ASPECTS OF DEGENERACY

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1 INTRODUCTION

Without symmetry, degeneracies are considered to be 'accidential', reflecting the fact that for a typical Hamiltonian $\hat{H}$, representing a bound quantal system, no two of the energy levels E_n will coincide. But just as with road accidents the chance of a degeneracy can rise from negligible to inevitable if instead of considering individual Hamiltonians one embeds $\hat{H}$ in a population smoothly parameterised by variables $\underset{\sim}{R}=(X,Y,Z....)$. In section 2 I review an old argument of Von Neumann and Wigner (1929) indicating that for typical families $\hat{H}(\underset{\sim}{R})$ of real Hamiltonians, two parameters are necessary to produce a degeneracy, while if $\hat{H}(\underset{\sim}{R})$ is Hermitian (and not real) three parameters are necessary.

In a semiclassical context (Berry 1983a) where Planck's constant $\hbar$ is considered as a small parameter, quantal spectra exhibit a hierarchy of structures (Berry 1983b), characterised by energy ranges δE which are successively smaller in comparison with $\hbar$. In this hierarchy, degeneracies are the finest structures, with $\delta E=0$. Next come splittings due to barrier penetration, with $\delta E \sim O(\exp\{-\hbar^{-1}\})$. Then come spacings between adjacent and near-degenerate levels, which for systems with N freedoms correspond to $\delta E<O(\hbar^N)$. The mean spacings themselves have $\delta E \sim O(\hbar^N)$. Next come oscillatory clusterings involving many levels and associated with classical closed orbits, for which the 'energy wavelength' is $\delta E \sim O(\hbar)$. On the coarsest scale, $\delta E>O(\hbar)$ and only the average level density can be perceived (this depends only on the phase-space volume of the classical energy surfaces).

In section 3 I will discuss a different semiclassical aspect of degeneracies, and connect the avoided crossings of levels when a single parameter is varied with the emergence of chaotic behaviour when a classically integrable system is nonintegrably perturbed.

In section 4 I will give two versions of an argument connecting the number of parameters $\underset{\sim}{R}$ necessary to produce a degeneracy with the form of the distribution of spacings of neighbouring energy levels.

Finally, in section 5 I will summarise the curious phase behaviour of quantum states when continued in parameter space close to degeneracies.

2 HOW ACCIDENTAL IS A DEGENERACY?

Suppose that at some point $\underset{\sim}{R}^*$ in parameter space two states $|\psi_1^*\rangle$ and $|\psi_2^*\rangle$ are degenerate, with energy $E=E^*$, i.e.

$$\hat{H}(R^*)\,|\psi_1^*\rangle = E^*|\psi_1^*\rangle,\quad \hat{H}(R^*)\,|\psi_2^*\rangle = E^*|\psi_2^*\rangle. \tag{1}$$

If now the system is perturbed by varying $\underset{\sim}{R}^*$, does the degeneracy persist or do the levels split? According to degenerate perturbation theory (Von Neumann and Wigner 1929, translated in Knox and Gold 1964), the new states $|\psi_1(\underset{\sim}{R})\rangle$ and $|\psi_2(\underset{\sim}{R})\rangle$ are, to lowest order in $\underset{\sim}{R}-\underset{\sim}{R}^*$, linear combinations of the old ones, i.e.

$$|\psi_i(\underset{\sim}{R})\rangle \sum_{i=1}^{2} a_{ij}(\underset{\sim}{R})\,|\psi_j^*\rangle \quad (i=1,2) \tag{2}$$

To find the coefficients a_{ij} and the new energies $E_1(\underset{\sim}{R})$ and $E_2(\underset{\sim}{R})$, Schrodinger's equation is written in the $|\psi_j^*\rangle$ basis. This involves matrix elements

$$H'_{ij}(\underset{\sim}{R}) \equiv \langle\psi_i^*|\,\hat{H}(\underset{\sim}{R})-\hat{H}(\underset{\sim}{R}^*)\,|\psi_j\rangle \tag{3}$$

and gives, for the energy splitting,

$$\Delta E(\underset{\sim}{R}) \equiv E_2(\underset{\sim}{R})-E_1(\underset{\sim}{R}) = \{[H'_{11}(\underset{\sim}{R})-H'_{22}(\underset{\sim}{R})]^2 + 4|H'_{12}(R)|^2\}^{\frac{1}{2}} \tag{4}$$

At a degeneracy, ΔE must be zero, and this requires

$$H'_{11}(\underset{\sim}{R})=H'_{22}(\underset{\sim}{R}),\quad \mathrm{Re}H'_{12}(\underset{\sim}{R})=0,\ \mathrm{Im}\,H'_{12}(\underset{\sim}{R})=0. \tag{5}$$

Consider first the case where the family $\hat{H}(\underset{\sim}{R})$ consists of Hermitian Hamiltonians which are not restricted to be real. This represents quantal systems without time-reversal symmetry, such as a particle bound by a scalar potential and in an external magnetic field. Then the three equations in (5) give independent restrictions on $\hat{H}(\underset{\sim}{R})$ and so at least three parameters $\underset{\sim}{R}$ are required in order to

satisfy them. If there are exactly three parameters, the degeneracy is isolated at the single point $\underset{\sim}{R}^*$ If there are M > 3 parameters, then equations (5) are satisfied on an M-3 dimensional manifold including $\underset{\sim}{R}^*$, so that the degeneracy is not isolated - for example in a four-parameter space a line of degenracy passes through $\underset{\sim}{R}^*$. This conclusion can be expressed as follows: for Hermitian operators, degeneracies have codimension three.

Now consider the case where $\hat{H}(\underset{\sim}{R})$ consists of <u>real</u> Hamiltonians (real symmetric matrices), representing quantal systems without time-reversal symmetry (no external magnetic fields). The last of equations (5) is now an identity, leaving just two independent conditions to be satisfied in order for a degeneracy to occur. If there are exactly two parameters $\underset{\sim}{R}$, the degeneracy is isolated at the single point $\underset{\sim}{R}^*$. For M > 2 parameters, the degeneracy is not isolated but lies on an M-2 dimensional manifold including $\underset{\sim}{R}^*$ - for example in a three-parameter space a line of degeneracy passes through $\underset{\sim}{R}^*$. This conclusion can be expressed as follows: for real symmetric operators, degeneracies have codimension two.

It is obvious that these arguments do not rely on there being any symmetry, and so really do establish conditions under which accidental degeneracies occur. If the family $\hat{H}(\underset{\sim}{R})$ consists of Hamiltonians with geometric symmetry, then group theory enforces different conditions for degeneracy, as explained by Arnol'd (1972 and appendix 10 of 1978) for the case of real operators.

For $\underset{\sim}{R}$ close to $\underset{\sim}{R}^*$, the perturbation matrix elements H_{ij} (equation 3) depend linearly on the components of $\underset{\sim}{R}-\underset{\sim}{R}^*$. If there are two parameters $\underset{\sim}{R}=(X,Y)$ and the Hamiltonians $\hat{H}(X,Y)$ are real, (4) implies that the level separation has the form

$$\Delta E(X,Y)=\{A(X-X^*)^2+ 2B(X-X^*)(Y-Y^*) + C(Y-Y^*)^2\}^{\frac{1}{2}} \qquad (6)$$

where the quadratic form is positive-definite and A,B,C depend on components of $\nabla_R\hat{H}$ at $\underset{\sim}{R}^*$. This is the equation of a double cone (Teller 1937) in the space $\Delta E,X,Y$, and the levels $E_1(X,Y)$ and $E_2(X,Y)$ also intersect conically in E,X,Y space (fig.1). The diabolo geometry which organises degeneracies in these typical quantal systems with real Hamiltonians makes it natural to refer to the degeneracies themselves as <u>diabolical points</u>.

In molecular physics, the importance of diabolical points in electronic levels (where the parameters $\underset{\sim}{R}$ are nuclear coordinates) has been emphasised by Vaz Pires et al (1978), Desouter-Lecomte et al (1979) and Dehareng et al (1983). In nuclear physics, the importance of diabolical points in nucleon spectra (where $\underset{\sim}{R}$ para--meterises nuclear shape) was emphasized by Hill and Wheeler (1952).

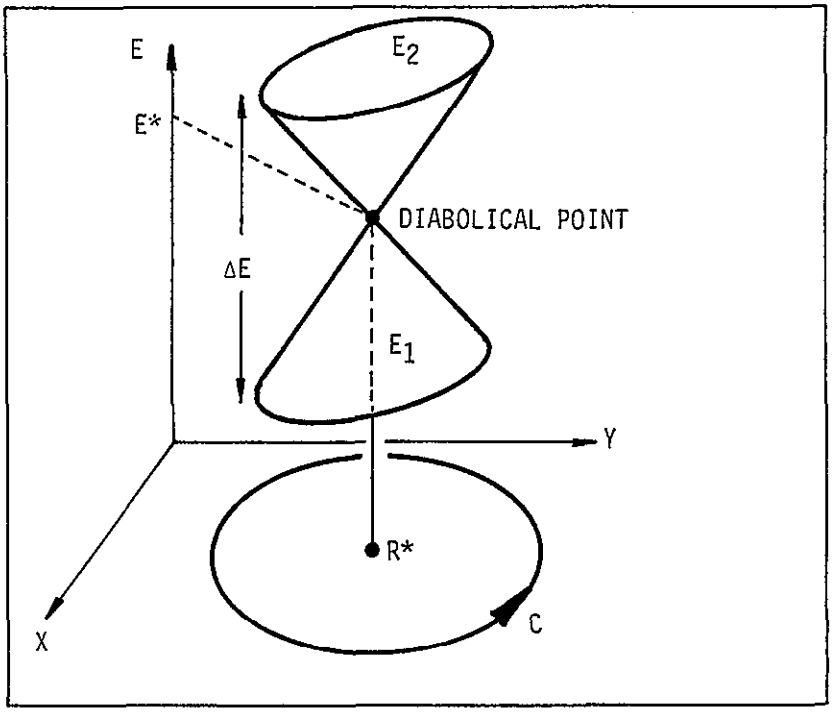

Fig.1. Geometry and notation near a diabolical point.

Berry and Wilkinson (1984) study diabolical points in the two-parameter family of'quantum triangles' (vibrations of triangular membranes) whose levels are determined by Schrödinger's equation for free motion within the triangles and vanishing wave function on the boundary. X and Y may correspond to any two angles (the third angle being determined and the size of the triangle causing trivial scaling of the levels). By exploring triangle space X,Y, a number of diabolical points were found numerically (their diabo--lical nature being established by a sign-change rule to be descri--bed in section 5). The lowest diabolical point involved levels 4 and 5 (the ground state being level 1) for the triangle 130.57°, 30.73° , 18.70° . This might be called the 'paradoxical triangle' on account of its being the non-special (generic) triangle with the special property that no other triangle has a lower pair of levels degenerating for reasons not connected with symmetry. (Of course there are lower degeneracies arising from symmetry such as levels 2, 3 for the equilaterial triangle, and levels 3,4 and 4,5 for certain isosceles triangles.)

For Hermitian Hamiltonians, the diabolical structure in E,X,Y space generalizes to a hyperconical intersection in the

four-dimensional space E,X,Y,Z, where Z is the third parameter required to produce the degeneracy. For example, Z might be the strength of a magnetic field perpendicular to the plane of a quantum triangle; in this case I expect degeneracies for Z=0 to disappear when the field is switched on, but that new ones will appear for finite values of Z (for different triangles X,Y).

3 AVOIDED CROSSINGS AND CHAOS IN QUASI-INTEGRABLE SYSTEMS

It is clear that a family of generic Hamiltonians $\hat{H}(X)$ (Hermitian or real) depending on a single parameter X will not exhibit degeneracies: in the plane E,X, the eigenvalue curves $E_n(X)$ will not cross. Instead, the curves will display avoided crossings whose local form (which can be considered to arise from a close approach to a degeneracy in an augmented parameter space) is that of a pair of hyperbolas (slices of a cone or hypercone). Such avoided crossings are now familiar in calculations of the quantal spectra of families classically nonintegrable systems: in nonlinearly coupled oscillators (Noid et al 1980, Marcus 1980), in chaotic quantum billiards (Berry 1981), in (pseudointegrable) rational quantum billiards (Richens and Berry 1981) and in triangle quantum billiards (Berry and Wilkinson 1984).

If the family consists of Hamiltonians $\hat{H}(X)$ which are not generic but are special in some way, then degeneracies can be expected to occur. An important case is families of separable systems. For example in two dimensions a particle in a rectangular box with side ratio X has levels labelled by quantum numbers m,n with energies $E_{m,n} \sim m^2+X^2n^2$, which can degenerate when X^2 is rational; and a particle in a central potential V(r;X) may exhibit degeneracies between states of different angular momentum as X alters the strength or shape of V (these should not be confused with the two-fold degeneracy for nonzero angular-momentum states for all X, which is a direct consequence of the circular symmetry).

A slight generalization is to one-parameter families of classically integrable systems, whose phase-space trajectories are confined to tori (see for example the review by Berry 1978 or the book by Lichtenberg and Lieberman 1983). Then degeneracies will occur in levels approximated semiclassically by torus quantization (Maslov and Fedoriuk 1982, Berry 1983a) which for N freedoms can be formulated as follows: the state with quantum numbers $\underline{m}=(m_1.....m_N)$ is associated with the torus whose actions $\underline{I}=(I_1 .....I_N)$ (corresponding to its N irreducible cycles) is

$$\underline{I}_{\underline{m}} = (\underline{m} + \underline{\alpha}/4)\hbar \qquad (7)$$

where $\underline{\alpha}$ is a vector of integers (Maslov indices) depending on the embedding of the torus in phase space. The energy $E_{\underline{m}}(X)$ of the

state $\underset{\sim}{m}$ is simply

$$E_{\underset{\sim}{m}}(X)=H(\underset{\sim}{I}_{\underset{\sim}{m}};X), \tag{8}$$

where $H(\underset{\sim}{I};X)$ is the Hamiltonian in action representation for the family of integrable systems.

Because torus quantization is only an approximation, the level crossings (degeneracies) predicted by (8) may in the exact quantal system be avoided crossings (near-degeneracies). A simple example occurs in one dimension for a particle in a double-well potential $V(x;X)$ whose form depends on X and is symmetric when X=0. In torus quantization (Bohr-Sommerfeld quantization in this case) the two wells are quantized separately, and there would be degeneracies when X=0; in reality, of course, these are split by barrier penetration, giving levels $E_n(X)$ with very narrow avoided crossings (splittings $O(\exp(-1/\hbar))$ as compared with spacings $O(\hbar)$).

A more interesting example is of families of multidimensional systems whose classical motion is quasi-integrable, i.e. perturba--tions of integrable systems. Then the torus quantization formula (8) is inexact in two senses: it is a semiclassical approximation to the quantum mechanics, and a torus approximation to the classical mechanics. For such cases, Marcus (1980), Noid et al (1980) and Ramaswamy and Marcus (1981) have associated multiple avoided cros--sings in the quantal spectrum $E_n(X)$ with chaos in the classical motion. This association is explained by the following simple argument, which was suggested to me by Ozorio de Almeida (private communication) and which does not appear explicitly in the papers cited although it is surely known to their authors.

On the basis of torus quantization (7 and 8), two states with quantum numbers $\underset{\sim}{m}_1$ and $\underset{\sim}{m}_2$ will degenerate for some parameter value X* if their tori $\underset{\sim}{I}_{\underset{\sim}{m}_1}$ and $\underset{\sim}{I}_{\underset{\sim}{m}_2}$ have the same energy, which if $\underset{\sim}{m}_1$ and $\underset{\sim}{m}_2$ are not too different implies

$$E_{\underset{\sim}{m}_1}(X^*)-E_{\underset{\sim}{m}_2}(X^*) \approx \hbar(\underset{\sim}{m}_1 - \underset{\sim}{m}_2)\cdot \nabla_I H(\underset{\sim}{I}_{\bar{\underset{\sim}{m}}};X^*) = 0, \tag{9}$$

where $\bar{\underset{\sim}{m}} \equiv (\underset{\sim}{m}_1 + \underset{\sim}{m}_2)/2$. Now

$$\nabla_I H(\underset{\sim}{I}) = \underset{\sim}{\omega}(\underset{\sim}{I}) \tag{10}$$

which denotes the set of frequencies $\omega_1 \ldots \omega_N$ with which the trajectory winds round the torus. Because $\underset{\sim}{m}_1 - \underset{\sim}{m}_2$ is a vector whose components are integers, (9) implies that the degenerating tori have rationally dependent frequencies. For small $\hbar$, these degeneracies, which torus quantization predicts near those para--meters X* for which quantized tori are rational tori, will occur

between many pairs of levels, i.e. those whose mean is $\bar{\underset{\sim}{m}}$ and whose difference $\underset{\sim}{m}_1 - \underset{\sim}{m}_2$ is small enough for the linear approximation (9) to hold.

But this prediction must fail in two ways. Firstly, torus quantization is not exact: because the family is generic (quasi-integrable), the exact quantal spectrum will exhibit not degeneracies but multiple avoided crossings. And secondly, the tori on which the prediction is based will not exist: because these tori have rationally dependent frequencies, they lie in narrow phase-space zones in which the nonintegrable perturbation destroys tori and replaces them (at least in part) by chaotic trajectories (see e.g. Berry 1978, Lichtenberg and Lieberman 1983). Thus nonexistent tori would predict nonexistent degeneracies, and actual chaos is associated with actual multiple avoided crossings.

The foregoing argument applies to quasi-integrable systems, and should not be misinterpreted to imply that multiple avoided crossings are always associated with classical chaos. In pseudo-integrable systems (rational billiards), for example, all trajectories are confined to N-dimensional invariant surfaces (multiple-handled spheres rather than tori), and there is no chaos in the sense of exponential separation; nevertheless, Richens and Berry (1981) found multiple avoided crossings in the spectrum of a family of such systems. (Isolated avoided crossings can occur even in integrable systems, as the earlier double-well example showed.)

4 DEGENERACIES AND LEVEL SPACINGS

In the semiclassical limit there is an intimate connection between the degeneracies of a family of systems and the distribution of level spacings for an individual system, which I will explain in two different ways. The spacings are defined so as to have the average value unity; this is achieved by magnifying the energy using the local smoothed level density $d\mathcal{N}(E)/dE$, where $\mathcal{N}(E)$ denotes the smoothed number of levels below E (Berry 1983a). For the system with parameters $\underset{\sim}{R}$, the n'th spacing is thus

$$S_n(\underset{\sim}{R}) \equiv (E_{n+1}(\underset{\sim}{R}) - E_n(\underset{\sim}{R}))\frac{d\mathcal{N}}{dE}(E_n;\underset{\sim}{R}) \qquad (11)$$

The level spacing distribution $P(S;E,\underset{\sim}{R})$ for the system $\underset{\sim}{R}$ at energy E is defined as

$$P(S;E,\underset{\sim}{R}) \equiv \left(\Delta E\frac{d\mathcal{N}}{dE}(E;\underset{\sim}{R})\right)^{-1} \sum_{n=\mathcal{N}(E-\Delta E/2;\underset{\sim}{R})}^{\mathcal{N}(E+\Delta E/2;\underset{\sim}{R})} \delta(S-S_n(\underset{\sim}{R})) \Bigg\}$$
$$\left(\begin{array}{l}\Delta E\to 0\\ \hbar^N/\Delta E\to 0\end{array}\right) \qquad (12)$$

This definition exploits the fact that semiclassically the level density is very large, so that in the limit it is possible to de-fine a distribution over infinitely many levels (spacing $\sim \hbar^N$) in an infinitesimal range ΔE, for an individual system $\underset{\sim}{R}$.

Of particular interest is the form of P(S) for small spa-cings. If P(S) vanishes as $S \to 0$, there is level repulsion; if P(S) tends to a constant as $S \to 0$, there is level clustering. Later I will show that these different types of behaviour occur for systems with different degeneracy structures.

In previous theories, developed to model the many-body physics of nuclei (Porter 1965), P(S) is defined not for an individual system but for an ensemble whose Hamiltonian matrix elements (real symmetric or Hermitian) are random (in fact with a Gaussian distribution). For semiclassical systems the connection between the ensemble and individual spacing distributions is made by realising that (by assumption) there is nothing particular about the system with parameters $\underset{\sim}{R}$, so that (12) would give the same P(S) for any other system close to $\underset{\sim}{R}$ in the family. Therefore (12) is unaffected by ensemble-averaging over a region of parameter space near $\underset{\sim}{R}$. Then, however, all terms in the summation over spa-cings of levels n close to $\mathcal{N}(E)$ become the same, so that the prefactor cancels and

$$P(S;E) = \langle \delta(S - S_{\mathcal{N}(E)}(\underset{\sim}{R}) \rangle_{\underset{\sim}{R}}, \qquad (13)$$

where $\langle \ \rangle_{\underset{\sim}{R}}$ denotes the ensemble average.

In the first way of understanding P(S), only small spacings are considered. The ensemble average (13) then contains contribu-tions only from parameter-space regions where the surfaces $E_{\mathcal{N}}(\underset{\sim}{R})$ and $E_{\mathcal{N}+1}(\underset{\sim}{R})$ (fig.2), which correspond to the spacing $S_{\mathcal{N}}$, are close to diabolical points. In these regions, the energy surfaces are well approximated by cones (eq.6 or fig.1) for generic real Hamil-tonians or hypercones for generic Hermitian Hamiltonians.

It is easiest to estimate not P(S) but its integral, namely

$$\begin{aligned} \int_0^S dS P(S) &= \text{probability that level spacing} < S \\ &= \text{fraction of parameter space for which } S_{\mathcal{N}}(\underset{\sim}{R}) < S \\ &\propto \text{measure of parameter space for which sheets of cone} \\ &\quad \text{have spacing} < S \\ &\propto S^2 \text{(real Hamiltonian, i.e. two parameters)} \\ &\propto S^3 \text{(Hermitian Hamiltonian, i.e. three parameters)}, \end{aligned} \qquad (14)$$

where the proportionalities S^2 and S^3 arise from the fact that when S is small the cones or hypercones expand linearly away from dege-neracies.

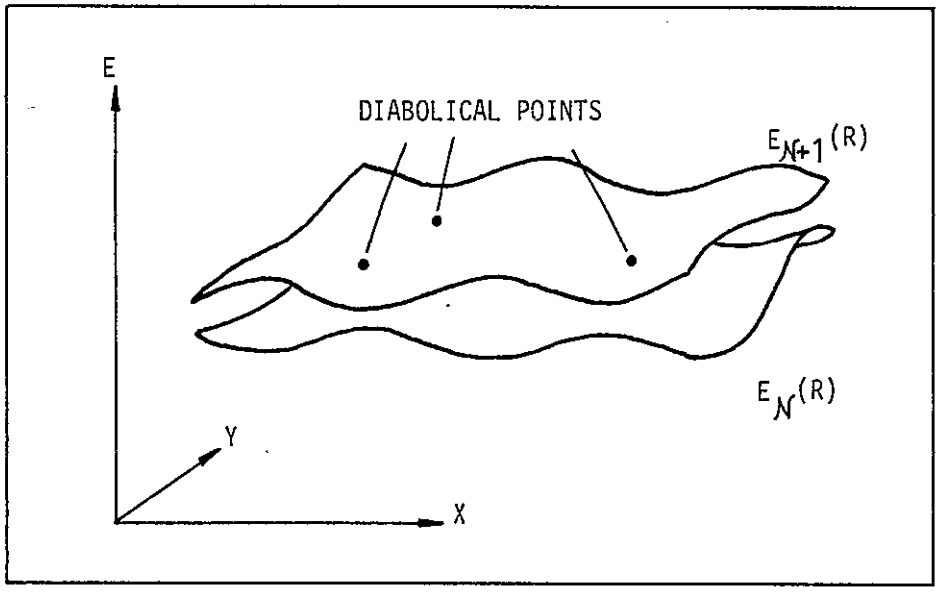

Fig.2. Neighbouring energy levels of generic real Hamiltonians, as a function of parameters $R=(X,Y)$. The surfaces are conically connected at diabolical points.

Thus

$$P(S) \propto \begin{cases} S \text{ (generic real Hamiltonian)} \\ S^2 \text{ (generic Hermitian Hamiltonian)} \end{cases} \text{(as } S \to 0) \qquad (15)$$

These results indicate that generically there is level repul--sion, whose nature depends on whether the Hamiltonian is real or Hermitian. For real Hamiltonians, there is accumulating evidence to support the linear level repulsion predicted by (15), based on computations of spectra for several different nonintegrable systems. These include: the stadium billiard (McDonald and Kaufman 1979) and the Sinai billiard (Berry 1981), both of which are chaotic; the square torus billiard (Richens and Berry 1981), which is pseudo--integrable; and irrational triangle billiards (Berry and Wilkinson 1984), which are nonintegrable but neither pseudointegrable nor fully chaotic.

For Hermitian Hamiltonians, (15) predicts quadratic level repulsion. To my knowledge this prediction has not been tested by computation. One such test would be to calculate the levels for a classically nonintegrable planar billiard, with a uniform magnetic field perpendicular to its plane.

As I have already pointed out, separable systems, and

integrable systems with torus quantization, are not generic in that they exhibit degeneracies when a single parameter X is varied. This leads to a simple modification of the argument in equation (14): locally linear level crossings in the E,X plane imply $\int_0^S dSP(S) \propto S$. Thus P(S) tends to a constant as $S \to 0$ so that there is level cluste--ring - a result obtained in a different way, and illustrated by several computations, by Berry and Tabor (1977).

An extension of the scaling argument leading to (15) enabled Berry and Wilkinson (1984) to estimate that for generic planar billiards the semiclassical density of degeneracies in $\underset{\sim}{R}=(X,Y)$ space, between any pair of levels, increases as $\hbar^{-3}$.

Now we turn to the second way of understanding the form of P(S) for classically chaotic systems. This is due to Pechukas (1983), whose argument (which is based on an idea of Dyson 1962 - reprinted in the book by Porter 1965) I will now paraphrase. Let a single parameter vary; think of this as time and denote it accordingly by t rather than X. Regard the levels as a system of particles distributed along the energy axis, with coordinates $E_n(t)$. P(S) (and much more) will be determined by the dynamics of the levels under the time-dependent Hamiltonian $\hat{H}(t)$. Pechukas chooses a function of $\hbar$ for his parameter, which is unfortunate because it excludes quantum billiards (whose levels merely scale homogeneously with $\hbar$); I will work with an arbitrary parameter t.

The dynamics of the levels are determined by Schrodinger's equation, which for the state $|n(t)>$ is

$$\hat{H}(t)\,|n(t)> = E_n(t)\,|n(t)>. \tag{16}$$

By elementary means, the velocity of the levels is obtained as

$$\dot{E}_n(t) = \dot{H}_{nn}(t) \tag{17}$$

and their accelerations as

$$\ddot{E}_n(t) = \ddot{H}_{nn}(t) + 2\sum_{m\neq n} \frac{|\dot{H}_{mn}(t)|^2}{E_n(t)-E_m(t)}\ , \tag{18}$$

where dots denote d/dt and

$$\dot{H}_{mn}(t) \equiv <m(t)\,|\frac{d\hat{H}(t)}{dt}\,|n(t)>\ . \tag{19}$$

The important equation is (18); its energy denominators show that the acceleration of the levels is dominated by strong interparticle repulsive forces which inhibit collisions (degeneracies).

The next step is to fix an energy E near which the spectrum

is to be studied, and introduce new coordinates $q_n(t)$ with E as origin and scaled so as to give a mean level spacing unity (cf 11 and its preceding paragraph); thus

$$E_n(t) \equiv E + \frac{q_n(t)}{d\mathcal{N}(E;t)/dE} \tag{20}$$

Now comes a crucial simplification. For classically chaotic systems, there is theoretical (Berry 1977, 1983a) and computational (McDonald and Kaufman 1979) evidence that quantum states resemble Gaussian random functions of their variables (e.g. position), which is a quantal reflection of classical exploration of the whole energy surface in phase space. This implies firstly that the matrix elements $\dot{H}_{mn}(t)$ in (18) couple the state n to many different states m with the same average strength, and secondly that $\dot{H}_{mn}(t)$ fluctuate rapidly with t. Dyson (1962), studying random matrices, treats these fluctuations as an underlying Brownian motion superposed on the interparticle repulsion. Pechukas (1983) makes the crucial simplification of simply replacing these fluctuating matrix elements by their t-averages. This amounts to the assumption that the time-scale of the fluctuations in $\dot{H}_{mn}$ is short in comparison with the time-scale of near-collisions resulting from interparticle bouncing; it is not clear how this assumption (which I expect to be valid in the semiclassical limit $\hbar \to 0$) might be justified.

With this simplification, the equations of motion become, in terms of the coordinates q_n (eq.20), and after subtracting any drift embodied in the average value of $\ddot{H}_{nn}$:

$$\ddot{q}_n(t) = \sum_{m \neq n} \frac{A_{mn}}{q_n(t) - q_m(t)} \tag{21}$$

where (with angle brackets now denoting an ensemble average over t)

$$A_{mn} \equiv 2\left(\frac{d\mathcal{N}(E)}{dE}\right)^2 \langle |\dot{H}_{mn}|^2 \rangle_t . \tag{22}$$

This describes the classical mechanics of particles distributed (with unit mean density) along the q axis, whose 'Hamiltonian' is

$$\mathcal{H}(\{q_n\}\{p_n\}) = \tfrac{1}{2} \sum_n p_n^2 + \sum\sum_{m<n} V_{mn}(q_m - q_n) \tag{23}$$

with interaction potential

$$V_{mn}(q_m - q_n) = - A_{mn} \ell n |q_m - q_n| . \tag{24}$$

The distribution of spacings $S_n (\equiv q_{n+1} - q_n)$, and other level statistics, is given by an average over t (cf 13).

Assuming that the interacting particles attain thermal equilibrium at some temperature $1/\beta$, this time average is also a thermal average, so that the joint probability distribution for all the levels is

$$P(\{q_n\}) \propto e^{-\beta\Sigma_{m<n} V_{mn}(q_m-q_n)} = \prod_{m<n} |q_m-q_n|^{\gamma_{mn}} \tag{25}$$

where

$$\gamma_{mn} \equiv A_{mn}\beta \tag{26}$$

To find the temperature $1/\beta$ we realise from (23) that this is the mean value of the fluctuations in (momentum)^2, which from (17) and (20) is

$$\frac{1}{\beta} = \langle p_n^2\rangle_t = \langle \dot{q}_n^2\rangle_t = \left(\frac{d\mathcal{N}(E)}{dE}\right)^2 \left(\langle \dot{H}_{nn}\rangle_t - \langle \dot{H}_{nn}\rangle_t^2\right) \tag{27}$$

Together with (26) and (22) this gives, for the exponent (25),

$$\gamma_{mn} = \frac{2\langle |\dot{H}_{mn}|^2\rangle_t}{\langle \dot{H}_{nn}^2\rangle_t - \langle \dot{H}_{nn}\rangle_t^2} \tag{28}$$

For few-neighbour statistics such as P(S), only the local interparticle forces, as embodied in γ_{mn} for $|m-n|$ not large, are important. To find these γ_{mn}, use is again made of the semiclassical chaos hypothesis, in the following explicit form: in the position representation the wavefunctions $\psi_m(\chi)$ and $\psi_n(\chi)$ of the states $|m\rangle$ and $|n\rangle$ are independent real or complex Gaussian random functions of χ with the same statistics, the ensemble being parameterized by t. Under this hypothesis, the averages appearing in (28) of the matrix elements

$$\dot{H}_{mn} = \int\cdots\int d\chi_1 d\chi_2\ \psi_m^*(\chi_1)\psi_n(\chi_2)\langle\chi_1|dH/dt|\chi_2\rangle \tag{29}$$

can be calculated (using elementary but lengthy algebra) and compared. The result is

$$\left.\begin{aligned}\gamma_{mn} &= 1 \text{ (real } \hat{H}\text{)}\\ &= 2 \text{ (Hermitian } \hat{H}\text{)}\end{aligned}\right\}. \tag{30}$$

The fact that γ_{mn} is independent of m and n is a time-averaged reflection of the fact that at any given t the operator dH/dt couples many semiclassically chaotic states with approximately equal strength. This behaviour contrasts with the coupling of semiclassical states in classically integrable

systems (Pechukas 1983). The fact that the values of γ_{mn} in (30) are so simple reflects a curious feature of the statistical mecha--nics of energy levels: the strength of the potential is related to the temperature (in different ways for real and Hermitian Hamiltonians).

When combined with (25) and the constraint of unit density, these values of γ_{mn} give the joint distribution of the energy levels. It implies exactly the same few-neighbour statistics as the eigenvalues of random matrices (Porter 1965), in particular the level repulsion laws (15) for P(S) as $S \to 0$ which we obtained by cone scaling. Bohigas and Giannoni (private communication)have found, for the levels of classically chaotic systems, strong computational evidence that few-neighbour statistics other than P(S) are also in good agreement with the predictions of random-matrix theory.

The universality of few-neighbour statistics for generic semiclassical systems and random matrices cannot extend to the statistics of distant levels. Even in random matrix theory, the distant correlations are model-dependent, being different for the orthogonal matrices of the circular ensemble and the symmetric matrices of the Gaussian ensemble (Porter 1965). Semiclassically, the distant correlations between levels separated by $O(\hbar)$ (i.e. for groups of $O(\hbar^{-(N-1)})$ levels in an N-freedom system) must reflect the nature of the eventual decay of the interaction-strength γ_{mn} from the values (30); in any case it is known (Berry 1983ab, see also Hannay's paper in this volume) that such distant correlations take the form of oscillatory clustering associated with individual classical closed orbits.

5 PHASE CHANGES NEAR DEGENERACIES

Near a degeneracy in parameter space $\underline{R}$, energy levels $E_n(\underline{R})$ have diabolical connections as discussed in section 2 (see fig.1) which depend on whether the Hamiltonian $H(\underline{R})$ is real or Hermitian. Now I will discuss the nature of the stationary states $|n(\underline{R})>$, by asking: how do the $|n(\underline{R})>$ behave under continuation in $\underline{R}$ space? In particular, if $\underline{R}$ is varied round a circuit C, how are the states at the beginning and end of the loop related? Without further information the answer can only be that the states are related by an arbitrary phase factor because the only restriction on $|n(\underline{R})>$ is that it is an eigenstate of $\hat{H}(\underline{R})$, and this leaves its phase undefined.

For real $\hat{H}(\underline{R})$, a natural restriction on $|n(\underline{R})>$ is that in some basis (e.g. the position representation $\underline{x}$) wavefunctions $\psi_n(\underline{x};\underline{R})$ remain real. Only the sign of ψ_n remains undetermined, and this can be fixed by requiring $\psi_n(\underline{x};\underline{R})$ (which depends smoothly on

x) to vary continuously with R. With this (implicit) convention Herzberg and Longuet-Higgins (1963) (see also Longuet-Higgins 1975) found by considering the multipliers a_{ij} in (2) that the quantum state changes sign if and only if C encloses an odd number of diabolical points (as in fig.1). Such enclosure is possible because degeneracies have codimension two for real Hamiltonians.

The sign change is a test for diabolical points, and is employed by Berry and Wilkinson (1984) for quantum triangles whose angles were taken round a cycle C of changes so as to surround a triangle for which two states were degenerate: the normal derivative of the wavefunction of either state was seen to change sign round C. Globally, the sign change implies that the nodal lines (or more generally nodal hypersurfaces) in x space must move as C is traversed. Korsch (1983) shows a particularly simple example involving two degenerate states of a square quantum billiard; in this case the degeneracy occurs because of symmetry. Fig.3 shows the nodal patterns associated with a sign reversal for a circuit of a degeneracy (which is not symmetry-generated) in a quantum triangle; for details see Berry and Wilkinson (1984).

For Hermitian $\hat{H}(R)$, continuity as C is traversed is not sufficient to determine the phase change of a quantum state. A natural physical principle which does determine the phase change is to consider C being traversed very slowly in time and defined by $R(t)$, so that $H(R(t))$ is a time-dependent Hamiltonian governing the (adiabatic) evolution of quantum states $|\psi_n(t)\rangle$ according to the time-dependent Schrödinger equation. If the traversal takes a (long) time T (so that $R(T)=R(o)$), the states at the beginning and end of C are related by

$$\langle\psi_n(o)|\psi_n(T)\rangle = e^{i\gamma_n(C)}\, e^{-\frac{i}{\hbar}\int_o^T dt\, E_n(R(t))} \qquad (31)$$

The second factor contains the dynamical phase associated with the evolution of any quantum state; it can be regarded as the system's way of recording time. The first factor contains the Hermitian generalization of the sign reversal associated with degeneracies of real Hamiltonians - a generalization which must be subtle because Hermitian degeneracies have codimension three and so cannot be enclosed by circuits C. I call $\exp\{i\gamma_n(C)\}$ the geometrical phase factor; it can be regarded as the system's way of recording where it has been in parameter space - a sort of 'quantum learning'.

Exactly how $\gamma_n(C)$ is determined by the natural continuation defined by the time-dependent Schrödinger equation, is explained by Berry (1984); here I simply summarise the main result, for the case where the parameter space $R=(X,Y,Z)$ is three-dimensional

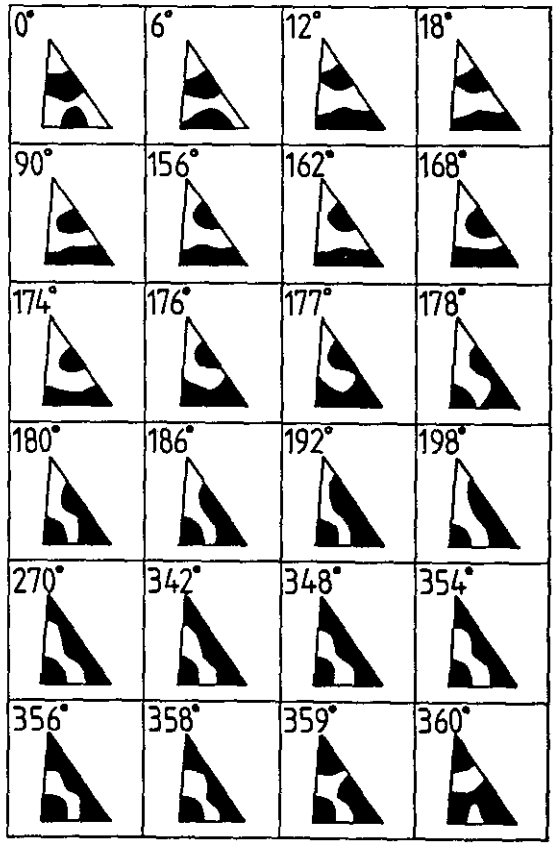

Fig.3. Sign reversal of a vibration mode for a triangle taken round a small circuit C, in angle space, surrounding a diabolical triangle; the indicated angles parameterise position on C.

(fig.4). It is that $\gamma_n(C)$ is determined by the flux through C of a vector field $\underset{\sim}{V}_n(\underset{\sim}{R})$ whose singularities are degeneracies involving the state $|n>$.

Explicitly,

$$\gamma_n(C) = -\iint_S \underset{\sim}{dS} \cdot \underset{\sim}{V}_n(\underset{\sim}{R}) \qquad (32)$$

where the integral is over any surface S spanning C and where

$$\underset{\sim}{V}_n(\underset{\sim}{R}) \equiv \mathrm{Im} \sum_{m \neq n} \frac{<n(\underset{\sim}{R})|\nabla_{\underset{\sim}{R}} \hat{H}(\underset{\sim}{R})|m(\underset{\sim}{R})> \times <m(\underset{\sim}{R})|\nabla_{\underset{\sim}{R}} \hat{H}(\underset{\sim}{R})|n(\underset{\sim}{R})>}{[E_m(\underset{\sim}{R}) - E_n(\underset{\sim}{R})]^2} \qquad (33)$$

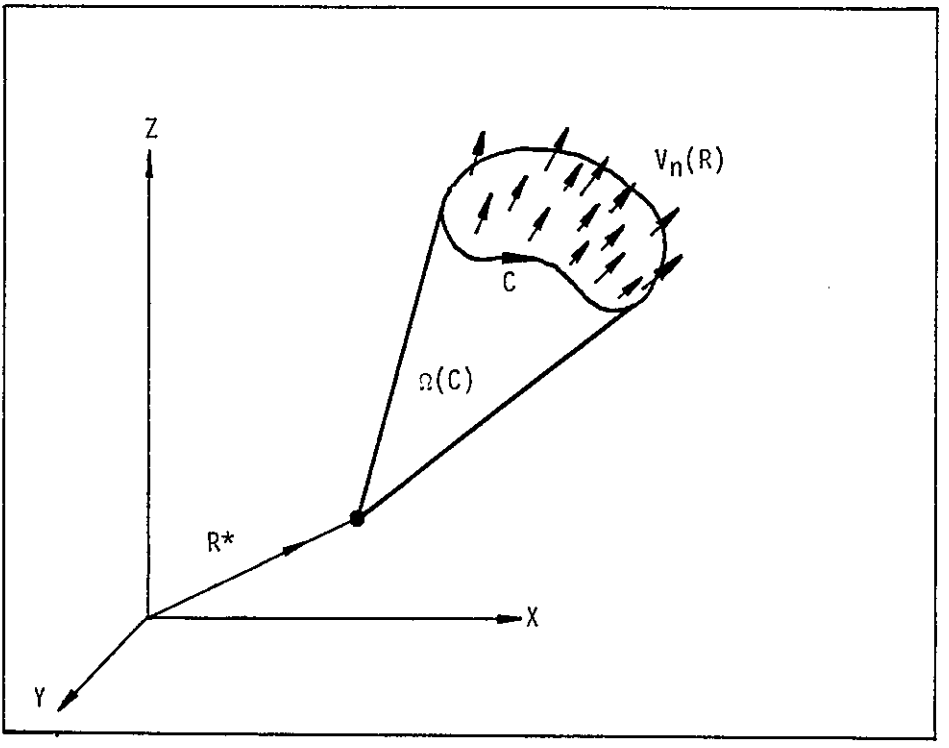

Fig.4 Circuit C near degeneracy $\underline{R}^*$ in $\underline{R}=(X,Y,Z)$ parameter space

In this formula, the arbitrary phases of the eigenstates $|n(\underline{R})>$ cancel, so $\underline{V}_n(\underline{R})$ is manifestly independent of their choice.

The energy denominators make it obvious that $\underline{V}_n$ is singular at degeneracies $\underline{R}^*$. Close to $\underline{R}^*$, the sum involves only the state $|m>=|n\pm1>$ with which $|n>$ degenerates. In this case the form of the singularity is particularly simple in the parameterization for which the 2×2 Hamiltonian coupling the two degenerating states has the standard form

$$\hat{H}(\underline{R}) = \tfrac{1}{2}\begin{pmatrix} Z-Z^*, & X-X^* - i(Y-Y^*) \\ X-X^*+iY-Y^*, & Z^*-Z \end{pmatrix} \qquad (34)$$

Then $\underline{V}(\underline{R})$ is the magnetic field of a monopole located at $\underline{R}^*$, with strength $\pm$ 1/2 if $|n>$ degenerates with $|n\mp1>$, and the phase factor associated with C is

$$e^{i\gamma_n(C)} = e^{\pm i\Omega(C)/2}, \qquad (35)$$

where $\Omega(C)$ is the solid angle (fig.4) subtended by C at the degeneracy.

For real Hamiltonians, $Y-Y^*=0$ in (34) and C lies in a plane and surrounds R^*. Then S subtends $\Omega=\pm 2\pi$ and (35) reproduces the sign-reversal rule. By topological arguments not requiring explicit formulae for $\gamma_n(C)$, Stone (1976) proved that if C is expanded from one point R and contracted onto another so as to sweep out a closed surface enclosing R^*, then the geometrical phase factor traverses a circle in its Argand plane; this property (which is easy to prove using (35)) is the Hermitian generalization of the sign-reversal test for degeneracy.

Apart from generalizing the sign-reversal rule near degene--racies, the geometrical phase factor defined by (31-33) has other interesting aspects. As described by Berry (1984), $\exp\{i\gamma_n(C)\}$ implies observable interference effects for spinning particles (bosons as well as fermions) in slowly-rotated magnetic fields, and contains the Aharonov-Bohm effect as a special case. Mead (1979, 1980,1983) and Mead and Truhlar (1979) describe how phase changes in molecular electronic states resulting from changes in nuclear configuration must affect the states and energies of nuclear motion.

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