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J. Phys. A: Math. Gen. 36 (2003) 1289-1297

PII: S0305-4470(03)39975-5

Fluctuations of wavefunctions about their classical average

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Received 23 July 2002, in final form 3 December 2002 Published 22 January 2003 Online at stacks.iop.org/JPhysA/36/1289

Abstract

Quantum-classical correspondence for the average shape of eigenfunctions and the local spectral density of states are well-known facts. In this paper, the fluctuations of the quantum wavefunctions around the classical value are discussed. A simple random matrix model leads to a Gaussian distribution of the amplitudes whose width is determined by the classical shape of the eigenfunction. To compare this prediction with numerical calculations in chaotic models of coupled quartic oscillators, we develop a rescaling method for the components. The expectations are broadly confirmed, but deviations due to scars are observed. This effect is much reduced when both Hamiltonians have chaotic dynamics.

PACS numbers: 05.45.-a, 05.45.Mt, 03.65.Sq

1. Introduction

At the turn of the century the study of the quantum manifestations of classically chaotic systems suffered a significant change. Earlier, spectral statistics were amply discussed and it was shown that they follow the random matrix theory (RMT) predictions [1, 2]. The study of properties of wavefunction, however, presents inherent difficulties arising from the dependence on the basis used, forcing either to specify one or to define basis-independent quantities. Progress has been made in this respect in the study of average properties of eigenstates [3–5] and of the significant statistical deviations from RMT [9, 10]. Nevertheless, not much systematic work exists on the eigenfunction fluctuations in dynamical systems [3]. In this work we shall contribute to this last subject.

In a recent paper [5], it was found that the suitably rescaled overlaps between the eigenfunctions (EF) of two arbitrary Hamiltonians H_0 and H are well described in the

0305-4470/03/051289+09\$30.00 © 2003 IOP Publishing Ltd Printed in the UK

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semiclassical regime by a classical phase-space integral. Specifically, if we define ϕ_{α} , $E_{\alpha}^{(0)}$ to be the eigenfunctions and eigenvalues, respectively, of H_0 and ψ_i , E_i those of H, one finds to a good approximation

$$\langle |\langle \phi_{\alpha} | \psi_i \rangle|^2 \rangle = \tilde{g} \left(E_{\alpha}^{(0)}, E_i \right) \tag{1}$$

where $\tilde{g}(\epsilon, E)$ is given by

$$\tilde{g}(\epsilon, E) = \frac{g(\epsilon, E)}{(2\pi\hbar)^d \rho(E)\rho_0(\epsilon)}$$
(2)

and $g(\epsilon, E)$ is

$$g(\epsilon, E) = \int dp \, dq \, \delta(H_0(p, q) - \epsilon) \delta(H(p, q) - E)$$
(3)

which was called in [5] the *classical eigenfunction* for fixed *E*. Here $\rho_0(\epsilon)$ ($\rho(E)$) is the level density of $H_0(H)$ calculated by means of Weyl's formula. By the symmetry of equation (1), the local density of states can be calculated maintaining fixed ϵ in equation (2). For the details, in particular about the way in which the lhs of equation (1) must be averaged to obtain meaningful results, see [5]. This study was exemplified by two systems of anharmonic oscillators in one dimension, one coupled and the other uncoupled. We shall use these results in the present paper to analyse the *fluctuations* of the quantum wavefunctions around this classical limit in the chaotic case by comparing them with a simple random matrix model, presented in the next section. To be able to perform this comparison the component of the function has to be rescaled in a way that recalls the unfolding of the spectra, in order to compensate for average behaviour given by the classical limit. This rescaling has no free parameters and leads to a model-independent (universal) width of fluctuations, which is tested in numerical calculations in section 3.

2. A random matrix model

Random matrix models [1, 2] have a long history in the description of quantum systems whose classical analogue is chaotic, and relate to predictions of Gaussian distributions of wavefunctions [6, 8, 12] which have been discussed mainly in the context of billiards. Usually when one attempts a description of chaotic systems by random matrices, the restrictions implied by equations (1) and (2) are not present. Rather, one deduces the average properties of the eigenfunctions given the structure of the random matrix ensemble in some particular basis. Instead, here we choose pairs of matrices (H, H_0) of size $N \times N$ in such a way that the condition

$$\langle |\langle \phi_i | \psi_j \rangle|^2 \rangle = I_{i,j} \tag{4}$$

is always fulfilled, but the matrices are otherwise arbitrary. The angular brackets denote the average over the ensemble of matrix pairs and $I_{i,j}$ stand for any numbers given by outside constraints such as (1). Under these circumstances, we wish to determine the full distribution of the matrix elements $\langle \phi_i | \psi_j \rangle$. We then proceed to compare the predictions of this random matrix model with numerical results on models similar to that studied in [5].

To solve the above problem, we let ourselves be guided by the following considerations: the overlaps we need to model, namely the $\langle \phi_i | \psi_j \rangle$, are nothing other than the matrix elements of an orthogonal matrix (a unitary one in the case where time-reversal invariance is broken, but this does not affect our conclusions). We therefore need a random matrix model for orthogonal matrices of dimension *N* with prescribed expectation values for the intensities $I_{i,j}$. Note that,

in the large-*N* limit, the Haar measure over the group of orthogonal matrices can be replaced, up to corrections of order 1/N, by independent Gaussian distributions for all matrix elements $O_{i,j}$, all having a variance 1/N. In other words, what we need is a random matrix model where the average intensity $I_{i,j} = \langle |O_{i,j}\rangle|^2 \rangle$ is given. If $I_{i,j} \ll 1$, we can consider $1/I_{i,j}$ as an effective dimension and expect to get the desired result, up to corrections of order $O(I_{i,j})$, if we replace the average by a simple Gaussian average. We may then, to this level of accuracy, take the $O_{i,j}$ as independent Gaussian variables with variances given by $I_{i,j}$.

Note that we postulate a distribution for orthogonal matrices with the correct values for $I_{i,j}$. This directly relates the width of the distribution of amplitudes to the corresponding classical limit of the wavefunctions. For the particular case of a billiard [6] this variance is a reciprocal area, i.e. a classical quantity. We do not actually derive this distribution, but simply verify that it has all the required properties. If the classical wavefunction takes very large values and the eigenfunctions of H do not have a sufficiently large number of components in the basis of H_0 , it may happen that some $I_{i,j} \simeq 1$. Clearly, for these overlaps the model will not apply; we shall see later that this happens near peaks or singularities in the classical wavefunction, but then we cannot really make any comparison with the specific system anyway. However, for the vast majority of overlaps, we can expect that the amplitudes are Gaussian distributed and if we divide the amplitude $O_{i,j}$ by $\sqrt{I_{i,j}}$ we will find a standard Gaussian.

What deviations from the above predictions should we expect from a theoretical point of view? Clearly, scars [9] produce an excess of very small amplitudes, because a few exceptionally large amplitudes pick up more of the intensity than expected from the classical calculation. Would we also see the large amplitudes? Probably not in a statistical analysis against our model, because these will mainly occur in the region where the classical function is large and we will usually exclude this region: the condition $I_{i,j} \ll 1$ is violated there, unless we reach very high spectral densities, which is scarcely possible in a numerical experiment. In a real experiment, resolution might well make such a high-density region inaccessible as well. If, on the other hand, localization occurs due to disorder or due to the fact that the system does not cover the whole phase space on the Heisenberg timescale [11], then we may indeed also see irregularities beyond the realm of very small amplitudes.

However, all deviations mentioned above should only be important if one of the Hamiltonians, say H_0 , is integrable in the classical limit. If both are chaotic, and we exclude situations in which the two Hamiltonians are, in some sense, closely related, we can expect not to see any effect of the scars in the amplitudes. The reason for this can be understood in terms of the traditional picture due to Berry [12] of the eigenfunctions in phase space: for a chaotic Hamiltonian, they are expected to cover phase space in an essentially uniform way, up to rather small concentrations on periodic orbits. In integrable systems, on the other hand, eigenfunctions are localized on well-defined tori, with only half the dimension of the full phase space. The overlap between two chaotic states is therefore far less likely to become anomalously large than one between an integrable state and a chaotic one.

3. Numerical results

We now test the Gaussian property against anharmonic oscillator models. We shall choose the expansion of a chaotic system in terms of an integrable one; in particular, we have chosen two particles in a quartic oscillator potential. This ensures a system with scaling properties, for which the classical properties do not change as a function of energy. We restrict our attention to antisymmetric wavefunctions since in this case we reach the semiclassical limit much more rapidly than otherwise. The calculation is performed using the basis of the uncoupled



Figure 1. Averaged eigenfunction around (a) ψ_{100} , (b) ψ_{500} and (c) ψ_{900} , all three for H_1 with respect to H_0 with the parameters given in the text, with $E_{100} = 203.182$, $E_{500} = 576.267$ and $E_{900} = 846.680$, respectively. The smooth curve represents the corresponding classical EF. Note the general exponential decay and oscillations in the classically forbidden region.

oscillators, which in turn we approximate in a harmonic oscillator basis [5]. The Hamiltonian used is

$$H = \sum_{i=1}^{n} \frac{p_i^2}{2} + \alpha \sum_{i=1}^{n} x_i^4 + \beta \sum_{1 \le i < j}^{n} x_i^2 x_j^2 + \gamma \sum_{1 \le i < j}^{n} \left[x_i x_j^3 + x_i^3 x_j \right]$$
(5)

where in this case *n* is equal to two. We have also considered the case n = 4 with overall similar results [13]. We shall use two Hamiltonians: one with the same parameters as in [5], namely $\alpha = 10$, $\beta = -5.5$ and $\gamma = 5.6$, which we call H_1 ; the other with the parameters $\alpha = 10$, $\beta = \gamma = -4.15$, which we call H_2 . The H_0 Hamiltonian will have $\alpha = 10$ and $\beta = \gamma = 0$.

We analyse the eigenfunctions in terms of the classical eigenfunction as given in equation (2) at fixed energy E. The integral is calculated by the Monte Carlo method. We find very good agreement as shown in figure 1. There the classical EF and an average over 101 EFs of the perturbed Hamiltonian are plotted using the method of [5]. Note that the quantum functions are not reliable at the upper end of the classical energy range of H_0 for the higher lying states, although their energies are quite reliable. At the lower end of the spectra, on the other hand, the amplitudes are very good, and we find a consistent approximation to an exponential decay of intensities in the classically forbidden region as shown in figure 1, with some system-dependent oscillations (these disappear in the four-particle case [13]).



Figure 2. Eigenfunction tail zones B and C considered for analysis. The extreme cutoffs are determined by the quantum–classical agreement, and renormalized for unfolding. The centre window is 4Δ and 80Δ width for the corresponding cases analysed here.

We now proceed to analyse the amplitude fluctuations. We do this in the wings of the wavefunctions far from the peak, in regions where the classical function varies slowly and is sufficiently small to ensure $I_{i,j} \ll 1$; of course, we restrict our attention to reliable amplitudes. To this end, we first cut out the parts of the wavefunction which are either too high in energy so that they are not reliable, or which lie outside the classically allowed region. We further cut four states on either side of the singularity at the peak of the classical EF. We do this because the fluctuations around the peak are large and the peak itself at energy *E* is a singularity of the classical EF. We set the norm of the rest to one in both EF and the classical EF. Then we proceed to rescale the EF dividing the quantum EF by the classical one,

$$C_i^j = \frac{\langle \phi_i | \psi_j \rangle}{\sqrt{\tilde{g}(E_i^{(0)}, E_j)}}.$$
(6)

Note that C_i^j is normalized to N, more precisely to N_{eff}^j , that is, the effective number of components that we consider in the reliable zones described above. In practice, N_{eff}^j can be considered as a constant in a window of perturbed energies E_j inside which we take the average. The variance of C_i^j is one if the rhs of (6) corresponds to the random matrix model (4). In order to compare the different rescaled EFs we normalize them to one, the distributions of this normalized quantity are the object of the following analysis.

The corresponding regions in the wings, labelled B and C in figure 2, are the ones with the best quantum–classical correspondence. We use the intensity shape instead of amplitudes for clarity, but all the calculations were performed on the latter. In order to avoid the rapidly varying region, for the cases shown below we drop a window of four mean energy level spacings Δ centred in the eigenfunction for H_1 and one of 80Δ for H_2 ; the end of the C region is 400Δ away from the centre for both Hamiltonians. (The values of Δ are, respectively,



Figure 3. Amplitude distribution for 100 unfolded EF around the states with energies $E_{100} =$ 204.013 (a), (b) and $E_{900} = 846.680$ (c), (d) in zones B and C. The Gaussians with the same moments as the distributions are indicated by the continuous lines. Note that (b) is plotted on a semilogarithmic scale.

0.826 and 0.729.) As we cannot perform ensemble averages, we will perform energy averages within these windows after dividing the amplitudes by the square root of the local average intensity obtained from the classical function, which agrees well with the quantum average. As the centre of each EF changes in energy, the window centre changes but its width remains constant. The amplitude distributions we find, are plotted in figure 3 for the superposition of the results of regions B and C on 101 EFs; for low-lying states the shape is far from Gaussian while for high-lying states we find fair agreement with the Gaussian behaviour except for the excess of small intensities, which we expect due to scars. Such scars were seen in the two-body system as exceptional states with much narrower intensity distributions and smaller participation ratios [5]; similar results are found for the four-body system [13]. Nevertheless, a semi-log plot of the amplitude distribution shows a good parabolic shape in the wings, even for the zone C in a low-lying state around ψ_{100} (see figure 3(b)). This shows that fluctuations are more sensitive to non-classical effects than the average EF: compare the strong deviations for the states near ψ_{100} in figure 3 with the reasonable agreement shown in figure 1 for the same states.

We now test our assumption that scar effects are not seen when we expand the chaotic Hamiltonian in a basis of another chaotic Hamiltonian, instead of an integrable one. For such an expansion we put the EF of the H_2 Hamiltonian in terms of the H_1 EFs. The quantumclassical correspondence is shown in figure 4. In this case the exponential decay in the classically forbidden area shows a hump, for which we have no explanation. The B zone is



Figure 4. Averaged eigenfunction around ψ_{500} for H_2 Hamiltonian in the H_1 basis with the parameters given in the text and at energy $E_{500} = 611.717$. The smooth curve represents the corresponding classical EF.



Figure 5. Amplitude distribution for 100 unfolded states around the unfolded EF with energy $E_{500} = 611.717$ of the H_2 Hamiltonian in the zones B (*a*) and C (*b*). The Gaussians with the same moments as the distributions are shown by the continuous lines.

wider and in consequence the statistics are better as we show below. The amplitude distribution in the same region as in the previous case fits the Gaussian better, as shown in figure 5. The excess of small amplitudes decreases and the agreement is better in a wider energy regime. A similar result is observed if we drop localized states in the statistics for the previous case.



Figure 6. Histogram of the amplitude distribution in a window of width 20 energy units for 100 EFs around (*a*) ψ_{900} of H_1 and (*b*) ψ_{500} of H_2 . The normalization corresponds to the number of events per bin, the total number of events being 2525 and 2595 for (*a*) and (*b*), respectively. The corresponding values of χ^2 are $\chi^2_{16} = 12.289$ and $\chi^2_{16} = 14.483$. The continuous lines correspond to Gaussian curves with the same moments as the histograms.

Beyond all these features, if we consider small windows in the tail of eigenfunctions we find statistically good Gaussians for both cases. In figure 6 we show some of them. The window width is of 20 mean level spacings in order to have a sufficient number of amplitudes (~1000) of the 101 EFs considered for the average. They have energies between 1000 and 1020 in figure 6(*a*) for the state 900 of H_1 and from 640 to 660 for the state 500 of H_2 in figure 6(*b*). The fluctuations in figure 6 are larger than in the previous figures, but all of them are inside the statistical deviation, as shown by using the χ^2 test per bin, which is $\chi^2_{16} = 12.289$ for (*a*) and $\chi^2_{16} = 14.483$ for (*b*). For clarity, we plot the histograms with larger bins and normalized to (total number of events) × (bin width). We cannot get such a good fit to the Gaussian distribution for all energy ranges; the larger the window width, the worse the observed fit.

For the random matrix model the expected variance for C_k^i of equation (4) is one. In the dynamical problem it fluctuates around one for the small windows in unperturbed energy. For the large windows a tendency exists: in zone C this is to grow slowly from 0.95 for state ψ_{200} to 1.10 for state ψ_{800} . In zone B the tendency is to fall from 1 to 0.90 in the same interval of states. In zone A the variance fluctuates around 1. However the fluctuations are large and this result is not conclusive.

4. Conclusion

We have analysed the fluctuations of quantum-mechanical eigenfunctions with respect to their classical limit. Using a simple random matrix model, the amplitudes are shown to follow a

Gaussian distribution whose width is determined by the classical limit and rescaled to unity. This is confirmed by a numerical calculation using systems of two particles interacting through anharmonic potentials after carrying out the proper rescaling and normalization; agreement improves as we move up the spectrum, but more slowly for the fluctuations than for the average EF. We further find evidence for scars in an excess of small amplitude values as compared to the theoretical prediction if we express the eigenstate of the chaotic Hamiltonian in terms of an integrable one. This effect decreases markedly when both Hamiltonians have chaotic dynamics.

Acknowledgments

This work was partially supported by the DGAPA(UNAM) project IN-109201 and the CONACyT(México) grant nos 25192-E, 34668-E and 33773-E. One of the authors (HHS) acknowledges the financial support by DGEP(UNAM) and PAEP-PCF(UNAM).

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