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Statistics of energy levels without time-reversal symmetry: Aharonov–Bohm chaotic billiards

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Abstract. A planar domain D contains a single line of magnetic flux Φ. Switching on Φ breaks time-reversal symmetry (T) for quantal particles with charge q moving in D, whilst preserving the geometry of classical (billiard) trajectories bouncing off the boundary ∂D. If ∂D is such that these classical trajectories are chaotic, we predict that T breaking will cause the local statistics of quantal energy levels to change their universality class, from that of the Gaussian orthogonal ensemble (GOE) of random-matrix theory to that of the Gaussian unitary ensemble (GUE). In the semiclassical limit this transition is abrupt; for statistics involving the first N levels, GUE behaviour requires that the quantum flux $\alpha \equiv q\Phi/h \gg 0.13N^{-1/4}$. The special flux $\alpha = 1/2$ corresponds to 'false T breaking' and for this case we predict GOE statistics. These predictions are confirmed by numerical computation of spectral statistics for a classically chaotic billiard without symmetry, for which ∂D is a cubic conformal image of the unit disc.

1. Introduction

For a bound quantal system with time-reversal symmetry (T), energy levels are determined by diagonalising a Hamiltonian matrix which is real and symmetric. When T is broken (for example by applying an external magnetic field) the Hamiltonian becomes, in general, complex, that is, fully Hermitian. Our purpose here is to show by means of an example that, in cases where the system has a classical counterpart whose trajectories are chaotic, such symmetry breaking has a dramatic effect on the spectrum: it changes the universality class of the local statistics of high-lying (semiclassical) energy levels.

There is good reason to expect this effect. High-lying levels of classically chaotic systems are eigenvalues of large complicated matrices, which can be regarded as typical members of an appropriate ensemble as studied in random-matrix theory (Porter 1965, Mehta 1967). With T (or an equivalent anti-unitary symmetry (Robnik and Berry 1985)) the Gaussian orthogonal ensemble (GOE), consisting of real symmetric matrices, is appropriate; without T, the Gaussian unitary ensemble (GUE), consisting of complex Hermitian matrices, is appropriate. Strong evidence has now accumulated for a variety of classically chaotic systems with T that shows that the quantal spectral statistics are indeed those of the GOE (see the review by Bohigas and Giannoni (1984)). In contrast, energy levels in the case where T is broken have so far been studied in only one system: Seligman and Verbaarschot (1985) demonstrated GUE behaviour for a particle moving in a combination of inhomogeneous magnetic and scalar force fields. (In addition, GUE statistics have been found by Izraelev (1984) for the quasi-energies of a chaotic quantum map and by Odlyzko (reported by Bohigas and Giannoni (1984)) for the imaginary parts of the zeros of Riemann's zeta function.)

The statistics we shall study are the *level spacings distribution* $P(S)$ and the *rigidity* $\Delta(L)$. $P(S)$ describes fine-scale spectral structure, because it is the distribution of spacings of *neighbouring* levels (with S measured in terms of the local mean level spacing). An important difference between the GOE and GUE universality classes is their behaviour as $S\to 0$: GOE predicts the 'linear level repulsion' $P\propto S$, whilst GUE predicts the 'quadratic level repulsion' $P\propto S^2$ (a simple explanation of this difference, in terms of the codimension of degeneracies of families of real and complex Hermitian matrices, is given by Berry 1985a). Useful approximate formulae for $P(S)$ are

$$\begin{aligned} P_{\mathrm{GOE}}(S) &\approx (\pi/2)S\exp(-\pi S^2/4) \\ P_{\mathrm{GUE}}(S) &\approx (32S^2/\pi^2)\exp(-4S^2/\pi). \end{aligned} \tag{1}$$

The rigidity $\Delta(L)$ is the local average least squares deviation of the spectral staircase $N(E)$ for a straight line, over an energy range of L mean level spacings. Thus

$$\Delta(L)\equiv\left\langle \min_{(A,B)}\frac{\langle d(E)\rangle}{L}\int_{-L/2\langle d\rangle}^{+L/2\langle d\rangle}\mathrm{d}\varepsilon[N(E+\varepsilon)-A-B\varepsilon]^2\right\rangle. \tag{2}$$

In this formula $\langle d(E)\rangle$ is the mean level density near energy E, $N(E)$ is the spectral staircase

$$N(E)\equiv\sum_{j=1}^{\infty}\Theta(E-E_j) \tag{3}$$

where E_j are the energy levels and Θ denotes the unit step function, and $\langle\ \rangle$ denotes averaging (over an ensemble of spectra, or over a classically small energy range centred on E). Rigidity was introduced by Dyson and Mehta (1963) (they called it $\Delta_3(L)$); it describes spectral structure over a range of scales. As $L\to 0$, $\Delta(L)\to L/15$ for all systems of the class we consider here. For large L, random-matrix theory predicts that $\Delta(L)$ increases logarithmically, with different constants for GOE and GUE

$$\left.\begin{aligned} \Delta_{\mathrm{GOE}}(L) &\to (1/\pi^2)\ln L-0{\cdot}006\,95 \\ \Delta_{\mathrm{GUE}}(L) &\to (1/2\pi^2)\ln L+0.0590 \end{aligned}\right\}\qquad (L\gg 1) \tag{4}$$

These formulae have recently been derived by Berry (1985b) for the case of classically chaotic systems, using not random-matrix theory but an asymptotic representation of the spectrum in terms of the set of *closed classical trajectories*; in this semiclassical theory, the difference between GOE and GUE arises from the fact that with T each closed orbit combines coherently with its time-reversed counterpart, whereas without T this does not occur—a fact we will fully exploit later. The semiclassical theory also predicts that at a certain value $L_{\max}$, $\Delta(L)$ will deviate from the universal random-matrix asymptotic formula (4) and will display non-universal behaviour determined by the shortest classical closed orbits; for $L\gg L_{\max}$, $\Delta(L)$ will reach a (non-universal) saturation value.

The system we shall study is a particle with charge q and mass m confined by hard walls to a planar domain D ('billiard table') threaded by a single line of magnetic flux Φ. If the flux line is at the origin of the plane $\boldsymbol{r}=(x,y)$, the vector potential $\boldsymbol{A}(\boldsymbol{r})$ can be chosen as any vector field satisfying

$$\nabla_{\wedge} \boldsymbol{A}(\boldsymbol{r}) = \hat{\boldsymbol{n}} \Phi \delta(\boldsymbol{r}) \tag{5}$$

(where $\hat{\boldsymbol{n}}$ is a unit vector normal to D) and energy levels are determined by Schrödinger's equation

$$(1/2m)(-\mathrm{i}\hbar\nabla - q\boldsymbol{A}(\boldsymbol{r}))^2 \psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}) \tag{6}$$

where $\psi(\boldsymbol{r})$ is single-valued and $\psi = 0$ on ∂D.

This situation is the bound-state analogue of scattering from a single flux line, first calculated by Aharonov and Bohm (1959) and later studied extensively (see, e.g., Morandi and Menossi (1984) and the review by Olariu and Popescu (1985)). As in the scattering problem, the fact that the magnetic field is zero except at $\boldsymbol{r} = 0$ means that the geometry of classical trajectories is unaffected by the flux Φ (except for the set of measure zero of paths which pass through $\boldsymbol{r} = 0$), whilst the fact that the vector potential $\boldsymbol{A}(\boldsymbol{r})$ cannot be set equal to zero in (6) means that quantum mechanics, and in particular the energy levels, are altered when Φ is non-zero. Switching on Φ therefore means switching off T without changing the geometry of classical trajectories, and if the boundary ∂D is chosen without symmetry and such that these trajectories are chaotic, we predict an abrupt transition of spectral statistics from GOE (when $\Phi = 0$) to GUE (when $\Phi \neq 0$).

In § 2 we show that the quantum spectrum depends on Φ via the *quantum flux parameter*

$$\alpha \equiv q\Phi/h \tag{6a}$$

and show how the dependence has a semiclassical origin in spite of the fact that the geometry of trajectories is unaffected by Φ. This semiclassical picture is used in § 3 to study the softening of the GOE–GUE transition when only a finite number of levels is included in the computation of spectral statistics.

Section 4 is devoted to an exposition of the technique we use to solve equation (6) and so determine the energy levels. This is an adaptation of the method of conformal transformation introduced by Robnik (1983, 1984) to study classical and quantum billiards without flux. The method easily suggests a natural class of boundaries without symmetry. In § 5, one member of this class is chosen and the results of computations of $P(S)$ and $\Delta(L)$ for several values of α are presented, confirming the prediction that T-breaking changes the spectral statistics from GOE to GUE.

An obvious alternative to Aharonov–Bohm billiards as a class of model systems for studying T-breaking is billiards with *uniform* magnetic field, but this has two disadvantages. Firstly, it changes the classical trajectories from sequences of straight line segments to circles and sequences of circular arcs; this gives rise to interesting new dynamics (Robnik and Berry 1985) but complicates the study of T-breaking itself. Secondly, it makes the quantum levels harder to calculate (however, we are pursuing these calculations because they reveal interesting phenomena not directly connected with time reversal).

2. Quantal and classical reversibility

Violation of T for the Aharonov–Bohm billiard is reflected in the fact that the Hamiltonian operator in (6) is complex (the term linear in $\boldsymbol{A}$ has a factor i). A gauge-invariant expression of this complex Hermiticity can be obtained by formally eliminating the vector potential using the Dirac substitution

$$\psi(\boldsymbol{r}) \equiv \chi(\boldsymbol{r}) \exp\left(\frac{\mathrm{i}q}{\hbar} \int_{\boldsymbol{r}_0}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}') \cdot \mathrm{d}\boldsymbol{r}'\right) \tag{7}$$

where $\boldsymbol{r}_0$ is an arbitrary reference point. This transformation is however multivalued because, for any circuit C,

$$\oint_C \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{r} = W_C \Phi \tag{8}$$

where W_C is the winding number of C about the flux line. Therefore, in order that ψ be single valued, χ must acquire a phase factor

$$\exp\left(-\frac{\mathrm{i}q}{\hbar} \oint \boldsymbol{A} \cdot \mathrm{d}\boldsymbol{r}\right) = \exp\left(-\frac{\mathrm{i}q}{\hbar}\Phi\right) = \exp(-2\pi\mathrm{i}\alpha) \tag{9}$$

for each positive circuit of the flux line. Schrödinger's equation (6) now becomes, using polar coordinates (r, θ) for $\boldsymbol{r}$,

$$\begin{aligned} &(-\hbar^2/2m)\nabla^2\chi(r, \theta) = E\chi(r, \theta) \\ &\chi(r, \theta+2\pi) = \exp(-2\pi\mathrm{i}\alpha)\chi(r, \theta) \qquad \chi = 0 \text{ on } \partial D. \end{aligned} \tag{10}$$

It is clear from (10) that the quantum mechanics of this system can be made to depend on the solution of a *real* equation with a *real* boundary condition, but with a continuation condition which is in general *complex*, so that the operator is complex Hermitian, leading to the prediction of GUE spectral statistics. However, there are two exceptional cases for which the operator (10) is wholly real, leading us to predict GOE statistics. The first is when α is an *integer* (χ unchanged in a circuit of the flux line). The second is when α is a *half-integer* (χ changes sign during a circuit of the flux line). This latter case is an example of 'false T-breaking' leading to GOE statistics when GUE might have been expected, because a non-trivial real representation of the Hamiltonian can be found (in this case (10)); this phenomenon can also arise from geometric symmetry (of ∂D, for example), giving rise to an anti-unitary symmetry different from T, as we explain in detail elsewhere (Robnik and Berry 1985). (Half-integer flux also plays a special role in the ordinary Aharonov-Bohm effect, as discussed in detail by Berry *et al* (1980).)

The following symmetries of the spectrum $\{E_j(\alpha)\}$ follow trivially from (10):

$$E_j(\alpha+1) = E_j(\alpha) \qquad E_j(-\alpha) = E_j(\alpha). \tag{11}$$

Therefore, the Aharonov-Bohm quantum billiard spectrum need only be studied on the range $0 \leqslant \alpha \leqslant 1/2$.

Now we give the *semiclassical interpretation* of the dependence on α. At first this appears impossible, because the geometry of the classical trajectories is unaffected by the flux. However, quantum theory depends not on the Newtonian trajectories in configuration space but on the *Hamiltonian orbits* in *phase space*. These orbits involve the canonical momentum $\boldsymbol{p}$, which differs from the kinetic momentum $m\boldsymbol{v}$ by $q\boldsymbol{A}(\boldsymbol{r})$—a term which cannot be transformed away because $\boldsymbol{A}$ must satisfy the flux condition (5) and so cannot be made to vanish.

In particular, as emphasised by Gutzwiller (1978) and Balian and Bloch (1974), the quantal spectrum depends on the actions of *classical closed orbits*. The action of a closed orbit, in units of $\hbar$ (that is, the semiclassical phase), is

$$\frac{S}{\hbar}=\frac{1}{\hbar}\oint \boldsymbol{p}\cdot \mathrm{d}\boldsymbol{r}=\frac{m}{\hbar}\oint \boldsymbol{v}\cdot \mathrm{d}\boldsymbol{r}+\frac{q}{\hbar}\oint \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{r}$$

$$=\frac{S_0}{\hbar}+2\pi W\alpha. \tag{12}$$

where S_0 is the action for zero flux and W the winding number of the orbit about the flux line. That fact that this α dependence of the action is directly connected with time reversal is indicated by the existence of a non-zero phase difference between a closed orbit (+, with winding number W) and its time-reversed counterpart (−, with winding number $-W$), namely

$$(S_+-S_-)/\hbar=4\pi W\alpha. \tag{13}$$

W is, of course, an integer, so there is phase coherence between an orbit and its time-reversed counterpart whenever α is an integer or a half-integer, a conclusion fully concordant with our earlier quantal arguments based on (10). For other values of α, there will be a degree of phase incoherence between an orbit and its time-reversed counterpart, whose quantitative estimation is the subject of the next section.

3. Switching off time-reversal symmetry

The level density $d(E)$, whose singularities are the eigenvalues E_j, can be expressed as a semiclassical sum in which each classical closed orbit, with action S, contributes a term containing the phase factor $\exp(\mathrm{i}S/\hbar)$. Important spectral statistics can be expressed as averages of quadratic functionals of $d(E)$; these include the rigidity $\Delta(L)$, and the pair correlation of the levels (Mehta 1967) whose short-range behaviour is the same as that of $P(S)$ and which therefore manifests the linear or quadratic level repulsion of GOE or GUE. For such statistics, the effect on the spectrum of the T breaking induced by the flux depends on the average of

$$|\exp(\mathrm{i}S_+/\hbar)+\exp(\mathrm{i}S_-/\hbar)|^2 \tag{14}$$

over all relevant pairs of orbits (+) and their time-reversed counterparts (−).

It is natural now to define a *coefficient of T breaking* by

$$K(\alpha)\equiv\langle 2\cos^2[(S_+-S_-)/2\hbar]-1\rangle=\langle\cos(4\pi W\alpha)\rangle, \tag{15}$$

where use has been made of (13). The average $\langle\ \rangle$ is over the winding numbers of all the closed orbits which are involved in determining the levels. Complete phase coherence gives $K=1$ and GOE statistics; complete phase incoherence gives $K=0$ and GUE statistics. We now estimate $K(\alpha)$ for spectral statistics computed using the first N levels (the semiclassical limit is $N\to\infty$).

The energy E of the Nth level is approximately given by the Weyl rule (for example, see Berry 1983)

$$N\approx \mathscr{A}mE/2\pi\hbar^2 \tag{16}$$

where $\mathscr{A}$ is the area of the billiard. Therefore the spacing between neighbouring levels is

$$\Delta E=\langle d(E)\rangle^{-1}=2\pi\hbar^2/m\mathscr{A}. \tag{17}$$

A closed orbit of period T contributes spectral structure on an energy scale h/T, therefore the spectrum is approximately determined by those orbits giving structure on ΔE, that is, those with periods

$$T \approx h/\Delta E = m\mathscr{A}/\hbar. \tag{18}$$

The geometrical length $l = vT$ of these orbits is obtained by combining this result with (16), giving

$$l \approx 2(\pi N \mathscr{A})^{1/2}. \tag{19}$$

Because N is large, these are long orbits, consisting of $n(N)$ chords connected by specular reflection at ∂D, where $n(N)$ is obtained by dividing l by the mean chord length $\pi\mathscr{A}/\mathscr{L}$, where $\mathscr{L}$ is the length of the boundary (Joyce 1975). Thus

$$n(N) \approx 2\mathscr{L}(N/\pi\mathscr{A})^{1/2}. \tag{20}$$

To calculate the coefficient of T breaking (15) we require the distribution of winding numbers W over the large number of closed n-chord orbits. In the appendix we show that this distribution is a discrete Gaussian with a variance which depends on the position of the flux line, but whose average $W^2(n)$ is given approximately by

$$W^2(n) \approx (1{\cdot}69n/\mathscr{L})(\mathscr{A}/2\pi)^{1/2}. \tag{21}$$

Evaluating the average in (15) using the Poisson summation formula and the fact that $W^2(n) > 1$, we obtain the coefficient of T breaking for flux α and N levels as

$$K(\alpha; N) \approx \sum_{m=-\infty}^{\infty} \exp[-8\pi^2 W^2(n(N))(\alpha - m/2)^2]. \tag{22}$$

Use of (20), (21) and restriction to $\alpha < 1/4$ gives, for large N,

$$K(\alpha; N) \approx \exp(-60{\cdot}1\alpha^2 N^{1/2}). \tag{23}$$

Note that in this approximation no details of billiard geometry appear.

To get GUE spectral statistics, K must be small. This requires

$$\alpha \gg 0.13 N^{-1/4}. \tag{24}$$

In the semiclassical limit of infinite N, this implies that the transition from GUE to GOE takes place abruptly as soon as the flux is non-zero, as previously asserted. Pandey (1981) and Mehta and Pandey (1983), working within the framework of random-matrix theory, have given an analogous treatment of the way in which a symmetry-breaking perturbation produces a transition between different universality classes of spectral fluctuation, which is abrupt in the limit of infinite matrices.

4. The conformal transformation technique

Any boundary ∂D of a simply-connected domain D can be regarded as a conformal transformation of the unit circle. If the circle lies in the complex plane $z \equiv x + iy$, any non-singular complex function

$$w(z) = u(x, y) + iv(x, y) \tag{25}$$

with non-vanishing derivative in D produces, as the boundary of the conformal image of the unit disc, the simple closed curve given parametrically by

$$u = \mathrm{Re}\, w(\exp(\mathrm{i}\theta)) \qquad v = \mathrm{Im}\, w(\exp(\mathrm{i}\theta)) \tag{26}$$

(see figure 1).

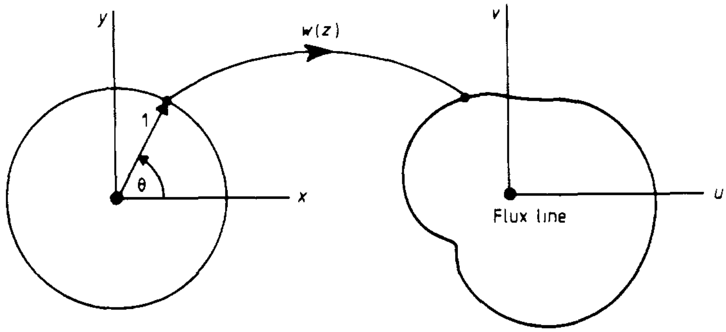

Figure 1. Conformal transformation from the unit disc in $z = x + \mathrm{i}y$ to the billiard domain in $w = u + \mathrm{i}v$. The boundary shown is generated by the mapping function (40) with parameters (41).

We begin the transformation of Schrödinger's equation (6) (whose domain D now resides in the uv plane) by choosing a non-divergent gauge in which the lines of the vector potential $\boldsymbol{A}$ are the contours of a scalar function $f(u, v)$. Using (5) we therefore write

$$\boldsymbol{A}(u, v) = (\Phi/2\pi)(\partial f/\partial v, -\partial f/\partial u, 0) \tag{27}$$

where

$$\nabla^2_{uv} f = -2\pi\delta(u)\delta(v). \tag{28}$$

Thus, for the wavefunction $\psi(u, v)$, (6) becomes

$$\nabla^2_{uv}\psi - 2\mathrm{i}\alpha\left(\frac{\partial f}{\partial v}\frac{\partial}{\partial u} - \frac{\partial f}{\partial u}\frac{\partial}{\partial v}\right)\psi - \alpha^2\left[\left(\frac{\partial f}{\partial u}\right)^2 + \left(\frac{\partial f}{\partial v}\right)^2\right]\psi + k^2\psi = 0 \tag{29}$$

with $\psi = 0$ on ∂D and where

$$k \equiv (2mE)^{1/2}/\hbar. \tag{30}$$

Changing to the disc coordinates $\boldsymbol{r} = (x, y)$ is a straightforward procedure based on (25). Defining

$$F(\boldsymbol{r}) \equiv f(u(\boldsymbol{r}), v(\boldsymbol{r})) \qquad \text{and} \qquad \Psi(\boldsymbol{r}) \equiv \psi(u(\boldsymbol{r}), v(\boldsymbol{r})) \tag{31}$$

we obtain

$$\begin{aligned} &\nabla^2\Psi(\boldsymbol{r}) - 2\mathrm{i}\alpha\left(\frac{\partial F}{\partial y}\frac{\partial}{\partial x} - \frac{\partial F}{\partial x}\frac{\partial}{\partial y}\right)\Psi(\boldsymbol{r}) - \alpha^2|\nabla F|^2\Psi(\boldsymbol{r}) + k^2|w'(z)|^2\Psi(\boldsymbol{r}) = 0 \\ &\Psi = 0 \qquad \text{if} \qquad x^2 + y^2 = 1, \end{aligned} \tag{32}$$

in which the last term (involving $w'(z)$) encodes all information about the shape of ∂D.

Next, we choose

$$F(\boldsymbol{r}) = -\ln|\boldsymbol{r}| \tag{33}$$

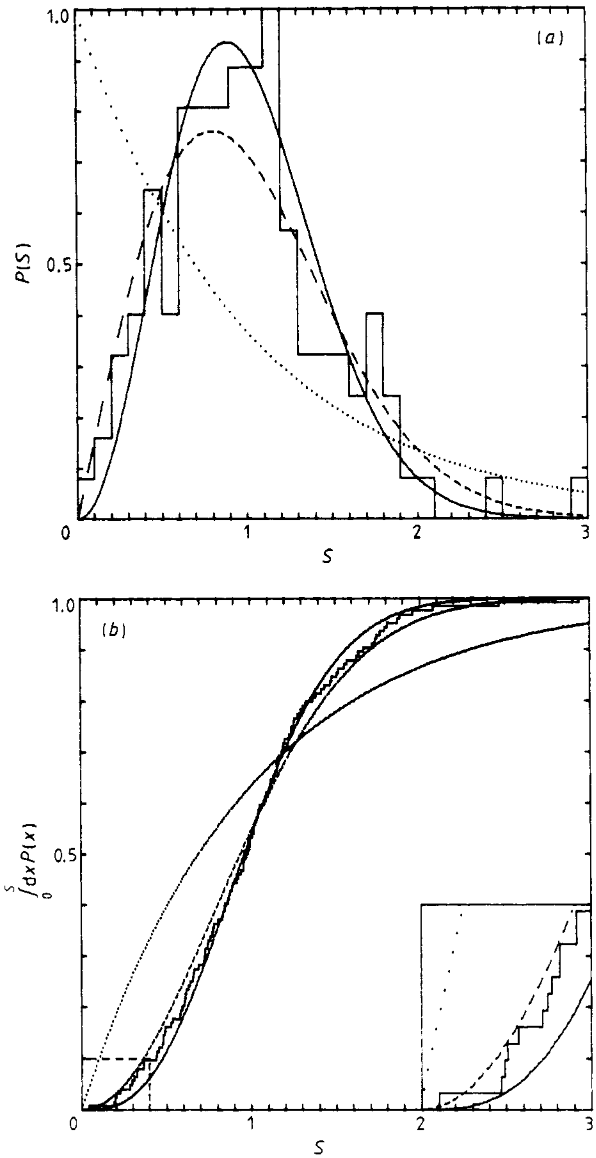

Figure 2.

so that

$$f(u, v) = -\tfrac{1}{2}\ln(x^2(u, v) + y(u, v)), \tag{34}$$

a function which satisfies the flux condition (28). (This gauge has the property that the lines of $\boldsymbol{A}$ are tangential to ∂D.) Thus (32) becomes the final form of the Schrödinger equation, namely (using polar coordinates $\boldsymbol{r} = (r, \theta)$)

$$\nabla^2\Psi - \frac{2\mathrm{i}\alpha}{r^2}\frac{\partial\Psi}{\partial\theta} - \frac{\alpha^2}{r^2}\Psi + k^2|w'(z)|^2\Psi = 0$$

$$\Psi(1, \theta) = 0. \tag{35}$$

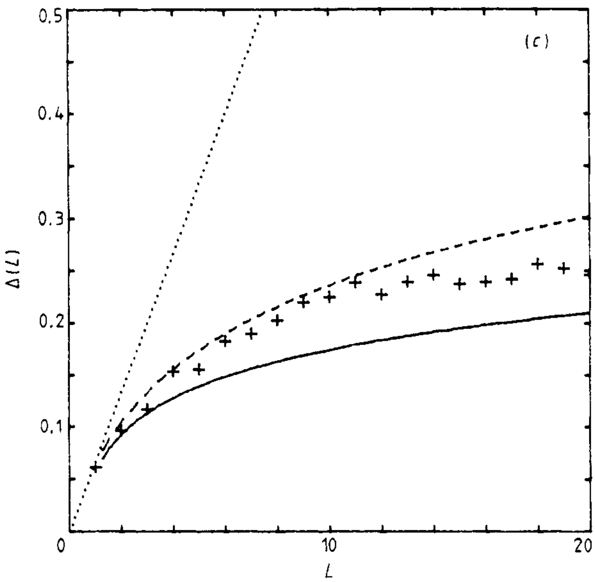

Figure 2. Spectral statistics for quantum billiard with boundary generated by (26), (40) and (41) and shown in figure 1, with zero magnetic flux α, for which there is time-reversal symmetry. (a) Level spacings distribution $P(S)$; (b) cumulative level spacings distribution $\int_0^S \mathrm{d}x\, P(S)$; ($c$) spectral rigidity $\Delta(L)$. The full, broken and dotted curves give the predictions of the GUE, GOE and Poisson statistics respectively.

To solve this equation, we expand Ψ in terms of eigenstates of the unit disc plus central flux line. Thus

$$\Psi(r, \theta) = \sum_{n=1}^{\infty} \sum_{l=-\infty}^{\infty} \frac{c_{nl} N_{nl}}{a_{nl}} \exp(\mathrm{i}l\theta) J_{|l-\alpha|}(a_{nl} r), \tag{36}$$

where c_{nl} are expansion coefficients, a_{nl} is the nth zero of the Bessel function $J_{|l-\alpha|}$ and N_{nl} are normalisation constants given by

$$N_{nl}^{-1} = \sqrt{\pi} |J'_{|l-\alpha|}(a_{nl})|. \tag{37}$$

Substitution of (36) into (35) leads to

$$\sum_{n'l'} c_{n'l'} M_{n'l'nl} = c_{nl}/k^2, \tag{38}$$

where

$$M_{n'l'nl} = \frac{N_{nl} N_{n'l'}}{a_{nl} a_{n'l'}} \int_0^1 \mathrm{d}r\, r \int_0^{2\pi} \mathrm{d}\theta \exp[\mathrm{i}(l-l')\theta] J_{|l-\alpha|}(a_{nl} r) J_{|l'-\alpha|}(a_{n'l'} r) |w'(z)|^2. \tag{39}$$

Solution of the Aharonov-Bohm quantum billiard problem can therefore be accomplished by diagonalising the matrix $M_{n'l'nl}$. It is remarkable that the only effect of the flux line is to change the order of the Bessel functions from integer to fractional; apart from this, the technique is the same as that devised by Robnik (1984) to determine the levels of quantum billiards without flux.

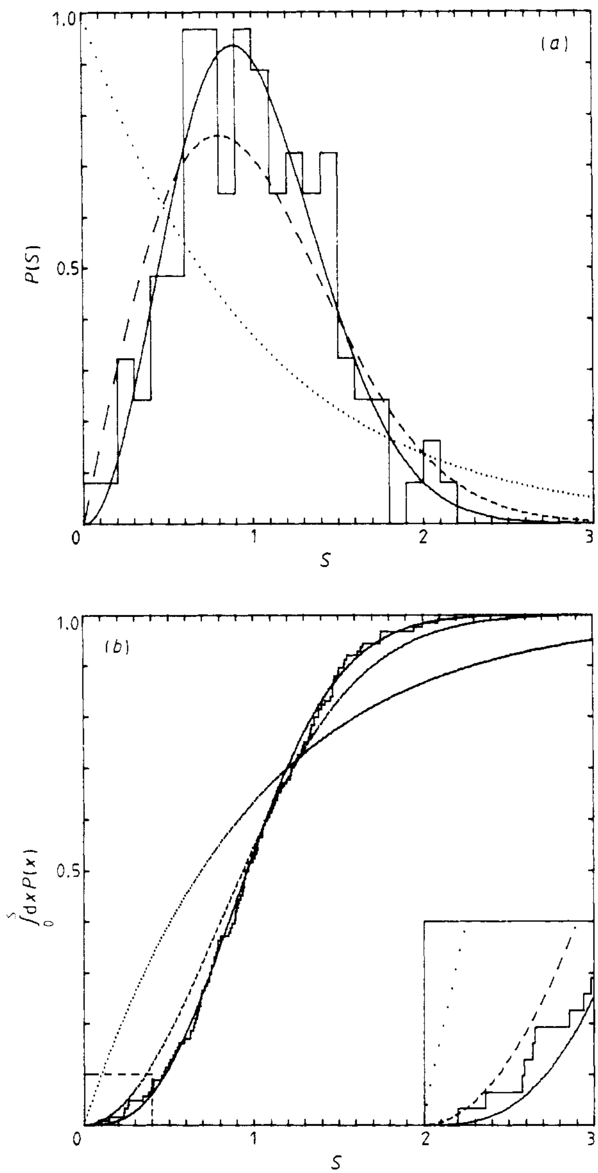

Figure 3.

5. Numerical illustrations and discussion

In choosing a complex function $w(z)$ to generate a billiard boundary via (26), three considerations are important. Firstly, computation of the matrix elements (39) must be made as easy as possible. This can be achieved by choosing $w(z)$ to be a low-order polynomial, because this makes the θ integration trivial (and moreover the matrix is almost diagonal in l). Secondly, in order to avoid false T breaking and so generate GOE instead of GUE, ∂D should not possess reflection symmetry (Robnik and Berry 1985). Thirdly, ∂D should generate classically chaotic motion. These conditions can

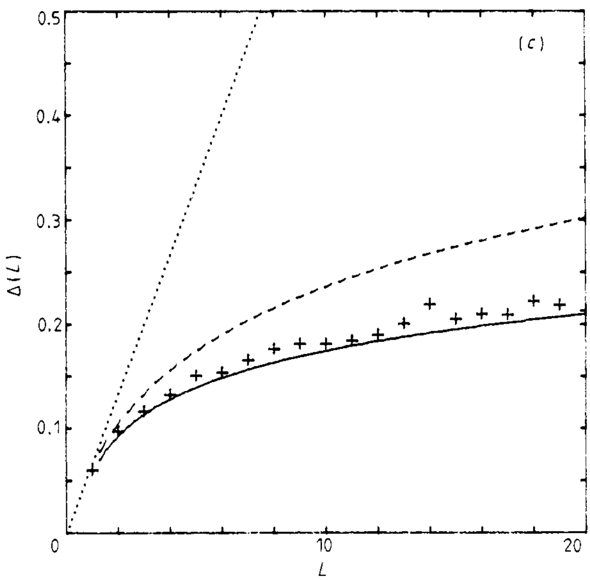

Figure 3. As figure 2, with $\alpha = \frac{1}{2}(\sqrt{5}-1)$ (the golden flux, equivalent to $\alpha = 0.382$), for which time-reversal symmetry is broken.

be satisfied by a cubic polynomial, whose most general form can be reduced by translation, rotation and scaling to

$$w(z) = z + Bz^2 + C\exp(\mathrm{i}\phi)z^3, \tag{40}$$

in which B, C and ϕ are all real and (to avoid symmetry) non-zero.

After some numerical investigation we selected the following parameters:

$$B = C = 0.2, \qquad \phi = \pi/3. \tag{41}$$

The boundary ∂D generated by this choice is shown in figure 1; its area and perimeter are

$$\mathscr{A} = 3.7699, \qquad \mathscr{L} = 7.1012. \tag{42}$$

The classical trajectories are chaotic. This follows from two facts. Firstly, ∂D is not convex and its concave portions are powerful sources of instability, as demonstrated by Robnik (1983). Secondly, the shortest closed orbits (each with two bounces, involving diameters of ∂D), whose neighbourhoods dominate a large fraction of the phase space, are all unstable. Computation of the bounce map for 10^5 iterations confirms the expectation that the classical orbits are irregular; numerical evidence is consistent with ergodicity and shows no trace of tiny islands of regularity amidst the chaos (although of course we cannot exclude this possibility).

By diagonalising the matrix (39), the spectrum was computed for several values of α, with Bessel functions calculated by recursion and matrix elements evaluated by numerical radial integration. For each α, 500 levels were computed, and of these the lowest 125 were used to calculate spectral statistics; we are confident that numerical errors do not exceed 5% of the mean level spacing. Of course with $N = 125$ we do not expect exact agreement with random-matrix theory—for that, we would need the

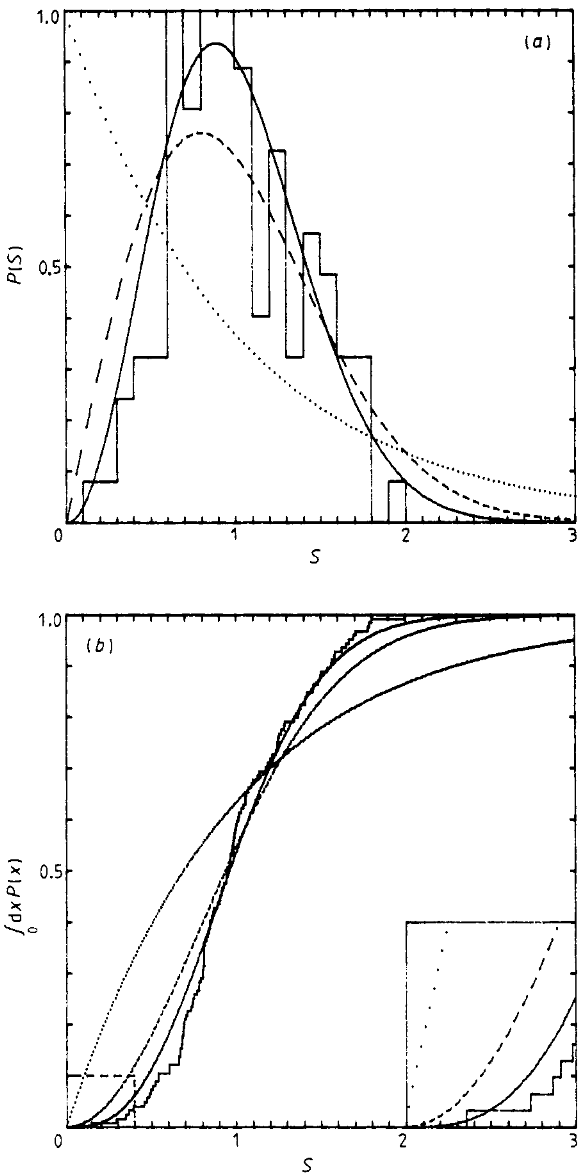

Figure 4.

semiclassical limit $N \to \infty$. For each spectrum, the staircase $N(E)$ was checked for gross errors by comparing it with the Weyl rule plus corrections (Baltes and Hilf 1976).

The first set of statistics (figure 2) is for the case of zero flux ($\alpha = 0$). Figure 2(a) shows the level spacings distribution presented in the customary way as a histogram obtained by dividing the data into bins. The data appear to favour GOE statistics, as expected for this quantum billiard with T as its only symmetry. However, it is much better to present the data cumulatively, as $\int_0^S dx P(x)$, because this avoids both the large statistical fluctuations with small bins and the smoothing of data with large bins; figure 2(b) shows the result. Evidently GOE statistics give a better fit for small S,

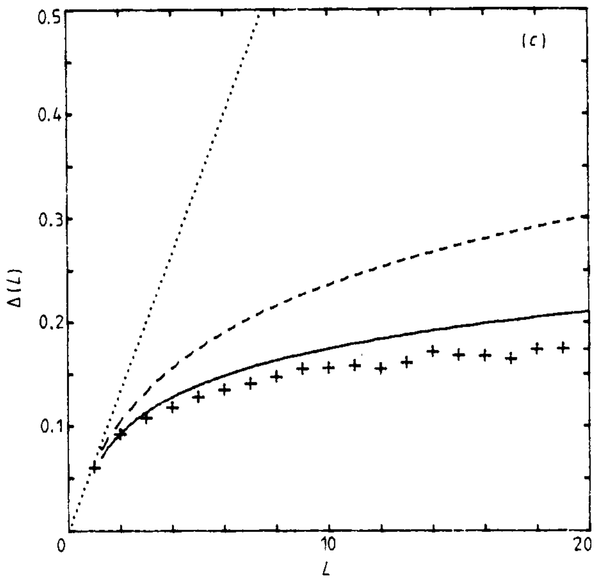

Figure 4. As figure 2, with $\alpha = \frac{1}{4}$, for which time-reversal symmetry is broken.

indicating linear level repulsion (the deviations from the GOE curves are within the ranges expected for $N = 125$).

Figure 2(c) shows the rigidity $\Delta(L)$ for this case of zero flux computed by spectral averaging of (2) over $125/L$ non-overlapping level sequences. The data lie close to the GOE curve until $L \sim 15$ and then rise more slowly. The GOE behaviour for $L \leq 15$ agrees with earlier studies (Bohigas and Giannoni 1984, Bohigas *et al* 1984) which were restricted to approximately the same range of values. Semiclassical theory (Berry 1985b) predicts that $\Delta(L)$ may deviate from GOE when L reaches a value for which a rough estimate is

$$L_{\max} = h\langle d\rangle / T_{\min} \tag{43}$$

where $T_{\min}$ is the period of the shortest classical closed orbit. The behaviour of $\Delta(L)$ for $L \sim L_{\max}$ is non-universal and determined by the particular detailed structure of the shortest few closed orbits. We calculate $L_{\max}$ using the Weyl rule for $\langle d\rangle$, with the result (the same with and without flux)

$$L_{\max} = 2(\pi \mathscr{A} N)^{1/2} / l_{\min}, \tag{44}$$

where $l_{\min}$ is the length of the shortest closed orbit (twice the shortest diameter). For our billiard, with $N = 125$, $L_{\max} \approx 20$—a reasonable agreement considering the roughness of the estimates.

Figure 3 shows the effect of T breaking, with α chosen as the golden number to make the quantum flux maximally irrational. Thus $\alpha = \frac{1}{2}(\sqrt{5} - 1)$, which is equivalent to $1 - \alpha = 0.382$. For this value, the condition (24) for GUE statistics is amply satisfied: the coefficient of T breaking (23) is $K \sim \exp(-9)$. The effect is striking; in figures 3(a) and 3(b), $P(S)$ and its integral now agree with GUE predictions over the whole range of spacings and in particular the level repulsion as $S \to 0$ is approximately quadratic. As figure 3(c) shows, the data cling to the GUE curve over the whole range $0 \leq L \leq 20$.

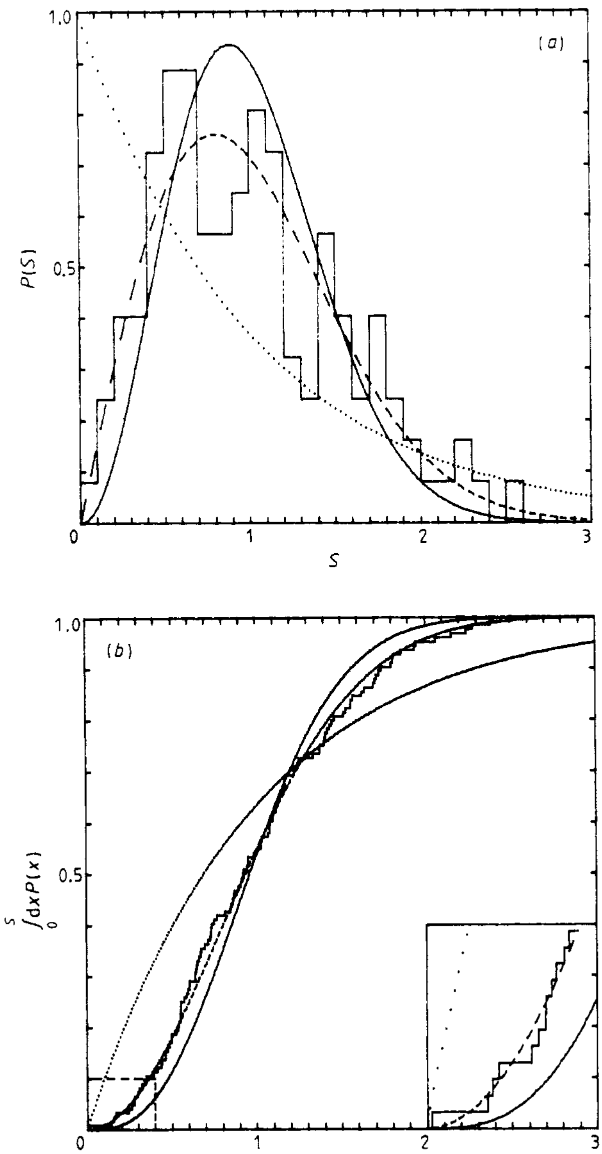

Figure 5.

For $\alpha = \frac{1}{2}(\sqrt{5}-2) = 0.118$, the spectral statistics (not shown here) also agree well with GUE in the expected range. However, beyond $L \sim 15$, $\Delta(L)$ does not agree with the GUE curve as in figure 3(c) but rises more slowly (cf analogous behaviour for $\alpha = 0$ in figure 2(c)).

Figure 4 shows the spectral statistics for $\alpha = \frac{1}{4}$, chosen because it is furthest from the extremes $\alpha = 0$ and $\alpha = \frac{1}{2}$ (for which the Hamiltonian is real) and therefore ought to exhibit the effects of T breaking most strongly. The results confirm this expectation: the level spacings (figures 4(a) and 4(b)) again agree with GUE, although with larger fluctuations than for the golden flux. The rigidity (figure 4(c)) again agrees with GUE

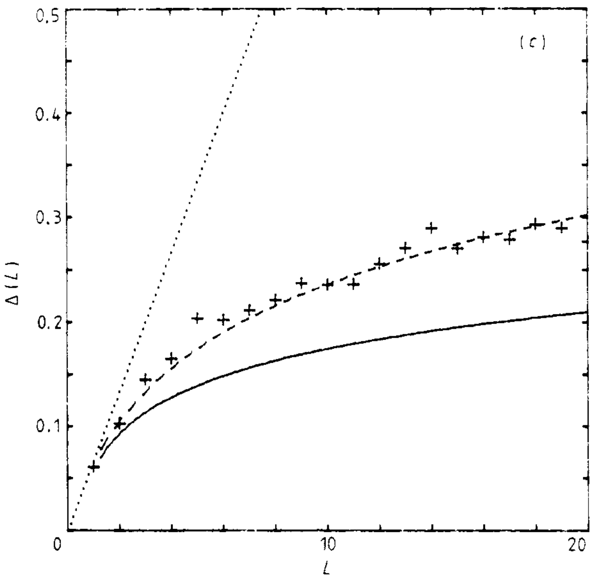

Figure 5. As figure 2, with $\alpha = \frac{1}{2}$, for which there is false time-reversal symmetry-breaking.

for small L, but then rises more slowly (cf analogous behaviour for $\alpha = 0$ in figure 2(c)). This stronger-than-GUE long-range level correlation might arise from the fact that when $\alpha = \frac{1}{4}$ the quantity $\cos(4\pi W\alpha)$, whose average is the coefficient of T breaking (15), can take only the values ± 1 (depending on whether the winding number is even or odd).

A central prediction of § 2 was that $\alpha = \frac{1}{2}$ is a special value which corresponds to false T breaking and so should have GOE spectral statistics. Figure 5 confirms that this is the case over the whole plotted range of S and all the expected range of L.

To show the effect of symmetry-breaking beyond any doubt, we show in figures 6(a) and 6(b) the spacings statistics for the combined data for the two cases with real Hamiltonian ($\alpha = 0$ and $\alpha = \frac{1}{2}$) and in figures 6(c) and 6(d), the corresponding statistics for the three cases with complex Hamiltonian ($\alpha = \frac{1}{2}(\sqrt{5} - 1)$, $\alpha = \frac{1}{4}$ and $\alpha = \frac{1}{2}(\sqrt{5} - 2)$).

The foregoing computations concern the billiard (41) which has no symmetry. In cases where ∂D has reflection symmetry, we can show (Robnik and Berry 1985) that even though the flux line destroys T in quantum (and Hamiltonian) mechanics, it is nevertheless possible to find a non-trivial basis in which the Hamiltonian operator is real, so that GOE and not GUE statistics are predicted for non-zero flux if the classical motion is chaotic. This case of false T breaking was confirmed by computations (not shown here) with the golden α for the heart-shaped billiard with $B = 0.4$ and $C = 0$, previously studied with zero flux classically and quantally by Robnik (1983, 1984).

We summarise our conclusions as follows. Breaking the time-reversal symmetry of a quantal system whose corresponding classical motion is, and continues to be, chaotic causes the local spectral fluctuations to change their universality class from that of the Gaussian orthogonal ensemble of random-matrix theory to that of the Gaussian unitary ensemble. This has been illustrated in the simplest possible way by the Aharonov–Bohm quantum billiard, for which switching on the flux breaks quantum mechanical time-reversal symmetry whilst preserving the geometry of classical trajectories.

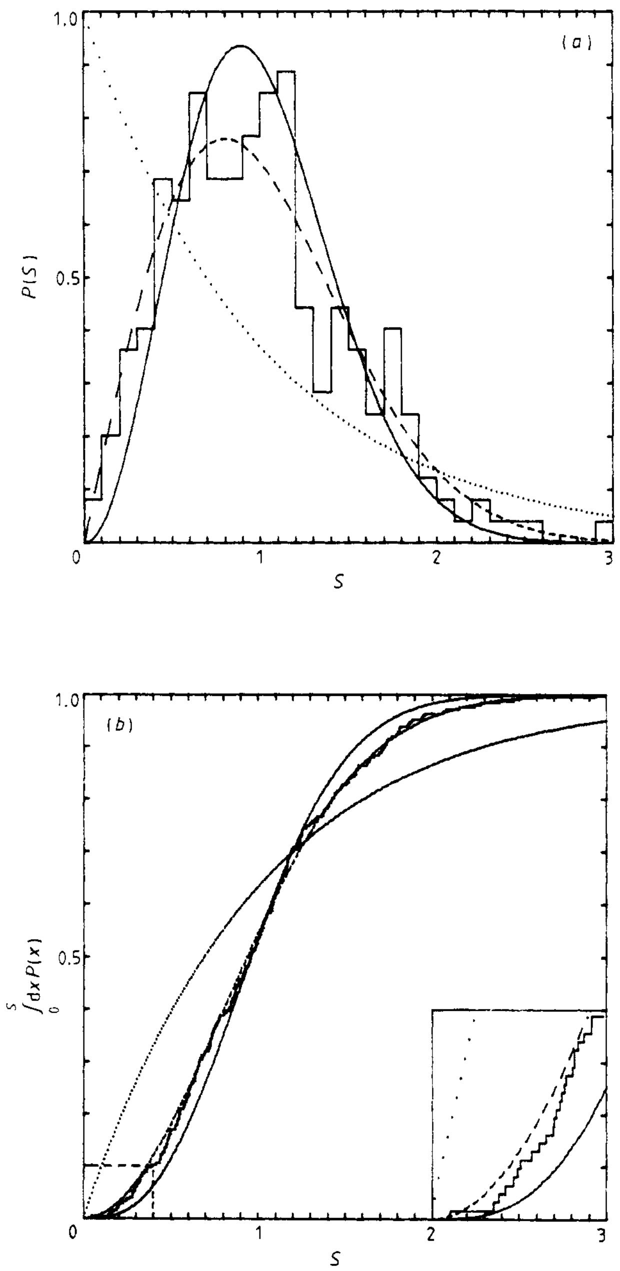

Figure 6.

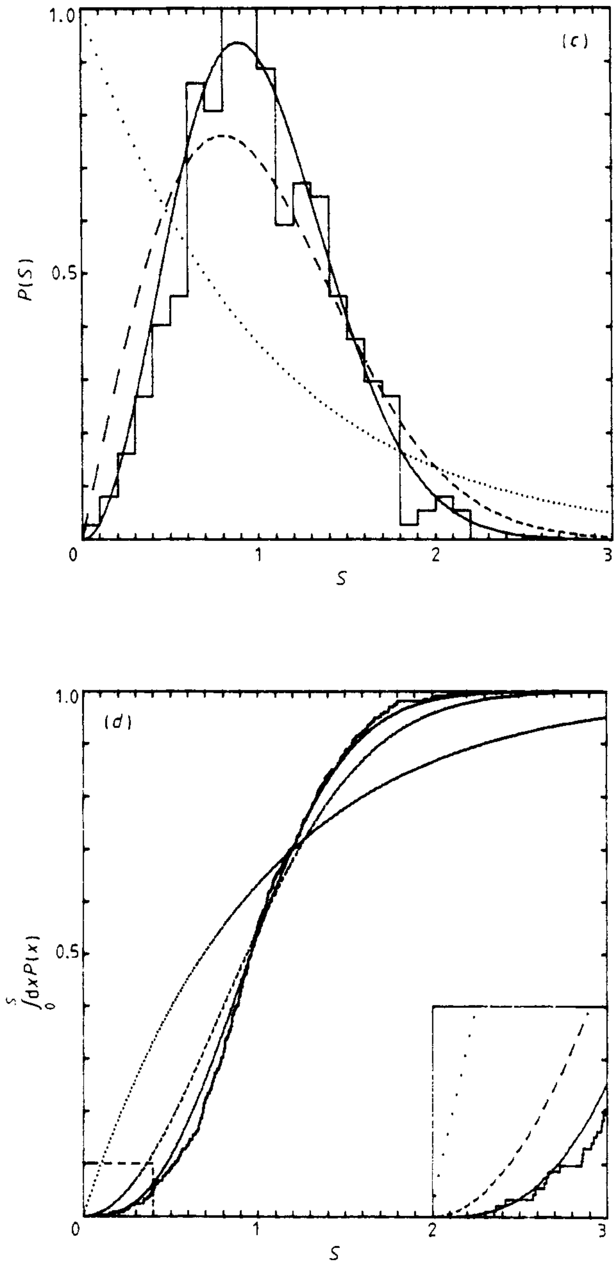

Figure 6. (a) Level spacings distribution combining data from $\alpha = 0$ (figure 2(a)) and $\alpha = \frac{1}{2}$ (figure 5(a)); (b) cumulative level spacings distribution $\int_0^S dxP(x)$ combining data from $\alpha = 0$ (figure 2(b)) and $\alpha = \frac{1}{2}$ (figure 5(b)); (c) level spacings distribution combining data from $\alpha = \frac{1}{2}(\sqrt{5}-1)$ (figure 3(a)), $\alpha = \frac{1}{4}$ (figure 4(a)), and $\alpha = \frac{1}{2}(\sqrt{5}-2)$; ($d$) cumulative level spacings distribution combining data from $\alpha = \frac{1}{2}(\sqrt{5}-1)$ (figure 3(b)), $\alpha = \frac{1}{4}$ (figure 4(b)) and $\alpha = \frac{1}{2}(\sqrt{5}-2)$. ($a$) and ($b$) show clear GOE behaviour (broken curves) whilst (c) and (d) show clear GUE behaviour (full curves).

Acknowledgments

We thank Dr J H Hannay for the idea which led to the appendix. MVB thanks the Institut de Physique Nucléaire (Paris-Sud) for hospitality whilst this paper was written. MR thanks the UK Science and Engineering Research Council for financial support. No military agency supported this research.

Appendix. Statistics of winding numbers of long closed orbits†

For any particular n-step closed orbit the winding number will be an integer-valued function of position, $W(\boldsymbol{r})$, which changes by ± 1 whenever the flux line $\boldsymbol{r}$ crosses the orbit and which vanishes on the boundary ∂D. As $n \to \infty$ the orbits tend to cover D densely and so in any small displacement $\boldsymbol{R}$ the number of crossings will be constant and equal to $2n|\boldsymbol{R}|/\mathscr{L}$ (as can be seen by choosing $\boldsymbol{R}$ close to the boundary and parallel to it and realising that each of the n chords meets the boundary twice). Because the increments of W are randomly ± 1 for large n, the mean *square* increment of W in a displacement $\boldsymbol{R}$ (averaged over all n-step orbits) equals the number of crossings, i.e.

$$\langle [W(\boldsymbol{r}+\boldsymbol{R}) - W(\boldsymbol{r})]^2 \rangle = 2n|\boldsymbol{R}|/\mathscr{L}. \tag{A1}$$

Therefore $W(\boldsymbol{r})$ is a *Brown plane-to-line function* (Mandelbrot 1982) and so has a Gaussian distribution, whose variance $\langle W^2(\boldsymbol{r})\rangle$ we seek to estimate. We begin by noting that $W(\boldsymbol{r})$ can be represented by an expansion in terms of any convenient complete set of functions; it is natural to choose the eigenfunctions of the Laplacian in D. Thus we can write

$$W(\boldsymbol{r}) = \sum_{j=1}^{\infty} \frac{a_j}{k_j^{\mu}} \psi_j(\boldsymbol{r}) \tag{A2}$$

where

$$\nabla^2 \psi_j + k_j^2 \psi_j = 0 \text{ in } D, \qquad \psi_j = 0 \text{ on } \partial D, \tag{A3}$$

and the a_j are independent random variables with zero mean and, for large j, a common variance $\langle a_j^2 \rangle$ which, along with the index μ, is to be determined by requiring the statistics of $W(\boldsymbol{r})$ to conform to (A1).

Thus

$$2\langle a_j^2 \rangle \sum_{j=1}^{\infty} \frac{\langle \psi_j^2(\boldsymbol{r})\rangle - \langle \psi_j(\boldsymbol{r})\psi_j(\boldsymbol{r}+\boldsymbol{R})\rangle}{k_j^{2\mu}} = \frac{2n|\boldsymbol{R}|}{\mathscr{L}}. \tag{A4}$$

Here we have carried out not only an ensemble average over the a_j but also a local space average near $\boldsymbol{r}$ and $\boldsymbol{r}+\boldsymbol{R}$. For the eigenfunctions of classically ergodic systems these averages (mean square probability density and spatial autocorrelation function) were worked out by Berry (1977), and give

$$\frac{2\langle a_j^2 \rangle}{\mathscr{A}} \sum_{j=1}^{\infty} \frac{1 - J_0(k_j|\boldsymbol{R}|)}{k_j^{2\mu}} = \frac{2n|\boldsymbol{R}|}{\mathscr{L}}. \tag{A5}$$

Now $|\boldsymbol{R}|$ is small and each individual term vanishes as $|\boldsymbol{R}|^2$, so that the value of the

† Based on an idea of Dr J H Hannay.

sum is determined by its high terms and can therefore be replaced by an integral, using the Weyl rule

$$\sum_j \to \int \mathrm{d}k\, k\mathscr{A}/2\pi. \tag{A6}$$

Thus (A5) becomes

$$\frac{\langle a_j^2\rangle}{\pi}\int_0^\infty \frac{\mathrm{d}k}{k^{2\mu-1}}(1-J_0(k|\boldsymbol{R}|))=\frac{2n|\boldsymbol{R}|}{\mathscr{L}}. \tag{A7}$$

By scaling k to bring $|\boldsymbol{R}|$ outside the integral we identify $\mu=\frac{3}{2}$ and

$$\langle a_j^2\rangle=\frac{2n\pi}{\mathscr{L}}\left(\int_0^\infty \frac{\mathrm{d}x}{x^2}(1-J_0(x))\right)^{-1}=\frac{2n\pi}{\mathscr{L}}. \tag{A8}$$

From (A2) the variance of winding number now becomes

$$\langle W^2(\boldsymbol{r})\rangle=\frac{2n\pi}{\mathscr{L}}\sum_{j=1}^\infty \frac{\psi_j^2(\boldsymbol{r})}{k_j^3}. \tag{A9}$$

The average value of $\langle W^2(\boldsymbol{r})\rangle$ over D, which we now denote by W_n^2, is found from (A9) by using the normalisation of the ψ_j:

$$W_n^2=\frac{2n\pi}{\mathscr{A}\mathscr{L}}\sum_{j=1}^\infty k_j^{-3}. \tag{A10}$$

This expression involves the zeta function of the eigenvalues k_j. An approximation adequate for the estimates of § 3 is obtained by a slight refinement of the Weyl rule, namely

$$j-\tfrac{1}{2}\approx \mathscr{A}k_j^2/4\pi \tag{A11}$$

which gives

$$\begin{aligned} W_n^2 &\approx \frac{n}{\mathscr{L}}\left(\frac{\mathscr{A}}{2\pi}\right)^{1/2}\sum_{j=1}^\infty (2j-1)^{-3/2} \\ &= \frac{n}{\mathscr{L}}\left(\frac{\mathscr{A}}{2\pi}\right)^{1/2}(1-2^{-3/2})\zeta(\tfrac{3}{2}). \end{aligned} \tag{A12}$$

Evaluating the Riemann zeta function, we obtain equation (21) of § 3.

References

Aharonov Y and Bohm D 1959 *Phys. Rev.* **115** 485–91
Balian R and Bloch C 1974 *Ann. Phys., NY* **85** 514–45
Baltes H P and Hilf E R 1976 *Spectra of finite systems* (Mannheim: B-I Wissenschaftsverlag)
Berry M V 1977 *J. Phys. A: Math. Gen.* **10** 2083–91
—— 1983 *Chaotic Behavior of Deterministic Systems* ed G Iooss, R H G Helleman and R Stora (Amsterdam: North-Holland) pp 171–271
—— 1985a *Proc. R. Soc.* A **400** 299–51
—— 1985b *Proc. Como Conf. on Quantum Chaos* ed G Casati (London: Plenum) pp 123–40
Berry M V, Chambers R G, Large M D, Upstill C and Walmsley J C 1980 *Eur. J. Phys.* **1** 154–62

Bohigas O and Giannoni M J 1984 *Mathematical and Computational Methods in Nuclear Physics* ed J S Dehesa, J M G Gomez and A Polls (*Lectures Notes in Physics* **209**) (New York: Springer) pp 1-99
Bohigas O, Giannoni M J and Schmit C 1984 *Phys. Rev. Lett.* **52** 1-4
Dyson F J and Mehta M L 1963 *J. Math. Phys.* **4** 701-12
Gutzwiller M C 1978 *Path Integrals and their Applications in Quantum, Statistical and Solid-State Physics* ed G J Papadoulos and J T Devreese (New York: Plenum) pp 163-200
Izraelev F M 1984 *Preprint, 84-63* Novosibirsk
Joyce W B 1975 *J. Acoust. Soc. Am.* **58** 643-55
Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
Mehta M L 1967 *Random Matrices and the Statistical Theory of Energy Levels* (New York: Academic)
Mehta M L and Pandey A 1983 *J. Phys. A: Math. Gen.* **16** 2655-84
Morandi G and Menossi E 1984 *Eur. J. Phys.* **5** 49-58
Olariu S and Popescu I 1985 *Rev. Mod. Phys.* **57** 339-436
Pandey A 1981 *Ann. Phys., NY* **134** 110-27
Porter C E 1965 *Statistical Theories of Spectra: Fluctuations* (New York: Academic)
Robnik M 1983 *J. Phys. A: Math. Gen.* **16** 3971-86
—— 1984 *J. Phys. A: Math. Gen.* **17** 1049-74
Robnik M and Berry M V 1985 *J. Phys. A: Math. Gen.* **18** 1361-78
Seligman T H and Verbaarschot J J M 1985 *Phys. Lett.* **108A** 183-7