

Home Search Collections Journals About Contact us My IOPscience

A Brownian motion model for the parameter dependence of matrix elements

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 1995 J. Phys. A: Math. Gen. 28 6143 (http://iopscience.iop.org/0305-4470/28/21/017)

View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 171.66.16.70 The article was downloaded on 02/06/2010 at 03:50

Please note that terms and conditions apply.

A Brownian motion model for the parameter dependence of matrix elements

Michael Wilkinson and Paul N Walker

Department of Physics and Applied Physics, John Anderson Building, University of Strathclyde, Glasgow G4 0NG, UK

Received 7 March 1995, in final form 11 July 1995

Abstract. We introduce a Brownian motion model for the parametric evolution of eigenstates of a complex quantum system, modelled by a random matrix. The model is analogous to Dyson's model for the evolution of the eigenvalues. We use this approach to analyse correlation functions describing the parameter dependence of diagonal and off-diagonal matrix elements of a generic operator. In the case of diagonal matrix elements, we compare our results with a semiclassical approach, which relates sums of matrix elements to periodic classical orbits. For systems with a chaotic classical limit, the semiclassical correlation function agrees exactly with the random matrix theory.

1. Introduction

In this paper we consider the sensitivity of the eigenstates of a Hamiltonian $\hat{H}(X)$ to variations of a parameter X, using a random matrix model. We characterize the parameter dependence of the eigenstates $|\phi_n(X)\rangle$ through statistics of the matrix elements $U_{nm}(X', X) = \langle \phi_n(X') | \phi_m(X) \rangle$, describing the overlap between eigenstates at X' and those at X. We calculate the mean value $\langle U_{nm}(X', X) \rangle$ of these overlap matrix elements and the overlap probabilities $P_{nm} = \langle |U_{nm}(X', X)|^2 \rangle$; the angle brackets denote an average over the random matrix ensemble. We use these statistics to analyse the parameter dependence of the matrix elements $A_{nm}(X) = \langle \phi_n(X) | \hat{A} | \phi_m(X) \rangle$ of an operator \hat{A} which is independent of the Hamiltonian. There are several physical problems for which it is important to understand the parameter dependence of matrix elements of this type. One application is to the analysis of the adiabatic form of the Schrödinger equation, in which these matrix elements appear [1]. Another application is to understanding fluctuations of transition strengths of atomic, molecular, or mesoscopic systems as a parameter (such as an externally applied electric or magnetic field) is varied.

In common with other theories based on random matrix Hamiltonians, the results are expected to apply to 'real' quantum systems which have no symmetries or constants of motion: random matrix models have been very successful in describing complex nuclear spectra [2], and systems with few degrees of freedom which have chaotic classical dynamics [3]. As well as providing a good description of the statistical properties of the spectrum, random matrix models can also describe the parametric dependence of energy levels [4]. This is important in analysing the response of systems to large perturbations [5], and to perturbations which induce a shift in the parameter as well as a transition between levels [6]. We demonstrate the applicability of our random matrix results by comparing one of our statistics with semiclassical results, for a system with a chaotic classical limit. Despite the very different basis of the two approaches, the results agree exactly.

The parameter dependence of the matrix elements A_{nm} can be characterized by their correlation functions: we will consider correlations of both diagonal and off-diagonal matrix elements:

$$\langle A_{nn}(X)A_{n'n'}(X')\rangle \tag{1.1a}$$

$$\langle A_{nm}(X)A_{n'm'}^*(X')\rangle. \tag{1.1b}$$

The angle brackets denote an average over the random matrix ensemble; to apply the results to specific quantum systems this average would be replaced by an average over matrix elements for states with energies E_n , E_m close to a given energy E; we give an example of such an average in (1.2) below.

It is difficult to calculate these correlation functions directly, using a model in which the Hamiltonian depends smoothly on the parameter X. Instead, we will consider a Brownian motion model, in which the Hamiltonian matrix evolves diffusively, as a function of a fictitious time variable τ . The Brownian motion model was invented by Dyson [7], and used to study parameter dependencies in the spectra of random matrices by Beenakker and Rejaei [8, 9]. In section 2 we discuss the relationship between the Brownian motion model as smooth parametrization of the random matrix Hamiltonian.

The equations of motion of the energy levels in the Brownian motion model were discussed by Dyson [7]. In section 3 we give Langevin equations of motion for the overlap matrix elements U_{nm} , which are analogous to the Dyson model for the eigenvalues. We discuss the solution of these equations of motion in section 4, and give results for the averages of the elements U_{nm} and the overlap probabilities $|U_{nm}|^2$ in the limit where τ is large. Our results are complementary to some recent work by Kusnezov and Lewenkopf [10]. They describe a considerably less general Brownian motion model for the wavefunctions which only treats the diagonal elements U_{nn} , but they also consider a variant of the model in which the matrix elements undergo anomolous diffusion.

In section 5 we apply these results to the correlation functions (1.1). It is desirable to check these predictions of random matrix theory against other approaches. In section 6 we compare our results for the diagonal matrix elements with a semiclassical theory [11] for the statistic

$$f(E, X) = \sum_{n} A_{nn} \delta_{\epsilon} (E - E_n)$$
(1.2)

where $\delta_{\epsilon}(x)$ is a 'smoothed delta function', i.e. a function supported on an interval of length ϵ at x = 0, with unit weight (an example is $\delta_{\epsilon}(x) = \exp(-x^2/2\epsilon^2)/\epsilon\sqrt{2\pi}$). This statistic represents an average value of the diagonal matrix elements of \hat{A} for states $|\phi_n\rangle$ with energies within a tolerance ϵ of E. We find that the semiclassical and random matrix theory predictions for the correlation function of f agree exactly. Section 7 contains some concluding remarks.

2. Relationship between the parametrized Gaussian ensembles and the Dyson model

The natural model for analysing parameter-dependent quantities is the following parametrization of the standard Gaussian ensembles [4]:

$$\hat{H}(X) = \cos X \hat{H}_1 + \sin X \hat{H}_2$$
 (2.1)

where \hat{H}_1 and \hat{H}_2 are independent samples from the same Gaussian symmetry-invariant ensemble: the relevant symmetry classes are orthogonal, unitary, or symplectic [2, 12]. The dimension N of the matrices \hat{H}_1 and \hat{H}_2 should be large. We will only discuss the cases of the Gaussian unitary and orthogonal ensembles. In the case of the unitary ensemble the Hamiltonian is a Hermitean matrix with elements of the real and imaginary parts independently Gaussian distributed, satisfying

$$\langle H_{ij} \rangle = 0 \tag{2.2}$$

and

$$\langle H_{ij}H_{i'j'}^*\rangle = \delta_{ii'}\delta_{jj'} \qquad \langle H_{ij}H_{i'j'}\rangle = \delta_{ij'}\delta_{i'j}. \tag{2.3}$$

The elements of the orthogonal ensemble are real and (2.3) is replaced by

$$\langle H_{ij}H_{i'j'}\rangle = \delta_{ii'}\delta_{jj'} + \delta_{ij'}\delta_{i'j} . \tag{2.4}$$

In this paper we will show that matrix elements decorrelate over a very short range of X; in this case the periodicity of (2.1) in X is irrelevant, and the Hamiltonian can be approximated by

$$\hat{H}(X) = \hat{H}_1 + X\hat{H}_2.$$
(2.5)

Random matrix models provide a good statistical description of the spectrum of many systems, after the energy levels are scaled to have the same density of states ρ as the random matrix ensemble. When we extend the random matrix model to describe the parameter dependence of energy levels, another scaling parameter must be introduced to describe the sensitivity of energy levels to a perturbation. The most natural choice [4] is the variance of the off-diagonal matrix elements of $\partial \hat{H} / \partial X$:

$$\mu^{2}(E) = \left\langle \left| \left(\frac{\partial H}{\partial X} \right)_{nm} \right|^{2} \right\rangle_{E_{n} \sim E_{nt} \sim E} \,. \tag{2.6}$$

The matrix elements are evaluated in the eigenbasis of \hat{H} , and only matrix elements for which E_n and E_m are close to the energy of interest are included in the average. It follows from the invariance properties of the Gaussian ensembles that for our random matrix models (2.1) or (2.5) we have $\mu = 1$. The general definition of μ^2 , and formulae for calculating it in semiclassical systems, are discussed in [4, 13].

The X dependencies of the matrix elements A_{nm} obey a complex set of equations of motion similar to those discussed by Pechukas [14]; the direct solution of these equations is very difficult. Instead, we will relate the parameter dependence of the model (2.1) to that of the 'Brownian motion model' discussed by Dyson [7], which is considerably simpler to analyse. This correspondence was first discussed by Beenakker [8], who noted that if the Brownian motion model and the smooth parametrization are to agree, the parameter X and the time variable τ must be related by $X^2 \sim \tau$ for small τ . Our discussion below makes the connection with (2.1) clearer, in that it shows that the relationship between X^2 and τ is linear for all τ .

In the Dyson model, the matrix elements of the Hamiltonian undergo a diffusive evolution as a function of a fictitious time variable τ . In the unitary case the change

 δH_{ij} in the elements of the random matrix Hamiltonian due to an infinitesimal increment $\delta \tau$ in the time variable satisfies

$$\langle \delta H_{ij} \delta H_{i'j'}^* \rangle = \delta_{ii'} \delta_{ji'} D \delta \tau \qquad \langle \delta H_{ij} \delta H_{i'j'} \rangle = \delta_{ij'} \delta_{i'j} D \delta \tau \qquad (2.7)$$

where D is a constant. The corresponding rule for the orthogonal case follows by analogy with (2.3). The increment $\delta \hat{H}$ is also assumed to be independent of the Hamiltonian \hat{H} . The invariance properties of the Gaussian invariant ensembles show that (2.7) remains true when the matrix $\delta \hat{H} = \{\delta H_{ij}\}$ is transformed to the eigenbasis of \hat{H} ; we use the notation $\delta H'_{nm} = \langle \phi_n | \delta \hat{H} | \phi_m \rangle$ for these transformed matrix elements. In the version originally formulated by Dyson, the mean value of δH_{ij} is non-zero in order to ensure that the matrix elements do not have a secular increase. The matrix element correlations which we consider decay very rapidly, and we can ignore this refinement and write

$$\langle \delta H_{ij} \rangle = 0. \tag{2.8}$$

The reader can verify that neglecting the mean value makes no difference to the correlation functions which we calculate.

We will show explicitly that the dynamics of the deterministic model (2.1) and of the stochastic model described by (2.7) and (2.8) are related if the increment of the fictitious time variable is related to the parameter X by the relation

$$\mu^2 X^2 = D\tau \,. \tag{2.9}$$

In order to clarify the connection between these two random matrix models, we introduce a multidimensional version of (2.1), in which the parameter space is d dimensional, with components X_1, X_2, \ldots, X_d ; we will be concerned with the limit in which $d \gg 1$. We consider the following generalization of (2.1):

$$\hat{H}(X) = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} \cos(\sqrt{d}X_i) \hat{H}_{2i-1} + \sin(\sqrt{d}X_i) \hat{H}_{2i}.$$
(2.10)

Note that both $\hat{H}(X)$ and $\partial \hat{H}/\partial X_i$ have the same statistical properties as (2.1). We will contrast the behaviour of the elements of this Hamiltonian matrix along two different paths in the multidimensional parameter space. One of these paths will be a random walk; along this path the elements of the Hamiltonian matrix evolve diffusively, in exactly the same manner as for the Brownian motion model. The second path is a straight line joining the beginning and end points of this random walk. Along this path, the evolution of the Hamiltonian matrix is smooth and deterministic, and is similar to (2.1).

First we consider the case of the random-walk path, in which for each time interval $\delta \tau$ we make a step of length $\pm \delta X_i$ along a randomly chosen axis (the *i*th, say). The corresponding change in the Hamiltonian matrix is

$$\delta \hat{H} = \left[-\sin(\sqrt{d}X_i) \hat{H}_{2i-1} + \cos(\sqrt{d}X_i) \hat{H}_{2i} \right] \delta X_i .$$
(2.11)

If we take the magnitude of δX_i to be $|\delta X_i| = \sqrt{D\delta \tau}/\mu$, it is clear that the statistical properties of the increment (2.10) are identical to those of the Dyson model, specified by (2.7) and (2.8). Furthermore, because the increments of the Hamiltonian in each of the *d* different directions are independent random matrices, the successive time steps become

uncorrelated in the limit where $d \gg 1$. In the limit where d is large, the evolution of the Hamiltonian therefore corresponds to that of the Dyson model.

The random walk reaches a position $X(\tau)$ after time τ . The Euclidean distance travelled, R = |X|, satisfies $\langle R^2 \rangle = D\tau/\mu^2$, and the probability distribution P[R]dR of R is

$$P[R] dR = CR^{d-1} \exp(-d\mu^2 R^2/2D\tau) dR$$
(2.12)

for some constant C. In the limit of large d, this distribution is very sharply peaked at $R = \sqrt{D\tau}/\mu$, implying that although the direction travelled is random, the final distance from the starting point has very small fluctuations.

We now consider an alternative path, in which the end point of the random walk is reached by following a straight line, parametrized by a coordinate λ : we write

$$X(\lambda) = \lambda s \tag{2.13}$$

where $X(\tau)$ is the final position of the random walk at time τ , and $s = X(\tau)/\sqrt{D\tau}$ is a vector which, in the limit $d \gg 1$, has a length which is almost always very close to unity. The Hamiltonian at coordinate λ along this path is

$$\hat{H}(\lambda) = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} \cos(\sqrt{d}\lambda s_i) \hat{H}_{2i-1} + \sin(\sqrt{d}\lambda s_i) \hat{H}_{2i} \sim \hat{H}'_1 + \lambda \hat{H}'_2$$
(2.14)

where in the second relation we assume that $\lambda \sqrt{d} \ll 1$, and where

$$\hat{H}'_{1} = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} \hat{H}_{2i-1} \qquad \hat{H}'_{2} = \sum_{i=1}^{d} s_{i} \hat{H}_{2i}$$
(2.15)

are two independent GUE or GOE matrices with statistics specified by (2.2)–(2.4). Along the straight line path parametrized by λ , the model (2.10) is therefore equivalent to the smooth parametrization, equation (2.5), provided that $\lambda\sqrt{d} \ll 1$. This model can be used to analyse the decay of correlations if the support $\Delta\lambda$ of the correlation function satisfies $\Delta\lambda\sqrt{d} \ll 1$. Our results will show that $\Delta\lambda\rho\mu \sim 1$: for the random matrix ensemble, $\rho \sim \sqrt{N}$ and $\mu = 1$ [2], implying that we should choose N and d in (2.10) such that $N \gg d \gg 1$.

By considering the evolution of (2.10) along two different paths, we have shown that the Brownian motion model is equivalent to the smoothly parametrized ensemble when $\lambda = \sqrt{D\tau}$. The correlation of a function in the smoothly parametrized model can therefore be obtained from that in the Dyson model using (2.9), provided that the function is independent of the path.

3. A Dyson model for the evolution of eigenstates

The eigenfunctions $|\phi_n\rangle$ of a chaotic system are very sensitive to variation of a parameter in the Hamiltonian. The parameter dependence can be characterized by the set of Dirac brackets

$$U_{nm}(X', X) = \langle \phi_n(X') | \phi_m(X) \rangle.$$
(3.1)

The matrix $\tilde{U} = \{U_{nm}\}$ describes a change of basis, and is therefore unitary. We will consider a model for which the correlation functions depend only upon the separation X - X', and consider only the case where X' = 0. This is reasonable, because the correlations of functions decay very quickly.

We will derive a Brownian motion model for the overlaps $\langle \phi_n(0) | \phi_m(\tau) \rangle$; results for a smooth Hamiltonian can be obtained using (2.9). The objective is to model the evolution of the matrix elements U_{nm} as a function of τ by a set of Langevin equations. The starting point for deriving these equations is to apply Rayleigh-Schrödinger perturbation theory to second order. In the case of the energy levels this gives

$$\delta E_n(\tau) = E_n(\tau + \delta \tau) - E_n(\tau) = \delta H'_{nn} + \sum_{m \neq n} \frac{|\delta H'_{nm}|^2}{E_n - E_m} + \mathcal{O}(\delta H'^3)$$
(3.2)

where $\delta H'_{nm} = \langle \phi_n | \delta \hat{H} | \phi_m \rangle$; in the case of functions

$$\begin{split} |\delta\phi_{n}(\tau)\rangle &= |\phi_{n}(\tau + \delta\tau)\rangle - |\phi_{n}(\tau)\rangle = \sum_{m \neq n} \frac{\delta H'_{mn}}{E_{n} - E_{m}} |\phi_{m}(\tau)\rangle \\ &+ \sum_{m \neq n} \sum_{k \neq n} \frac{\delta H'_{mk} \delta H'_{kn}}{(E_{n} - E_{m})(E_{n} - E_{k})} |\phi_{m}(\tau)\rangle - \sum_{m \neq n} \frac{\delta H'_{nn} \delta H'_{mn}}{(E_{n} - E_{m})^{2}} |\phi_{m}(\tau)\rangle \\ &- \frac{1}{2} \sum_{k \neq n} \frac{|\delta H'_{nk}|^{2}}{(E_{n} - E_{k})^{2}} |\phi_{n}(\tau)\rangle + O(\delta H'^{3}) \,. \end{split}$$
(3.3)

The wavefunction remains normalized (up to second order in $\delta H'$), and satisfies

$$\langle \phi_n(\tau) | \delta \phi_n(\tau) \rangle = 0 \tag{3.4}$$

to lowest order. In the unitary case (3.4) can be seen as a connection rule [15] which determines the phases of the states, given an arbitrary choice at $\tau = 0$; for the orthogonal case the wavefunction is always real. Defining

$$\Delta U_{nm}(\tau) = \langle \phi_n(\tau) | \phi_m(\tau + \delta \tau) \rangle \tag{3.5}$$

we find that the overlap $U_{nm}(\tau) = \langle \phi_n(0) | \phi_m(\tau) \rangle$ evolves as follows:

$$U_{nm}(\tau + \delta\tau) = \sum_{k} U_{nk}(\tau) \Delta U_{km}(\tau) .$$
(3.6)

The coefficients ΔU_{km} can be obtained from (3.3). The change in the overlap matrix element U_{nm} due to a perturbation of the Hamiltonian with elements $\delta H'_{nm}$ is therefore

$$\delta U_{nm}(\tau) = U_{nm}(\tau + \delta \tau) - U_{nm}(\tau) = \sum_{k} U_{nk}(\tau) \Big[\Delta U_{km}(\tau) - \delta_{km} \Big]$$

=
$$\sum_{k \neq m} U_{nk} \Big[\frac{\delta H'_{km}}{E_m - E_k} + \sum_{j \neq m} \frac{\delta H'_{kj} \delta H'_{jm}}{(E_m - E_j)(E_m - E_k)} - \frac{\delta H'_{mm} \delta H'_{km}}{(E_k - E_m)^2} \Big]$$

-
$$\frac{1}{2} U_{nm} \sum_{k \neq m} \frac{|\delta H'_{mk}|^2}{(E_m - E_k)^2} .$$
 (3.7)

Brownian motion model

6149

If the matrix elements $\delta H'_{nm}$ evolve diffusively according to (2.7) and (2.8), equations (3.2) and (3.7) can be replaced by Langevin equations. The Langevin equation corresponding to (3.2) was discussed by Dyson [7]: the change in the energy level E_n in time $\delta \tau$ is the sum of a random impulse δF_n and a drift with velocity v_n ,

$$\delta E_n = \delta F_n + v_n \delta \tau \,. \tag{3.8}$$

The drift velocity is given by

$$v_n \delta \tau = \langle \delta E_n \rangle = \sum_{m \neq n} \frac{\langle \delta | H'_{nm} |^2 \rangle}{E_n - E_m} = D \delta \tau \sum_{m \neq n} \frac{1}{E_n - E_m}$$
(3.9)

and the random impulse $\delta F_n = H'_{nn}$ satisfies

$$\langle \delta F_n \rangle = 0 \qquad \langle \delta F_n^2 \rangle = \langle \delta H'_{nn}^2 \rangle = 2\beta^{-1} D \delta \tau$$
 (3.10)

(where $\beta = 1$ in the orthogonal case, $\beta = 2$ in the unitary case). The overlap matrix elements satisfy a similar Langevin equation

$$\delta U_{nm} = \delta F_{nm} + v_{nm} \delta \tau$$

=
$$\sum_{k \neq m} U_{nk} \frac{\delta H'_{km}}{E_m - E_k} + \langle \delta U_{nm} \rangle$$
 (3.11)

where the second line defines both the random impulse term and the drift velocities. The Langevin equation is fully specified by calculating the drift term $\langle \delta U_{nm} \rangle$ and the correlations of the impulse terms, which are the same (to leading order in $\delta \tau$) as the correlations of the δU_{nm} :

$$\langle \delta F_{nm} \delta F_{n'm'} \rangle = \langle \delta U_{nm} \delta U_{n'm'} \rangle + \mathcal{O}(\delta \tau^2) \,. \tag{3.12}$$

We now consider the statistical properties of the elements δU_{nm} , treating the unitary and orthogonal cases separately. Using equations (2.7) and (2.8), and discarding all terms of higher order than $\delta H^{\prime 2}$, we find that the leading order contributions to the changes in the matrix elements U_{nm} therefore have the following statistical properties:

$$\langle \delta U_{nm}(\tau) \rangle = -\frac{1}{2} D \delta \tau U_{nm} \sum_{k \neq m} \frac{1}{(E_m - E_k)^2}$$
 (3.13)

$$\langle \delta U_{nm} \delta U_{kl} \rangle = (1 - \delta_{ml}) D \delta \tau U_{nl} U_{km} \frac{1}{(E_m - E_l)^2}$$
(3.14)

$$\langle \delta U_{nm} \delta U_{kl}^* \rangle = \delta_{ml} D \delta \tau \sum_{j \neq m} \frac{1}{(E_m - E_j)^2} U_{nj} U_{kj}^*$$
(3.15)

(and the r.h.s. of (3.14) is zero when m = l). In the orthogonal case we write $O_{nm}(\tau) = \langle \phi_n(0) | \phi_m(\tau) \rangle$; the equation for $\langle \delta O_{nm} \rangle$ is identical to the unitary case (3.13), but the result for the correlations of the impulses is

$$\langle \delta O_{nm} \delta O_{kl} \rangle = (1 - \delta_{ml}) D \delta \tau \frac{1}{(E_m - E_l)^2} O_{nl} O_{km} + \delta_{ml} D \delta \tau \sum_{j \neq m} \frac{1}{(E_m - E_j)^2} O_{nj} O_{kj}.$$
(3.16)

Equations (3.11) and (3.13)-(3.16) define our Brownian motion model for the wavefunctions. It is important to note that the impulses driving the energy levels are given by the diagonal elements $\delta H'_{nn}$, whereas the impulses driving the stochastic evolution of the wavefunctions depend only on the off-diagonal elements $\delta H'_{nm}$. This decoupling greatly simplifies the calculation of ensemble averages. We can consider the evolution of the wavefunctions using (3.11) with the τ dependence of the energy levels frozen, and then perform the average over the energy level fluctuations specified by (3.8). It will be useful to establish some notation for these averages. Averages over an infinitesimal time increment $\delta \tau$ will be denoted by plain angle brackets, as used above. Averages over the ensemble of Brownian paths will be indicated using a subscript e, for example $\langle F \rangle_e$. Averages over the off-diagonal fluctuations $\delta H'_{nm}$, with the energies frozen, will be written $\langle F \rangle_o$; these quantities depend on the history of the energy dependencies $E_n(\tau)$ because the energy levels appear in the equations of motion for the wavefunctions. The remaining average over the different histories of the energy levels will be written $\langle \cdot \cdot \rangle_d$, so that

$$\langle F \rangle_e = \langle \langle F \rangle_o \rangle_d . \tag{3.17}$$

Note that the ensemble average of the increment δF in an infinitesimal timestep $\delta \tau$ can be written

$$\langle\langle \delta F \rangle\rangle_e = \delta\langle F \rangle_e \,. \tag{3.18}$$

4. The overlap probabilities and amplitudes

In this section we calculate the overlap probability $P_{nm} = \langle |U_{nm}(\tau)|^2 \rangle_e$ and the mean overlap $\langle U_{nm}(\tau) \rangle_e$ in the limit $\tau \to \infty$. The approach in both cases is to derive and solve an equation of motion for the statistic of interest as a function of τ . Our calculations assume that there are a large number of levels and that the density of states ρ can be regarded as being independent of energy; these assumptions are valid for the Gaussian ensembles in the large $N \to \infty$ at fixed energy.

4.1. Overlap probabilities

The overlap probability is defined as

$$P_{nm}(\tau) = \langle |U_{nm}(\tau)|^2 \rangle_e \,. \tag{4.1}$$

Its increment δP_{nm} in time $\delta \tau$ is

$$\delta P_{nm} = \langle |U_{nm}(\tau + \delta \tau)|^2 \rangle_e - \langle |U_{nm}(\tau)|^2 \rangle_e$$

= $\langle |U_{nm}(\tau) + \delta U_{nm}(\tau)|^2 \rangle_e - \langle |U_{nm}(\tau)|^2 \rangle_e$
= $\langle \delta U_{nm} U_{nm}^* + U_{nm} \delta U_{nm}^* + |\delta U_{nm}|^2 \rangle_e$. (4.2)

Note that we can write

$$\langle \delta U_{nm} U_{nm}^* \rangle_e = \langle \langle \delta U_{nm} \rangle U_{nm}^* \rangle_e \tag{4.3}$$

and similar expressions for the other terms in (4.2). We therefore have

$$\delta P_{nm} = \langle \langle \delta U_{nm} \rangle U_{nm}^* \rangle_e + \langle U_{nm} \langle \delta U_{nm}^* \rangle \rangle_e + \langle \langle \delta U_{nm} \delta U_{nm}^* \rangle \rangle_e \tag{4.4}$$

(the $(\delta U)^2$ term is retained because it is of the same order in $\delta \tau$ as the δU terms). Using (3.13)-(3.15) to substitute for the averages over $\delta \tau$, we obtain

$$\delta P_{nm} = \langle \delta \langle |U_{nm}|^2 \rangle_o \rangle_d = D \delta \tau \left\langle \sum_{k \neq m} \frac{U_{nk} U_{nk}^* - |U_{nm}|^2}{(E_m - E_k)^2} \right\rangle_e$$
$$= D \delta \tau \left\langle \sum_{k \neq m} \frac{\langle |U_{nk}|^2 \rangle_o - \langle |U_{nm}|^2 \rangle_o}{(E_m - E_k)^2} \right\rangle_d.$$
(4.5)

We can extract from (4.5) a rate equation for the partially averaged overlap probabilities

$$P_{nm}' = \langle |U_{nm}|^2 \rangle_o \tag{4.6}$$

obtained by averaging over the off-diagonal fluctuations $\delta H'_{nm}$, with the τ dependence of the energy levels frozen. These partially averaged probabilities obey the rate equation

$$\frac{\mathrm{d}P'_{nm}}{\mathrm{d}\tau} = D \sum_{j \neq n} \frac{(P'_{nj} - P'_{nm})}{(E_m - E_j)^2} \,. \tag{4.7}$$

This equation is to be solved subject to the initial condition $P_{nm}(0) = \delta_{nm}$. In the limit of large τ , the probability spreads diffusively, and the P'_{nm} may be regarded as a slowly varying function of n: in this limit we can approximate the $P'_{nm}(\tau)$ by a continuous function of n-m. Also, because of the rigidity properties of the distribution of energy levels given by the Dyson model, we can assume that $\Delta E = E_n - E_m$ is approximately equal to $(n-m)/\rho$, where ρ is the mean density of states. We will therefore consider P to be a smooth function of ΔE in the long-time limit. Replacing the sum in (4.7) by an integral, we approximate (4.7) by a continuum equation of the form

$$\frac{\partial P(\Delta E, \tau)}{\partial \tau} = \int_{-\infty}^{\infty} dE' R(\Delta E - E') P(E', \tau)$$
(4.8)

and the rate constant $R(\Delta E)$ is proportional to $1/\Delta E^2$ when $\rho|\Delta E| \gg 1$. The integral of $R(\Delta E)$ with respect to ΔE must be zero in order for probability to be conserved; we choose, for convenience, the following form for R which satisfies both of these conditions:

$$R(\Delta E) = \frac{\rho^3 D}{1 + \rho^2 \Delta E^2} - \pi \rho D \delta(\Delta E) \,. \tag{4.9}$$

The final result, equation (4.12), does not depend on the manner in which the $1/\Delta E^2$ divergence at small energy separations is eliminated. Equation (4.8) is solved by taking the Fourier transform; if t is the Fourier transform variable conjugate to ΔE , we have

$$\frac{\partial \tilde{P}(t,\tau)}{\partial \tau} = 2\pi \tilde{R}(t)\tilde{P}(t,\tau) \qquad \tilde{R}(t) = \frac{1}{2}\rho^2 D(\mathrm{e}^{-|t|/\rho} - 1). \tag{4.10}$$

In the limit of increasing τ , the Fourier transform $\tilde{P}(t,\tau)$ is supported on a decreasing interval of t, centred at t = 0: in this limit we can approximate $e^{-|t|/\rho} - 1$ by $-|t|/\rho$. The solution of the resulting equation is $\tilde{P} = C \exp(-\pi\rho D\tau |t|)$ for some constant C, chosen to normalize the integral of P to $1/\rho$. Inverting the Fourier transform, we find the following approximate solution of (4.8), valid for large τ :

$$P(\Delta E, \tau) = \frac{D\tau}{\Delta E^2 + (\pi \rho D\tau)^2}.$$
(4.11)

This result is independent of the τ dependence of the energy levels, indicating that there is no need to average over the energy level fluctuations. Equation (4.11) has been verified by a numerical simulation. Expressed in terms of the parameter X, and the state labels n, m, our final result for the overlap probability is

$$P_{nm}(X) = \frac{\mu^2 X^2}{(E_n - E_m)^2 + (\pi \rho \mu^2 X^2)^2}$$
(4.12)

which is valid in the limit $|X| \to \infty$. An identical result is obtained in the orthogonal case. A similar formula has been suggested by Kusnezov and Lewenkopf [10] for the case where n = m, and numerical evidence supporting this result is given in [16].

4.2. Overlap amplitudes

Next we consider the average of the overlap amplitude, $(U_{nm})_e$. Averaging (3.13) over the ensemble of Brownian paths, we obtain

$$\delta \langle U_{nm} \rangle_e = \langle \langle \delta U_{nm} \rangle \rangle_e$$
$$= -\frac{1}{2} D \delta \tau \left\langle U_{nm} \sum_{k \neq m} \frac{1}{(E_m - E_k)^2} \right\rangle_e.$$
(4.13)

We can write this result in the form

$$\langle \delta \langle U_{nm} \rangle_o \rangle_d = -\frac{1}{2} D \delta \tau \left\langle \langle U_{nm} \rangle_o \sum_{k \neq m} \frac{1}{(E_m - E_k)^2} \right\rangle_d.$$
(4.14)

A simple differential equation for the partial average $\langle U_{nm} \rangle_o$ can be extracted from (4.14); its solution is

$$\langle U_{nm}(\tau) \rangle_o = \delta_{nm} \exp[-F_n(\tau)] \tag{4.15}$$

where we have used the initial condition $U_{nm}(0) = \delta_{nm}$. Here the function $F_n(\tau)$ is

$$F_n(\tau) = \frac{1}{2} D \int_0^{\tau} \mathrm{d}\tau' \sum_{k \neq n} \frac{1}{[E_n(\tau') - E_k(\tau')]^2} \,. \tag{4.16}$$

The ensemble average is obtained by integrating (4.15) over the different histories of the energy levels $E_n(\tau)$:

$$\langle U_{nm}(\tau) \rangle_{e} = \delta_{nm} \langle \exp[-F_{n}(\tau)] \rangle_{d}$$

$$= \int_{0}^{\infty} dF P[F] e^{-F}$$

$$(4.17)$$

where P[F] is the probability distribution of the integrals F_n . The modal value of P[F] is

$$F_{\rm mode} \sim \rho^2 D\tau \tag{4.18}$$

and the integral (4.17) is dominated by the modal region of the distribution of F, so that in the limit of large τ

$$\langle U_{nm}(\tau) \rangle_{e} = \delta_{nm} \Gamma_{\beta} \exp(-\alpha_{\beta} \rho^{2} D \tau)$$
(4.19)

for some constants α_{β} , Γ_{β} . We have not been able to calculate these constants analytically. We confirmed (4.19) by simulating the Langevin equation (3.8) for the evolution of the energy levels, and calculating the average $\langle \exp[-F(\tau)] \rangle_d$. Our numerical simulations give the values $\alpha_1 \approx 3.84$ and $\Gamma_1 \approx 0.8$ in the orthogonal case ($\beta = 1$), and $\alpha_2 \approx 2.6$, $\Gamma_2 \approx 0.9$ for the unitary case. We remark that in the orthogonal case the mean value of F does not exist, due to the greater probability of near degeneracies where $E_n \approx E_k$, but this fact does not affect the existence of $\langle \exp(-F) \rangle$.

There is a significant difference in the interpretation of the results between the orthogonal and unitary cases. In the unitary case, the predictions of the Dyson model and the smooth parametrization (2.1) may not coincide, because the phases of the eigenfunctions $|\phi_n(X)\rangle$ depend on the path taken by the random walk in the multidimensional parameter space. The phases of the off-diagonal elements are determined by the connection rule (3.4), which is path-dependent: the difference in phase of the state $|\phi_n(X)\rangle$ between two paths is given by the integral of the curvature of the connection over a surface of which the two paths form the boundary [15]. The phases from different Brownian paths leading to the same point in the multidimensional parameter space may lead to a cancellation of the average of the off-diagonal matrix elements, and it is probable that in the unitary case the average $\langle U_{nm}(\tau) \rangle$ decays more rapidly than for the smooth parametrization. In the orthogonal case, the connection rule (3.4) simply ensures that the wavefunction remains real, and the phase is the same for all paths. Only in the orthogonal case can (4.19) be applied directly to the the case of a smoothly parametrized Hamiltonian, implying a Gaussian decay of correlations in the limit $|X| \to \infty$:

$$\langle O_{nm}(X) \rangle_e = \delta_{nm} \Gamma_1 \exp(-\alpha_1 \mu^2 \rho^2 X^2) \,. \tag{4.20}$$

5. Correlations of matrix elements

Now we will use the results of section 4 to derive information about correlations of matrix elements in the limit of large X. We consider the matrix elements $A_{nm}(X)$ of an arbitrary operator \hat{A} in the basis formed by the states $|\phi_n(X)\rangle$. The dependence of the matrix elements $A_{nm}(X) = \langle \phi_n(X) | \hat{A}(X) | \phi_m(X) \rangle$ on the parameter X is most strongly influenced by the parameter dependence of the basis states; we will therefore assume that the operator \hat{A} is independent of X. As in section 4, the results apply to the $N \to \infty$ limit of the random matrix problem.

Following the usual approach of random matrix theory, we assume that the matrix elements $A_{nm}(0)$ are uncorrelated Gaussian random variables, with mean value zero, and with a variance σ^2 , which can depend on $\bar{E} = \frac{1}{2}(E_n + E_m)$ and $\Delta E = (E_n - E_m)$. In semiclassical systems, the variance $\sigma^2(\bar{E}, \Delta E)$ varies on a scale which is $O(\hbar)$ in ΔE ,

but independent of \hbar in the variable \overline{E} [13]. For this reason, we will also simplify the calculation by assuming that σ^2 is a function of ΔE only.

In the case of systems without time-reversal invariance, for which the unitary ensemble is an appropriate model, we will assume that the matrix elements A_{nm} have the following statistical properties:

$$\langle A_{nm}(0)\rangle = 0 \tag{5.1}$$

and

$$\langle A_{nm}(0)A_{n'm'}^*(0)\rangle = \delta_{nn'}\delta_{mm'}\sigma_{nm}^2 \qquad \langle A_{nm}(0)A_{n'm'}(0)\rangle = \delta_{nm'}\delta_{n'm}\sigma_{nm}^2.$$
(5.2)

In 'real' systems the off-diagonal matrix elements have mean value zero [4], but the mean value of the diagonal matrix elements need not be zero [11]; our results can readily be extended to that case. In systems with orthogonal statistics the matrix elements are real, and we replace (5.2) by

$$\langle A_{nn'}(0)A_{mm'}(0)\rangle = (\delta_{nn'}\delta_{mm'} + \delta_{n'm}\delta_{nm'})\sigma_{nm}^2.$$
(5.3)

The matrix elements $A_{nm}(X)$ can be obtained from those at X = 0 using the coefficients of the unitary matrix $U_{nm}(X)$:

$$A_{nm}(X) = \langle \phi_n(X) | \hat{A} | \phi_m(X) \rangle$$

= $\sum_k \sum_l \langle \phi_n(X) | \phi_k(0) \rangle \langle \phi_k(0) | \hat{A} | \phi_l(0) \rangle \langle \phi_l(0) | \phi_m(X) \rangle$
= $\sum_k \sum_l U_{kn}^*(X) A_{kl}(0) U_{lm}(X)$. (5.4)

It can be assumed that the matrix elements $A_{nm}(0)$ and $U_{nm}(X)$ in (5.4) are uncorrelated, because \hat{A} is assumed to be independent of the Hamiltonian \hat{H} ; averages over the elements $U_{nm}(X)$ and $A_{kl}(0)$ can therefore be separated. We now consider both of the averages introduced in (1.1) in turn.

5.1. Diagonal matrix elements

First we consider the calculation of the correlation coefficient of the diagonal matrix elements:

$$\langle A_{nn}(X)A_{n'n'}(0)\rangle = \sum_{k} \sum_{l} \langle U_{kn}^{*}(X)U_{ln}(X)\rangle_{e} \langle A_{kl}(0)A_{n'n'}(0)\rangle.$$
(5.5)

The only non-vanishing contribution is from the term k = l = n', which (using equation (4.12)) gives

$$\langle A_{nn}(X)A_{n'n'}(0)\rangle = P_{n'n}\sigma_{nn}^2 \sim \frac{\sigma_{nn}^2\mu^2 X^2}{(E_n - E_{n'})^2 + (\pi\rho\mu^2 X^2)^2} \,. \tag{5.6}$$

This result shows that, although the matrix elements are initially uncorrelated at X = 0, the elements become correlated when evaluated at different values of the parameters. These

correlations decay as X^{-2} at large X. A similar result is obtained in the orthogonal case; the only difference is that the result is multiplied by a factor of two.

In many situations individual matrix elements are of little significance, but sums of matrix elements are related to observable properties. In the case of diagonal matrix elements it is natural to consider the statistic $f_{\epsilon}(E)$ defined by (1.2). The correlation function of this statistic, obtained by averaging over the energy E, can be obtained from (5.6):

$$K_d(\Delta E, X) = \langle f_{\epsilon}(\Delta E, X) f_{\epsilon}(0, 0) \rangle_E = \frac{1}{2\pi\epsilon^2} \sum_n \sum_{n'} \langle A_{nn}(X) A_{n'n'}(0) \rangle$$
$$\times \exp[-(\Delta E - E_n)^2 / 2\epsilon^2] \exp[-E_{n'}^2 / 2\epsilon^2] .$$
(5.7)

We now replace the summations by integrations, and approximate $P_{n'n}$ using a continuous function obtained from (4.12). We find, in the limit where $\rho \epsilon \gg 1$

$$K_d(\Delta E, X) = \frac{\rho^2 \sigma_{nn}^2}{2\pi\epsilon^2} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy P(x, X) \exp[-(x+y)^2/2\epsilon^2] \exp[-(\Delta E+y)^2/2\epsilon^2]$$
$$= \frac{\rho^2 \sigma_{nn}^2}{2\sqrt{\pi\epsilon}} \int_{-\infty}^{\infty} dx P(x, X) \exp[-(\Delta E-x)^2/4\epsilon^2].$$
(5.8)

The convolution theorem gives

$$K_d(\Delta E, X) = \frac{\rho \sigma_{nn}^2}{2\pi} \int_{-\infty}^{\infty} dt \exp(-\epsilon^2 t^2 - \pi \rho \mu^2 X^2 |t| - i\Delta Et)$$
(5.9)

which can be written in terms of the complimentary error function $\operatorname{erfc}(x)$:

$$K_d(\Delta E, X) = \frac{\rho \sigma_{nn}^2}{4\sqrt{\pi\epsilon}} \left[\exp(z^2) \operatorname{erfc}(z) + \exp(z^{*2}) \operatorname{erfc}(z^*) \right]$$

$$z = (\pi \rho \mu^2 X^2 + i\Delta E)/2\epsilon .$$
(5.10)

This result is valid when $\rho \in \gg 1$.

5.2. Off-diagonal matrix elements

Now we consider the correlation of a pair of off-diagonal matrix elements. The unitary and orthogonal cases are different and we discuss them separately, starting with the unitary case:

$$\langle A_{nm}(X)A_{n'm'}^{*}(0)\rangle = \sum_{k} \sum_{l} \langle U_{kn}^{*}(X)U_{lm}(X)\rangle_{e} \langle A_{kl}(0)A_{n'm'}^{*}(0)\rangle$$

= $\langle U_{n'n}^{*}U_{m'm}\rangle_{e}\sigma_{n'm'}^{2}.$ (5.11)

We can adapt the calculation of section 4.2 to estimate the coefficient $\langle U_{n'n}^* U_{m'm} \rangle_e$. Consider the average of the small increment in $U_{n'n}^* U_{m'm}$ occurring during the time interval $\delta \tau$:

$$\langle \delta(U_{n'n}^* U_{m'm}) \rangle = \langle \delta U_{n'n}^* \rangle U_{m'm} + U_{n'n}^* \langle \delta U_{m'm} \rangle + \langle \delta U_{n'n}^* \delta U_{m'm} \rangle$$

$$= -\frac{1}{2} D \delta \tau \Biggl[\sum_{k \neq n} \frac{1}{(E_n - E_k)^2} + \sum_{k \neq m} \frac{1}{(E_m - E_k)^2} \Biggr] U_{n'n}^* U_{m'm}$$

$$+ \delta_{nm} D \delta \tau \sum_{k \neq n} \frac{1}{(E_n - E_k)^2} U_{n'k}^* U_{m'k}$$
(5.12)

where equations (3.13) and (3.15) have been used to evaluate the averages. When $n \neq m$, the average of $U_{n'n}^* U_{m'm}$ with the energies frozen therefore obeys the rate equation

$$\delta \langle U_{n'n}^* U_{m'm} \rangle_o = -R(\tau) \langle U_{n'n}^* U_{m'm} \rangle_o \delta \tau$$
(5.13)

where

$$R(\tau) = \frac{1}{2} D \left[\sum_{k \neq n} \frac{1}{(E_k - E_n)^2} + \sum_{k \neq m} \frac{1}{(E_m - E_k)^2} \right].$$
 (5.14)

We now follow the argument at the end of section 4.2: solving (5.13), averaging over the energy fluctuations, and substituting the result into (5.11), we predict that the correlations of off-diagonal elements decay exponentially as $\tau \to \infty$:

$$\langle A_{nm}(\tau)A_{n'm'}^*(0)\rangle = \delta_{nn'}\delta_{mm'}\sigma_{nm}^2\Gamma_2'\exp(-\alpha_2'\rho^2 D\tau).$$
(5.15)

Here Γ'_2 and α'_2 are constants which are analogous to those introduced in (4.19), and which depend upon n - m. In the limit $|n - m| \gg 1$ the two sums in (5.14) are independent, and we will have $\alpha'_2 \to 2\alpha_2$, $\Gamma'_2 \to \Gamma^2_2$.

In the othogonal case we have

$$\langle A_{nm}(X)A_{n'm'}(0)\rangle = \langle O_{n'n}O_{m'm} + O_{n'm}O_{m'n}\rangle_e \sigma_{nm}$$
(5.16)

and using (3.13) and (3.16) we find that

$$\delta \langle O_{n'n} O_{m'm} + O_{n'm} O_{m'n} \rangle_o = -R(\tau) \langle O_{n'n} O_{m'm} + O_{n'm} O_{m'n} \rangle_o \delta \tau$$
(5.17)

where the rate constant is given by a slightly different expression from (5.14):

$$R(\tau) = \frac{1}{2} D \left[\sum_{k \neq n.m} \frac{1}{(E_n - E_k)^2} + \sum_{k \neq m.n} \frac{1}{(E_m - E_k)^2} \right].$$
 (5.18)

Again, the argument at the end of section 4 indicates that the correlation function is an exponential decaying function for large τ , with a different decay constant α'_1 . In terms of the dependence on X, the decay of correlations is Gaussian in the limit $\tau \to \infty$:

$$\langle A_{nm}(X)A_{n'm'}(0)\rangle = (\delta_{nn'}\delta_{mm'} + \delta_{n'm}\delta_{m'n})\sigma_{nm}^2\Gamma_1' \exp(-\alpha_1'\mu^2\rho^2 X^2).$$
(5.19)

6. Semiclassical theory for diagonal matrix elements

In this section we compare the random matrix theory prediction for the correlation function of the diagonal matrix elements with a semiclassical calculation, which applies to a system with chaotic classical motion. In the case of integrable classical motion, there is not expected to be any correspondence with random matrix theory.

It is not possible to write down an expression for a given matrix element of a chaotic system using semiclassical methods. The best that can be achieved is to write down an expression involving a summation over matrix elements in a small range of energy. For diagonal matrix elements, the appropriate sum is given by (1.2), and we will use a Gaussian weight for the smoothed delta function:

$$\delta_{\epsilon}(x) = \exp(-x^2/2\epsilon^2)/\epsilon\sqrt{2\pi} \,. \tag{6.1}$$

In the case where \hat{A} is the identity operator, the sum (6.1) reduces to the smoothed density of states n(E), for which Gutzwiller [3] has given an expression in terms of the periodic classical orbits of the system (which are unstable and isolated):

$$n_{\epsilon}(E) = \rho(E) + \sum_{j} \alpha_{j} \exp(\mathrm{i}S_{j}/\hbar) \exp(-\epsilon^{2}\tau_{j}^{2}/2\hbar^{2})$$
(6.2)

where $\rho(E)$ is the Weyl approximation to the density of states, and the index j labels the periodic orbits of the underlying classical system. Here $S_j(E)$ is the classical action of the jth periodic orbit at energy E, and α_j contains information about the stability of the orbit and the Maslov indices. By calculating tr{ $\hat{A\delta}(E - \hat{H})$ } using Gutzwiller's method, this result is easily extended to the quantity $f_{\epsilon}(E)$; the result [11] is

$$f_{\epsilon}(E) = \langle A \rangle + \sum_{j} \alpha_{j} \bar{A}_{j} \exp(iS_{j}/\hbar) \exp(-\epsilon^{2}\tau_{j}^{2}/2\hbar^{2})$$
(6.3)

where $\langle A \rangle$ is the microcanonical average of the classical limit A(q, p) of \hat{A} at energy E, and \bar{A}_i is the time average of A(q, p) of over the periodic orbit $(q_i(t), p_i(t))$

$$\bar{A}_{j} = \frac{1}{\tau_{j}} \int_{0}^{\tau_{j}} dt \, A(q_{j}(t), p_{j}(t)) \,. \tag{6.4}$$

Because we are concerned with the fluctuation properties of $f_{\epsilon}(E)$, we will assume that the term $\langle A \rangle$ vanishes. Now we consider the correlation function of $f_{\epsilon}(E)$

$$K_d(\Delta E, X) = \langle f_\epsilon(E + \Delta E, X) f_\epsilon(E, 0) \rangle_E$$
(6.5)

where the average is taken over an interval of energy for which S_j , α_j and \bar{A}_j are approximately constant. Using the periodic orbit expansion (6.4), we have

$$K_d(\Delta E, X) = \sum_j \sum_k \langle \alpha_j \alpha_k \bar{A}_j \bar{A}_k \exp[i(\bar{S}_j(E + \Delta E, X) - \bar{S}_k(E, 0))/\hbar] \times \exp[-\epsilon^2(\tau_j^2 + \tau_k^2)/2\hbar^2] \rangle_E.$$
(6.6)

In the semiclassical $(\hbar \to 0)$ limit the term involving $\exp[i(S_j - S_k)/\hbar]$ is highly sensitive to variations in the energy of the orbit and the parameter X, because \hbar appears in the denominator of the phase. The dependence of the factors α_j and \bar{A}_j on energy and X will therefore be neglected. Also, the \bar{A}_j can be regarded as random variables: in the case of a system without time-reversal symmetry the double sum is dominated by the diagonal term, j = k; when there is time reversal invariance the orbits exist as symmetry related pairs. In the former case the correlation function can therefore be written

$$K_d(\Delta E, X) = \sum_j \langle \alpha_j^2 \bar{A}_j^2 \rangle \left\langle \exp\left[\frac{i}{\hbar} \left(\frac{\partial S_j}{\partial X} X + \frac{\partial S_j}{\partial E} \Delta E\right)\right] \right\rangle_E \exp(-\epsilon^2 \tau_j^2 / \hbar^2) \,. \tag{6.7}$$

A result discussed in the appendix relates the parameter derivative of the actions of the periodic orbits to the parameter derivative of the Hamiltonian, integrated over the trajectory: it is shown that, for long periodic orbits

$$\left\langle \exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{\partial S_j}{\partial X}\right)X\right]\right\rangle = \exp\left[-\pi\rho\mu^2 X^2 \tau_j/\hbar\right]$$
 (6.8)

where the average is with respect to long orbits with periods close to τ_j . For long-period orbits the amplitudes α_j satisfy a sum rule discussed by Hannay and Ozorio de Almeida [17]:

$$\lim_{\tau \to \infty} \sum_{j} |\alpha_{j}|^{2} \delta_{\eta}(\tau - |\tau_{j}|) = \frac{2\tau}{(2\pi\hbar)^{2}}.$$
(6.9)

The mean value of A(q, p) evaluated along the periodic orbits can, in the case of long orbits, be related to the correlation function of A. Using a relationship between correlation functions and matrix elements which is discussed in [13], this can be expressed in terms of the mean square matrix elements of \hat{A} :

$$\langle \bar{A}_{j}^{2} \rangle = \frac{1}{\tau_{j}^{2}} \int_{0}^{\tau_{j}} dt \int_{0}^{\tau_{j}} dt' A_{j}(t) A_{j}(t') \sim \frac{1}{\tau_{j}} \int_{-\infty}^{\infty} dt \langle A(t)A(0) \rangle = 2\pi \rho \hbar \sigma^{2}(E, 0)/\tau_{j} \qquad (6.10)$$

where $\sigma^2(E, 0)$ is the variance of the off-diagonal matrix elements with $E_n \sim E_m \sim E$. Using equation (6.9) to replace the summation in (6.7) by an integral, and using (6.8) and (6.10), we have

$$K_{d}(\Delta E, X) = \frac{\rho \sigma^{2}}{\pi \hbar} \int_{0}^{\infty} d\tau \exp(-\epsilon^{2} \tau^{2} / \hbar^{2}) \exp(-(\pi \rho \mu^{2} X^{2} |\tau| + i \Delta E \tau) / \hbar)$$

$$= \frac{\rho \sigma^{2}}{4 \sqrt{\pi} \epsilon} \Big[\exp(z^{2}) \operatorname{erfc}(z) + \exp(z^{*2}) \operatorname{erfc}(z^{*}) \Big]$$

$$z = (\pi \rho \mu^{2} X^{2} + i \Delta E) / 2\epsilon.$$
 (6.11)

This is identical to the random matrix result for the unitary case, equation (5.10). For a system with time-reversal invariance, pairing the orbits with their time-reversed images doubles this result, in agreement with our findings for the orthogonal ensemble.

7. Concluding remarks

We have found a surprising difference between the correlation functions of diagonal matrix elements (which have correlations decaying with a power law), and off-diagonal elements (for which, in the orthogonal ensemble, the correlation function has a Gaussian decay). Also, we found that diagonal matrix elements which are uncorrelated at X = X' become correlated when $X \neq X'$: this follows from the fact that a pair of states $|\phi_n(X')\rangle$ and $|\phi_m(X)\rangle$ which are orthogonal when X = X' overlap when $X \neq X'$. These emergent correlations are absent from the off-diagonal matrix elements. Our conclusions concerning the off-diagonal matrix elements are consistent with a model for matrix element correlations introduced in an earlier paper [1], which discussed a model for the dynamics of complex systems. There is an extensive literature on the correlation function of dE_n/dX , which was investigated using random matrix methods by Altshuler and Simons [18] and by Beenakker and Rejaei [8, 9], and using semiclassical methods by Berry and Keating [19]. The parameter derivative of an energy level is a diagonal matrix element $(dE_n/dX = \langle \phi_n | d\hat{H}/dX | \phi_n \rangle)$ but our results are distinct from those of these earlier papers. This is because the matrix element dE_n/dX is correlated with the parameter dependence of the energy levels, whereas we have considered the case where the operator \hat{A} is unrelated to the Hamiltonian.

We made efforts to find a correspondence between our random matrix results on the statistics of the off-diagonal matrix elements, and a semiclassical theory [13] for the variance of the off-diagonal matrix elements. In this case we could not establish a correspondence; we believe that this is because the existing semiclassical theory is not sufficiently refined to reproduce the random matrix results.

We believe that the extension of the Dyson's approach to parametric dependencies of wavefunctions described in this paper will find many applications beyond those described in this paper. It is possible to use these methods to calculate averages of products of four overlap matrix elements U_{nm} , and we are applying this approach to correlation functions of transition strengths $|A_{nm}|^2$ and of the adiabatic curvature or Berry phase 2-form [15].

Acknowledgments

MW thanks CWJ Beenakker for the suggestion that the Dyson model could be extended to the eigenstates. This work was supported by the EPSRC, through a research grant reference GR/H94337, and a postgraduate studentship for PNW.

Appendix.

Goldberg *et al* [20] show that the parameter derivative of the action of a periodic orbit is related to the parameter derivative of the classical Hamiltonian as follows:

$$\frac{\partial S_j}{\partial X} = -\int_0^{\tau_j} dt \frac{\partial H}{\partial X}(q_j(t), p_j(t)).$$
(A.1)

In the limit of long periodic orbits these integrals can be assumed to have a Gaussian distribution. We will assume that the microcanonical average of $\partial H/\partial X$ vanishes; the calculation is easily extended to the general case. For orbits which are long compared to the characteristic timescale for the decay of classical correlations, the variance of $\partial S_j/\partial X$ can be expressed in terms of the classical correlation function

$$C_A(E,T) = \int \mathrm{d}q \int \mathrm{d}p \; \frac{\partial H}{\partial X}(q,p) \; \frac{\partial H}{\partial X}(q(t),p(t)) \; \delta(E-H(q,p)) \,. \tag{A.2}$$

Following the argument of Goldberg et al,

$$\left\langle \left(\frac{\partial S_j}{\partial X}\right)^2 \right\rangle = \tau_j \int_{-\infty}^{\infty} \mathrm{d}t \, C_A(E, t) \,. \tag{A.3}$$

In the semiclassical limit the integral over the correlation function can be expressed [13] exactly in terms of the variance of the matrix elements for states with nearly equal energies:

$$\left\langle \left(\frac{\partial S_j}{\partial X}\right)^2 \right\rangle = 2\pi\hbar\tau_j\sigma^2(E,0).$$
 (A.4)

If θ is a Gaussian distributed with mean value zero, we have $\langle \exp(i\theta) \rangle = \exp(-\frac{1}{2}\langle \theta^2 \rangle)$. Applying this to (A.4) gives

$$\left\langle \exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{\partial S_j}{\partial X}\right)X\right]\right\rangle = \exp\left[-\pi\sigma^2 X^2 \tau_j/\hbar\right].$$
 (A.5)

References

- [1] Wilkinson M and Austin E J 1995 J. Phys. A: Math. Gen. 28 2277-96
- [2] Porter C E (ed) 1965 Statistical Theories of Spectra: Fluctuations (New York: Academic)
- [3] Gutzwiller M C 1990 Chaos in Classical and Quantum Mechanics (New York: Springer)
- [4] Austin E J and Wilkinson M 1992 Nonlinearlity 5 1137-50
- [5] Wilkinson M 1988 J. Phys. A: Math. Gen. A 21 4021-37
- [6] Taniguchi N and Altshuler B L 1994 Phys. Rev. Lett. 71 4031
- [7] Dyson F J 1962 J. Math. Phys. 3 1191-8
- [8] Beenakker C W J 1993 Phys. Rev. Lett. 70 4126
- [9] Beenakker C W J and Rejaei B 1994 Physica 203A 61-90
- [10] Kusnezov D and Lewenkopf C H 1995 Yale university preprint
- [11] Wilkinson M 1988 J. Phys. A: Math. Gen. A 21 1173-90
- [12] Mehta M L 1991 Random Matrices 2nd edn (New York: Academic)
- [13] Wilkinson M 1987 J. Phys. A: Math. Gen. A 20 2415-23
- [14] Pechukas P 1983 Phys. Rev. Lett. 51 943-6
- [15] Shapere A and Wilczek F (eds) 1989 Geometric Phases in Physics (Singapore: World Scientific)
- [16] Kusnezov D and Mitchell D 1995 Yale university preprint
- [17] Hannay J H and Ozorio de Almeida A M 1984 J. Phys. A: Math. Gen. A 17 3429-40
- [18] Simons B D and Altshuler B L 1993 Phys. Rev. Lett. 70 4063
- [19] Berry M V and Keating J P 1994 J. Phys. A: Math. Gen. A 27 6167-76
- [20] Goldberg J, Smilansky U, Berry M V, Schweizer W, Wunner G and Zeller G 1991 Nonlinearity 4 1