system with pseudoregular motion. Richens (1983) has pointed out that the ergodicity probably arises from 'holes' in the smooth phase space surfaces, though which orbits can escape to explore the rest of the energy surface.

In this paper we are concerned with the quantum mechanics of the parallelogram. It is surely unphysical to suppose that an infinitely small change in the system can cause its behaviour to be so radically altered as the classical picture suggests. We believe that the finite size of Planck's constant smoothes out the classical distinctions and that our results reveal a quantum effect which is more general than the classical classifications.

## 2. Perturbation theory for the parallelogram

In this section we will develop a perturbation theory for the bound states of a rectangle, as its shape alters to that of a parallelogram. Let us assume that the base of the
rectangle is of length $a$ and that its height is $b$, while the perturbation is the angle $\varepsilon$, which measures the deviation of the parallelogram from the rectangle. The parallelogram is of the same height $b$, as the rectangle, as shown in figure 1. Perturbation problems of this sort are known as 'boundary perturbation problems', (Morse and Feshbach 1953), with certain specific properties of their own. More usual perturbation theory uses the set of eigenfunctions of the unperturbed Hamiltonian (in our case this is the Hamiltonian for the rectangle) as a basis in which the eigenfunctions of the perturbed Hamiltonian are expanded. However, in the perturbation problem shown in figure 1 , it is obvious that this method will fail: In the triangular area between the right-hand side of the parallelogram and the right-hand side of the rectangle, all the unperturbed eigenfunctions are exactly zero and therefore cannot be used there as the basis for expansion of the perturbed eigenfunctions. Nevertheless, it is possible to formulate a boundary perturbation theory, providing that the perturbed boundary is always within the unperturbed boundary. The problem is then solved using standard perturbation techniques.


Figure 1. Rectangle with sides $a, b$ perturbed by a small angle $\varepsilon$ to parallelogram of side $a$, height $b$.

Here we solve the boundary perturbation problem of the parallelogram without making any restrictions on the form of the perturbation, except that it be concave everywhere.

We define the following two sets of eigenfunctions: one in the $x$ and the other in the $y$ direction. For a fixed $y$, smaller than $b$, the unnormalised functions

$$
\begin{equation*}
\varphi_{m}(x)=\sin \left[m \pi a^{-1}(x-y \tan \varepsilon)\right] \tag{2}
\end{equation*}
$$

form a complete set on $S_{y}$ in figure 1 for any potential which is zero at $x=y \tan (\varepsilon)$ and $x=a+y \tan (\varepsilon)$. Likewise, on the path $S_{x}$ in figure 1, the set

$$
\begin{equation*}
\varphi_{n}(y)=\sin \left(n \pi b^{-1} y\right) \tag{3}
\end{equation*}
$$

is the basis in the $y$ direction. With reduced units, $\left(2 m / \hbar^{2}=1\right)$ any solution of the Schrödinger (Laplace) equation

$$
\begin{equation*}
\partial^{2} \Psi / \partial x^{2}+\partial^{2} \Psi / \partial y^{2}=\left(-E+V_{11 \mathrm{gram}}\right) \Psi \tag{4}
\end{equation*}
$$

for the parallelogram can be written as

$$
\begin{equation*}
\Psi(x, y)=\sum_{m, n} C_{m, n} \varphi_{m}(x) \varphi_{n}(y) \tag{5}
\end{equation*}
$$

At this point we cannot proceed in the usual way by defining a set of unperturbed eigenfunctions of (4), in order to find $C_{m . n}$ in (5) as a perturbation series. Instead we
use another perturbation approach which does not require definition of the unperturbed basis.

The idea is based on the fact that the eigenvalues of the Hamiltonian are also the roots of an equation of the type

$$
\begin{equation*}
F(E ; \varepsilon)=0 \tag{6}
\end{equation*}
$$

$F$ is the determinant of $H-E$, where $H$ is the Hamiltonian matrix, which in the basis (2) and (3) is given by

$$
\begin{align*}
H_{m_{0}, n_{0} ; m, n}= & \pi^{2}\left(\frac{m_{0}^{2}}{a^{2} \cos ^{2} \varepsilon}+\frac{n_{0}^{2}}{b^{2}}\right) \delta_{m, m_{0}} \delta_{n, n_{0}} \\
& +8 \frac{\tan (\varepsilon)}{a b} \frac{m m_{0} n n_{0}}{\left(m^{2}-m_{0}^{2}\right)\left(n^{2}-n_{0}^{2}\right)}\left[1-(-1)^{m+m_{0}}\right]\left[1-(-1)^{n+n_{0}}\right] \tag{7}
\end{align*}
$$

the indices taking only positive integer values. The matrix elements (7) are zero for $m=m_{0}$ and $n=n_{0}$.

Equation (6) rewritten as

$$
\begin{equation*}
\operatorname{Det}(H(\varepsilon)-E)=0 \tag{8}
\end{equation*}
$$

gives the eigenvalues of (4) as functions of $\varepsilon$. In the perturbation method, the eigenvalues are expanded in the series

$$
\begin{equation*}
E_{q}(\varepsilon)=E_{q}^{(0)}+E_{q}^{(1)} \varepsilon+E_{q}^{(2)} \frac{1}{2} \varepsilon^{2}+\ldots \tag{9}
\end{equation*}
$$

where the index $q$ designates a set of quantum numbers characterising bound states.
It has been shown how these expansion coefficients can be found (Bosanac 1980, 1982), and therefore we will only summarise the final results. We distinguish two cases: (a) the Hamiltonian matrix is degenerate/non-degenerate and $(b)$ the first-order perturbation in the Hamiltonian matrix is zero/non-zero on the diagonal.

To simplify the discussion we will assume that $H$ is non-degenerate for $\varepsilon=0$. It can be shown, by expanding (7) in powers of $\varepsilon$, that the first-order perturbation of the Hamiltonian matrix is zero on the diagonal, and hence, (Bosanac 1982) $E_{b}^{(1)}=0$. Therefore the leading perturbation coefficient in (9) is of $O\left(\varepsilon^{2}\right)$. To calculate this coefficient we require the expansion coefficients in $\varepsilon$ of (7), up to $O\left(\varepsilon^{2}\right)$. These coefficients are

$$
\begin{aligned}
& H_{m_{0} n_{0}: m n}^{(0)}=\Pi^{2}\left(m_{0}^{2} / a^{2}+n_{0}^{2} / b^{2}\right) \delta_{m m_{0}} \delta_{n m_{0}} \\
& H_{n_{0} n_{0} ; m n}^{(1)}=\frac{8}{a b} \frac{m m_{0} n n_{0}}{\left(m^{2}-m_{0}^{2}\right)\left(n^{2}-n_{0}^{2}\right)}\left[1-(-1)^{m+m_{0}}\right]\left[1-(-1)^{n+n_{0}}\right] \\
& H_{m_{0} n_{0} ; m n}^{(2)}=2 \pi^{2}\left(m_{0}^{2} / a^{2}\right) \delta_{m m_{0}} \delta_{n n_{0}},
\end{aligned}
$$

therefore

$$
\begin{equation*}
H(\varepsilon)=H^{(0)}+\varepsilon H^{(1)}+\frac{1}{2} \varepsilon^{2} H^{(2)}+\mathrm{O}\left(\varepsilon^{3}\right) \tag{11}
\end{equation*}
$$

Using these results, it can be shown that $E_{b}^{(2)}$ is (Bosanac 1982),

$$
\begin{equation*}
E_{m n}^{(2)}=H_{m n, m n}^{(2)}-2 \sum_{\mu, \nu \neq m, n} \frac{H_{m n ; \mu \nu}^{(1)} H_{\mu \nu ; m n}^{(1)}}{H_{\mu \nu ; \mu \nu}^{(0)}-E_{m n}^{(0)}} \tag{12}
\end{equation*}
$$

where the indices $m$ and $n$ designate the quantum numbers of the unperturbed eigenvalues

$$
\begin{equation*}
E_{m, n}^{(0)}=H_{m, n}^{(0)} . \tag{13}
\end{equation*}
$$

If we replace the coefficients in (12) by their explicit values in (10), we obtain

$$
\begin{equation*}
E_{m n}^{(2)}=H_{m n ; m n}^{(2)}-2 \sigma_{m n} \tag{14}
\end{equation*}
$$

where
$\sigma_{m n}=\frac{64 m^{2} n^{2}}{a^{2} b^{2}} \sum_{\mu \nu \neq m n} \frac{\mu^{2} \nu^{2}\left(1-(-1)^{m+\mu}\right)^{2}\left(1-(-1)^{n+\nu}\right)^{2}}{\left[\pi^{2}\left(\mu^{2} / a^{2}+\nu^{2} / b^{2}\right)-E_{m n}^{(0)}\right]\left(m^{2}-\mu^{2}\right)^{2}\left(n^{2}-\nu^{2}\right)^{2}}$.
In the double summation we can find the explicit value of one sum, say the sum over $\mu$. We designate this sum by $\sigma_{m n}^{\nu}$ which is given explicitly by

$$
\begin{equation*}
\sigma_{m n}^{v}=\sum_{\mu \neq m} \frac{\mu^{2}\left[1-(-1)^{m+\mu}\right]^{2}}{\left[\mu^{2}+\left(a^{2} / b^{2}\right) \nu^{2}-E_{m, n}^{(0)}\right]\left(m^{2}-\mu^{2}\right)^{2}} \tag{16}
\end{equation*}
$$

where

$$
\begin{equation*}
E_{m, n}^{(0)}=m^{2}+\left(a^{2} / b^{2}\right) n^{2} \tag{17}
\end{equation*}
$$

We will show how the sum (16) is calculated for $m=$ odd values, a similar derivation can be done for $m=$ even values.

Firstly, each term in the sum (16) can be separated into three terms, so that $\sigma_{m n}^{\nu}$ separates into three sums. These three sums are typically of the form, (Gradstein and Ryzhik 1965)

$$
\begin{align*}
& \sum_{\mu=1}^{\infty} \frac{1}{4 \mu^{2}-m^{2}}=\frac{1}{2 m^{2}}, \quad \sum_{\mu=1}^{\infty} \frac{1}{\left(4 \mu^{2}-m^{2}\right)^{2}}=\frac{\pi^{2}}{16 m^{2}}-\frac{1}{2 m^{4}} \\
& \sum_{\mu=1}^{\infty} \frac{1}{4 \mu^{2}+c^{2}}=-\frac{1}{2 c^{2}}+\frac{\pi}{4 c} \operatorname{coth}\left(\pi \frac{c}{2}\right) \tag{18}
\end{align*}
$$

where we have replaced $\mu$ by $2 \mu$. When the last results are taken into account, then (16) is rewritten as

$$
\begin{equation*}
\sigma_{m, n}^{\nu}=\frac{\pi b^{2}}{a^{2}\left(\nu^{2}-n^{2}\right)}\left(\pi-\frac{b^{2}}{a^{2}} \frac{\left(a^{2} \nu^{2} / b^{2}-E_{m n}^{(0)}\right)^{1 / 2}}{\nu^{2}-n^{2}} \cdot \operatorname{coth}\left[\frac{\pi}{2}\left(\frac{a^{2}}{b^{2}} \nu^{2}-E_{m n}^{(0)}\right)^{1 / 2}\right]\right) \tag{19}
\end{equation*}
$$

If we take only $n=$ odd values, then $\sigma_{m n}$ is

$$
\begin{align*}
\sigma_{m n}=\frac{64 m^{2} n^{2}}{\pi^{2} b^{2}} & \left(\frac{\pi^{4} b^{2}}{64 a^{2} n^{2}}-4 \pi \frac{b^{4}}{a^{2}} \sum_{\nu=\text { even }} \frac{\nu^{2}\left(a^{2} \nu^{2} / b-E_{m n}^{(0)}\right)^{1 / 2}}{\left(\nu^{2}-n^{2}\right)^{4}}\right. \\
& \left.\times \operatorname{coth}\left[\frac{\pi}{2}\left(\frac{a^{2}}{b^{2}} \nu^{2}-E_{m n}^{(0)}\right)^{1 / 2}\right]\right) \tag{20}
\end{align*}
$$

Likewise, if $n=$ even then the summation index $\nu$ in (20) takes only odd values. In the case where $m=$ even (earlier it was assumed that $m=o d d$ ), then (20) is the same except that the coth function is replaced by a tanh function. Of course, the summation index $\nu$ always takes values depending on the parity of $n$.

From the explicit form for $\sigma_{m n}$, given by (20), we can now obtain the explicit form for $E_{m, n}^{(2)}$ :
$E_{m n}^{(2)}=512 \frac{m^{2} n^{2} b^{2}}{\pi a^{4}} \sum_{\nu=\text { even }} \frac{\nu^{2}\left(a^{2} \nu^{2} / b^{2}-E_{m n}^{(0)}\right)^{1 / 2}}{\left(\nu^{2}-n^{2}\right)^{4}} \operatorname{coth}\left[\frac{\pi}{2}\left(\frac{a^{2}}{b^{2}} \nu^{2}-E_{m n}^{(0)}\right)^{1 / 2}\right]$
where $m=$ odd and $n=$ odd. For other combinations of the indices $m$ and $n$, the rules are the same as just mentioned above.

The expansion coefficients $E_{m, n}^{(2)}$ are finite and the sum over $\nu$ is rapidly convergent, the largest contribution coming from the vicinity of $\nu \sim n$. However, there are particular values of $\nu$ for which one of the perturbation coefficients is infinite. This is whenever

$$
\begin{equation*}
\left[\left(a^{2} / b^{2}\right) \nu^{2}-E_{m n}^{(0)}\right]^{1 / 2}=\mathrm{i} \lambda \tag{22}
\end{equation*}
$$

where $\lambda$ is an integer; for $m=$ odd, $\lambda$ is even and for $m=$ even, $\lambda$ is odd. The relationship (22) is equivalent to

$$
\begin{equation*}
\left(a^{2} / b^{2}\right)\left(\nu^{2}-n^{2}\right)=m^{2}-\lambda^{2} \tag{23}
\end{equation*}
$$

which has a pair of solutions

$$
\begin{equation*}
(a / b)(\nu-n)=m-\lambda, \quad(a / b)(\nu+n)=m+\lambda \tag{24}
\end{equation*}
$$

Of course, these are not the only solutions of (22). They give for $\lambda$ and $\nu$

$$
\begin{equation*}
\lambda / n=a / b, \quad m / \nu=a / b . \tag{25}
\end{equation*}
$$

Therefore, if the ratio of $a$ and $b$ is a rational number then there will always be a perturbation coefficient which is infinite. The infinities which appear in the coefficients are due to the incompleteness of the non-degenerate perturbation theory. These infinities would not be present if for such cases we use perturbation theory for degenerate states (condition (22) implies degeneracy in the states ( $m, n$ ) and ( $\lambda, \nu)$ ).

However, in general one cannot give a closed form of the perturbation coefficients for degenerates states, as was the case with (21), because finding them requires diagonalisation of the submatrix corresponding to the degenerate states. Such eigenvalues are usually not found in an analytic form. Here we will demonstrate how this theory works for the simplest case when only two channels are degenerate; say ( $m_{1}, n_{1}$ ) and ( $m_{2}, n_{2}$ ) in which case we can find the analytic solution. As it turns out, in the perturbation theory with degenerate states, the first-order perturbation coefficient $E_{m, n}^{(1)}$ is non-zero (Bosanac 1982). This coefficient is found from the equation

$$
\begin{equation*}
\operatorname{Det}\left(H_{\mathrm{d}}^{(1)}-E^{(1)}\right)=0 \tag{26}
\end{equation*}
$$

where $H_{\mathrm{d}}^{(1)}$ is the submatrix of (10) which corresponds to the degenerate channels. In our case

$$
\begin{equation*}
\left[H_{\mathrm{d}}^{(1)}\right]_{m_{1} n_{1} ; m_{2} n_{2}}=\frac{32}{a b} \frac{m_{1} m_{2} n_{1} n_{2}}{\left(m_{1}^{2}-m_{2}^{2}\right)\left(n_{1}^{2}-n_{2}^{2}\right)} \tag{27}
\end{equation*}
$$

hence the two solutions for $E^{(1)}$ are

$$
\begin{equation*}
E^{(1)}= \pm \frac{32}{a b} \frac{m_{1} m_{2} n_{1} n_{2}}{\left(m_{1}^{2}-m_{2}^{2}\right)\left(n_{1}^{2}-n_{2}^{2}\right)} \tag{28}
\end{equation*}
$$

which are of course finite.

## 3. Comparison of perturbation theory results with exact computations

The Schrödinger equation can of course be solved numerically for a two-dimensional enclosure with boundary conditions equivalent to a hard-walled parallelogram of chosen angle. We used the standard matrix diagonalisation technique in order to find the first fifty eigenvalues with $m, n=$ odd, odd or even, even, (for which the solution was fully converged), with an angle $\varepsilon=0.81$ (see figure 1 ). This angle is equivalent to a value $\frac{1}{2} \varepsilon^{2}=0.0001$ (see equation (9)). The results were compared with the results of the perturbation theory as shown in figure 2.

Each point represents the relative difference between an eigenvalue and its corresponding rectangle value. (For these low-lying states the perturbation theory did not predict any energy level crossings so that there was a straightforward correlation between rectangle, exact computation, and perturbation theory states.) The points were plotted against the rectangle eigenvalues and joined up by straight lines for clarity of ordering in the neighbourhood of near-degeneracies.

As mentioned above, the perturbation theory has not been extended to the case of actual degeneracies. Therefore, we chose irrationally related sides for the unperturbed rectangle:

$$
a^{2} / b^{2}=2 /(\sqrt{5}-1)
$$

such that the degeneracy condition,

$$
\left(m_{1}^{2}-m_{2}^{2}\right) /\left(n_{2}^{2}-n_{1}^{2}\right)=a^{2} / b^{2},
$$

can never be satisfied. All the following numerical results lie within the computational limits which do, of course, finally impose rationality on all calculations.

For most states the difference between the exact and perturbation theory result is so small as not to be visible at the scale drawn in figure 2. (When a larger discrepancy occurs the perturbation theory results are joined by broken lines.) Although the majority of eigenvalues can be seen to be only slightly different from their corresponding rectangle values, much larger perturbations occur at near-degeneracies. The corresponding discrepancies between exact and perturbation theory results are also much greater since the perturbation theory tends to predict a proportionately larger change in the eigenvalue.

It is generally the case that the relative difference between the exact and perturbation theory result is at least an order of magnitude smaller than the relative difference between the rectangle and exactly computed parallelogram eigenvalues. In that the perturbation theory is somewhat oversensitive to near-degeneracies, it occasionally predicts a considerably larger change in some eigenvalues, (which are also exactly relatively greatly disturbed) as can be seen in figure 2 This reflects the fact that the perturbation theory sees crossings of energy levels as $\varepsilon$ is varied although such actual degeneracies are rigorously forbidden (von Neumann and Wigner 1927) and result in 'avoided crossings' (Berry 1981a) exactly. In the present computation we did not calculate more states exactly than those shown in figure 2 , but similar comparisons carried out for different values of $a$ and $b$ showed consistently good agreement. It was never the case that the perturbation theory predicted a smaller change in the eigenvalues than that obtained exactly.

Figure 3 shows the variation of half the energy levels ( $m, n=$ odd-odd or even-even) as a function of $\varepsilon$. (For this figure only: $a=1.0, b=0.6$.)


Figure 2. The relative difference between the rectangle eigenvalues, $E^{0}$, and the corresponding eigenvalues of the parallelogram with perturbation angle $\varepsilon=0.81^{\circ}$. The exact results for the first fifty $m+n=$ even states are shown by full circles joined by full lines; open circles and broken lines indicate perturbation theory discrepancies which are visible on the scale drawn. The two horizontal broken lines on either side of the $E^{0}$-axis are boundaries beyond which the modulus of the relative difference between rectangle and parallelogram eigenvalues is greater than 0.001 -i.e. $Q>10$ in equation (29).


Figure 3. Comparison of exact (full curves) and perturbation theory (broken curves) energy levels as functions of perturbation angle $\varepsilon$. Only states with $n+m=$ even (for $\varepsilon=0$ ) are shown, so that crossings of the exact energy levels are rigorously forbidden. Note that for this figure only $a=1.0, b=0.6$.

The form of the exact energy levels is a complicated structure of multiple avoided crossings. The structure is similar to that seen for both ergodic and pseudointegrable systems individually (Berry 1981b, Richens and Berry 1981), although the variation of $\varepsilon$ causes the system to fluctuate classically between pseudointegrability and chaos. The perturbation theory, however, shows only a simple parabolic dependence on $\varepsilon$, (see $\S 2$ ) which cannot of course be expected to have any significance for large angles. Figure 3 shows clearly the strong sensitivity of the perturbation theory to neardegeneracies, and, of course, the expected actual crossings of energy levels. For small angles these actual crossings are closely associated with the exactly avoided crossings.

## 4. Eigenvalue dependence on perturbation

The eigenvalues of the rectangle can be obtained directly semi-classically by BohrSommerfeld quantisation of the classical actions. The quantum numbers $m, n$, simply pick out those classical tori separated by discrete numbers of Planck's constant, $h$, in the two classical action coordinates. Hence the unperturbed eigenvalues lie on a lattice in the classical action plane whose unit cell is of area $h^{2}$. Since our parallelogram is designed to represent a perturbation of the rectangle we seek to compare their eigenvalues using the action grid of the rectangle as a means of reference. Figure 4 shows a plot of 68040 states where each point is labelled by a particular $m$ and $n$. The spots mark those eigenvalues which are predicted by the perturbation theory to
be grossly perturbed as the rectangle's shape changes to that of a parallelogram, (the others being relatively undisturbed), according to the simple criterion

$$
\begin{equation*}
\frac{2}{\varepsilon^{2}}\left|\frac{E^{\text {pert }}-E_{m, n}^{\mathrm{rect}}}{E_{m, n}^{\text {rect }}}\right|>Q=10 \tag{29}
\end{equation*}
$$

The vast majority of these grossly perturbed states lie in well defined regions which roughly correspond to areas surrounding certain 'rational' tori of the rectangle. The rationally related frequencies on the two action circuits of these tori define centres of 'resonance'. The distribution of these regions was fitted according to the relation

$$
\begin{equation*}
\frac{m}{n}=\frac{a^{2}}{b^{2}}\left(\frac{r}{s} \pm \frac{K(\varepsilon)}{s^{2 \cdot 0}}\right) \tag{30}
\end{equation*}
$$

where $r, s$ define the frequency ratio of a particular torus, $K(\varepsilon)$ is a constant obtained empirically from examination of the largest $(1,1)$ resonance. It is clear from the straight lines in the figure, which are obtained from equation (30) that this fit is extremely good far away from the origin. Closer to the origin we see that the regions of grossly perturbed states divide into two parts which lie outside the predictions of equation (30).

Only half of the rational tori are apparent in figure 4. Those with 'odd-even' or 'even-odd' frequency ratios (i.e. $(r, s)=(2,1)$ or ( 3,2 ) etc) do not show large perturbations of their corresponding quantum eigenvalues. We can understand their absence by a closer examination of the perturbation theory and the mechanism whereby some states are grossly perturbed.

It is clear from equation (15) that a large perturbation occurs for near degeneracies such that the denominator is very small. We can obtain the condition for their existence very simply from the eigenvalue equation. A small energy difference is given as a function of $m$ and $n$ by

$$
\begin{equation*}
\Delta E=(\partial E / \partial m) \Delta m+(\partial E / \partial n) \Delta n \tag{31}
\end{equation*}
$$

$\Delta m, \Delta n$ are defined according to (15) to be

$$
\begin{equation*}
\Delta m=m-\mu \quad \Delta n=n-\nu . \tag{32}
\end{equation*}
$$

For a resonance we require (30) to be fulfilled such that

$$
\begin{equation*}
m / n \approx\left(a^{2} / b^{2}\right)(r / s), \tag{33}
\end{equation*}
$$

but we see immediately that (33) is identical with (31) when rewritten (for $\Delta E$ small):

$$
\begin{equation*}
\left(2 m / a^{2}\right)(m-\mu) \approx\left(2 n / b^{2}\right)(n-\nu) . \tag{34}
\end{equation*}
$$

Hence we can identify

$$
\begin{equation*}
r=n-\nu \quad s=m-\mu \tag{35}
\end{equation*}
$$

For 'odd-even' frequency ratios of the corresponding tori

$$
\begin{equation*}
r+s=n-\nu+m-\mu=(n+\nu)+(m+\mu)-2 \nu-2 \mu=\text { odd number. } \tag{36}
\end{equation*}
$$

However, the nominator in equation (15) is only non-zero if both ( $n+\nu$ ) and ( $m+\mu$ ) are odd numbers, which contradicts (36), and therefore excludes half the rational tori as evinced by figure 4.


Figure 4. The action grid of the rectangle enclosing 68040 states. Those eigenvalues (labelled by $m, n$ ) which are predicted by the perturbation theory to be grossly perturbed in the nearby parallelogram, are marked by black spots; they lie in 'resonant' regions, (as shown by straight lines) which are centred on certain rational tori of the classical rectangle (as labelled).

The actual widths of the resonances in figure 4 are also dependent on the empirically defined constant, $K(\varepsilon)$. The $\varepsilon$ dependence of our $K$ is implicit in the variable choice of value assigned to $Q$ in equation (29).

It is interesting to note that the form of the distribution as given by equation (30) is of the form of the classical KAM theorem. It describes the areas of destroyed tori in non-integrable systems which are formed by a small generic perturbation, $\varepsilon$, of integrable systems. We have as yet no explanation as to why it should fit the distribution in figure 4.

Much work has been devoted to conjectures concerning the quantum mechanical spectra of systems exhibiting different kinds of classical behaviour. In particular, it has been suggested by Percival (1973), that quantum eigenvalues corresponding to classically regular and irregular motion are distinguished according to their sensitivity to small perturbations. The eigenvalues of the so-called 'irregular spectrum' are expected to be much less stable than those obtained by torus quantisation. For recent discussions see Noid et al (1981) and Marcus (1983).

We appear to be seeing such a distinction, although what is known of the classical mechanics of the system does not suggest that any of the eigenvalues should correspond to regular torus motion. Had we subjected the rectangular enclosure to a Kam-type perturbation of the form of equation (1) the continued existence of tori separated by
areas of chaos may well have implied an eigenvalue distribution similar to figure 4. The boundary perturbation into a parallelogram implies an essentially chaotic system with perhaps some ordering due to the underlying pseudointegrability. There are certainly smooth phase space structures existing in the perturbed system e.g. the family of simple closed orbits moving vertically between the upper and lower edges of the parallelogram. These structures can be interpreted as tori punctured by holes, or alternatively, as loose handles of multiply-handled spheres.

The quantum mechanics does not distinguish between the classical alternatives of a highly complex pseudointegrable motion and possible ergodicity of the small- $\varepsilon$ parallelogram. It merely perceives a perturbation of an integrable system which radically alters some eigenvalues while leaving others relatively undisturbed. It can be hypothesised that those eigenvalues which are not greatly changed by the perturbation correspond to areas of the classical phase space still occupied by smooth surfaces, and that these surfaces can be quantised if their destruction under perturbation is limited to holes of size $\hbar$ or less. However, even if this hypothesis should prove correct, it does not at all explain why the distribution as shown in figure 4 should be describeable by the Kam-type equation (30). What is known of the classical mechanics of the parallelogram might have led one to expect a quite random distribution.

Nevertheless, it is worth pointing out that the index of $s$ in equation (30) is not the expected value of 2.5 for a two-dimensional classical system. Quite generally, moreover, the derivation of the кам theorem shows that no classical tori survive under a perturbation unless the index of $s$ is greater than 2 . Therefore our empirical finding of 2.0 , although not accurate to less than 0.1 , would certainly seem to imply more chaos in the system than is the case for a generic perturbation, and may also be taken as consistent with the absence of tori classically. Also, if the index of $s$ is not greater than 2 the resonant zones of figure 4 will eventually widen to the extent of overlapping, such that at very high energies almost all eigenvalues will be predicted to be grossly perturbed by the perturbation theory. Thus semiclassically, at least, the results may confirm the ergodicity hypothesis. As mentioned above, the ergodicity of the irrationalangled parallelogram has not been proved. If the value for the index of $s$ of 2.0 should be accurate and also interpretable in classical terms, it could indicate a 'marginal ergodicity', consistent with an 'almost existence' of classical tori.

## 5. Conclusions

The results obtained by the perturbation theory which we have presented here are unexpected and therefore not immediately explainable.

We have found a quantum mechanical effect which is independent of the rapidly fluctuating ergodic-pseudoregular underlying classical motion and which may be interpreted as an indicator of quantum chaos. Although the occurrence of large disturbances of certain eigenvalues under perturbation can be loosely tied to their near-degeneracy, we find no explanation for their 'classical кaм-type' distribution in the event of our arbitrarily chosen definition of such large disturbances. Given that
(1) the system is classically always infinitely close to pseudointegrable motion and
(2) the system under such small perturbation is in some sense close to regular motion,
we can hypothesise that the smooth surfaces which exist in the phase space due to statements (1) and (2) above, are strongly influencing the results.

There is some reason to suppose that we may be seeing indications of quantum mechanical behaviour which is of far greater generality than the classical mechanics. It is possible to conjecture that a 'KAM-type' distribution of the kind which we have found occurs quite generally in perturbed integrable quantum systems although classical theory, at least till now, imposes much stronger conditions on the use of such a description.

## References

Arnol'd V I 1978 Mathematical Methods of Classical Mechanics (New York: Springer)
Berry M V 1981a Semiclassical Mechanics of Regular and Irregular Motion, Lectures at Les Houches (Amsterdam: North-Holland)

- 1981b Ann. Phys., NY 131 163-216

Bosanac S 1980 Fiz., Zagreb 1277

- 1982 J. Math. Phys. 23213

Gradstein I S and Ryzhik I M 1965 Table of Integrals and Products (London: Academic)
Henyey F S and Pomphrey N 1982 Physica 6D 78
Hobson A 1975 J. Math. Phys. 162210
Lichtenberg A J and Lieberman M A 1983 Regular and Stochastic Motion (New York: Springer)
Marcus R A 1983 Faraday Discussion 75 preprint
Morse P M and Feshbach H 1953 Methods of Theoretical Physics (New York: McGraw-Hill)
von Neumann and Wigner E 1927 Physik Z 30467
Noid D W M, Koszykowski M L, Marcus R A 1981 Ann. Rev. Phys. Chem. 32 267-309
Percival I C 1973 J. Phys. B: At. Mol. Phys. 6 L229-32
Richens P J 1983 Private communication
Richens P J and Berry M V 1981 Physica 2D 495


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