The Effect of Scars on the Statistics of Transition Probabilities of Classically Chaotic Quantum Systems*

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We study the statistical properties of generalized intensities (squared matrix elements of Hermitian operators) for the hydrogen atom in strong magnetic fields in a range of parameters where the classical analogue of the system exhibits completely chaotic dynamics. In this way we extend previous work by Prosen and Robnik on the statistics of generalized intensities in *billiard* systems in the transition region with *mixed* classical dynamics. We observe deviations from the statistics found in that work, and demonstrate that these are due to the effect of scarring of wave functions by unstable periodic orbits.

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1. Introduction

Generalized intensities, i.e. off-diagonal matrix elements, are directly related to measured spectra and hence to experimental results. Thus it is of interest to investigate their characteristic features, which, in turn, depend on the properties of the underlying eigenfunctions. For quantum systems with classically chaotic counterparts the eigenfunctions are expected to cover the entire accessible phase space. Furthermore, the corresponding phase-space wave functions (e.g. Wigner distribution functions) fluctuate around the classical microcanonical distribution, as is implied by Shnirel'man's theorem (cf. [1]). This is equivalent to the statement that in the ergodic case almost all classical trajectories spread uniformly over the whole energy surface.

Starting from these ideas, many authors have shown that the distributions of quantum mechanical off-diagonal matrix elements of classically ergodic systems should be Gaussian (see e.g. [1, 2, 3]). For the squared matrix elements this implies a Porter-Thomas distribution [4]. In particular, Prosen and Robnik [3] analyzed the behaviour of transition probabilities of a billiard system with mixed dynamics and confirmed that the fluctuations obey the Porter-Thomas law. In the present note we wish to extend this type of analysis to a "real" physical system with classical chaos, namely the hydrogen atom in a strong magnetic field.

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2. Statistical analysis of matrix elements

The classical problem at hand is the well known diamagnetic Kepler problem (see e.g. [5]). A special feature of this system is its scaling property with respect to the ratio $\varepsilon = E\,\gamma^{-2/3}$ (where E is the energy in Hartrees (atomic units) and γ the magnetic field strength in units of 2.35×10^5 Tesla). Classical dynamics depends only on the value of this "scaled" energy ε, and not on energy and magnetic field strength separately. Hence the classical dynamics and the relations to quantum chaos are most adequately studied in that system at fixed scaled energy. In scaled quantum spectra the rôle of the new "energies" (i.e. eigenvalues), z, is taken by a power of the field strength, $z = \gamma^{-1/3}$. The scaling technique can be applied in studies of statistical properties of diagonal matrix elements [6]. It has also been applied in studies of transition amplitudes between initial and final states at constant scaled energy [7, 8], even though it must be noted that, experimentally, the magnetic field strength γ is kept constant in transitions, rather than ε.

To demonstrate the independence of the results from the choice of the operators we use the off-diagonal matrix elements of two different operators, viz. the dipole operator of $\Delta m = 0$ transitions ($\hat{A} = Z$) and the operator $\hat{A} = 1/\hat{P}^2$. The latter was chosen mainly for numerical convenience.

We investigate the statistical properties of matrix elements of the hydrogen atom in a magnetic field at fixed scaled energy $\varepsilon = -0.1$, where the classical phase space consists of a simply connected chaotic region without global stability islands to which regular eigenstates could be associated. All periodic orbits are unstable at that energy. However, the orbit parallel to the direction of the field is special in that it undergoes an infinite sequence of bifurcations up to the classical threshold energy $\varepsilon = 0$ [9, 10], and, in particular, turns stable at energies slightly below and above the value of the scaled energy we consider ($\varepsilon = -0.1$), viz. at $\varepsilon = -0.103602$ and $\varepsilon = -0.099873$.

The analysis presented here is based on the calculation of the first 2466 eigenstates with $z = \gamma^{-1/3} < 50$ (1247 for $m^\pi = 0^+$ and 1219 for $m^\pi = 0^-$). As expected, the matrix elements $A_{mn} = \langle m|\hat{A}|n\rangle$ cluster statistically around their classical limit, $\overline{A}$ ($m{=}n$) and zero ($m{\neq}n$), respectively.

An important point in our studies is the rescaling and unfolding of the matrix elements $\langle m|\hat{A}|n\rangle$ in such a way that, on the average, they become independent of the new energies $z = \gamma^{-1/3}$ (which are the eigenvalues of the individual states $|m\rangle$, $|n\rangle$ obtained in solving the scaled Schrödinger equation at fixed ε) and have constant variance $\overline{\sigma} = 1$. In the semiclassical approximation [11], the variance $\sigma^2(z, \Delta z)$ of non-diagonal matrix elements factorizes as

$$\sigma^2(z,\Delta z) = \rho_0(z)^{-1}\, C_A^{\mathrm{cl}}(\Delta z) \tag{1}$$

where $\rho_0(z)$ is evaluated at the mean of the eigenvalues of the initial and final state, $z = \frac{1}{2}(z_m + z_n)$, and $C_A^{\mathrm{cl}}(\Delta z)$ is the Fourier transform of the classical autocorrelation function of the Weyl transform $A(p,q)$ evaluated along an ergodic trajectory. The rescaling and unfolding of matrix elements is now achieved in two steps. The rescaling with respect to the variation of the mean level density $\rho_0(z)$ is accomplished by the transformation

$$\langle m|\hat{A}|n\rangle \to \sqrt{\rho_0(z)}\langle m|\hat{A}|n\rangle\ . \tag{2}$$

After rescaling, the renormalized quantum variance characterizing the distribution of off-diagonal transition amplitudes (see e.g. [2, 11]) reads

$$C_A^{\mathrm{qm}}(z,\Delta z) = \frac{1}{\rho_0(z)^2}\sum_{m,n}|A_{mn}|^2 \times$$
$$\delta_\eta\left(z - \frac{z_m + z_n}{2}\right) \times \delta_{\Delta\eta}\left(\Delta z - (z_m - z_n)\right)\ . \tag{3}$$

Because of the factorization (1) the variance of the rescaled matrix elements $C_A^{\mathrm{qm}}(z,\Delta z)$ becomes nearly independent of z. For the quantum variances of the operators $\hat{A} = Z,\ 1/\hat{P}^2$ for the hydrogen atom in a magnetic field the dependence of $C_A^{\mathrm{qm}}(z,\Delta z)$ on the spacings Δz is presented in figure 1 at $z = 30$.

The graphs for the operators $\hat{A} = Z$ and $\hat{A} = 1/\hat{P}^2$ differ significantly and illustrate the non-universal behaviour of $C_A^{\mathrm{qm}}(z,\Delta z)$. To allow for the discreteness of the spectrum, we have introduced

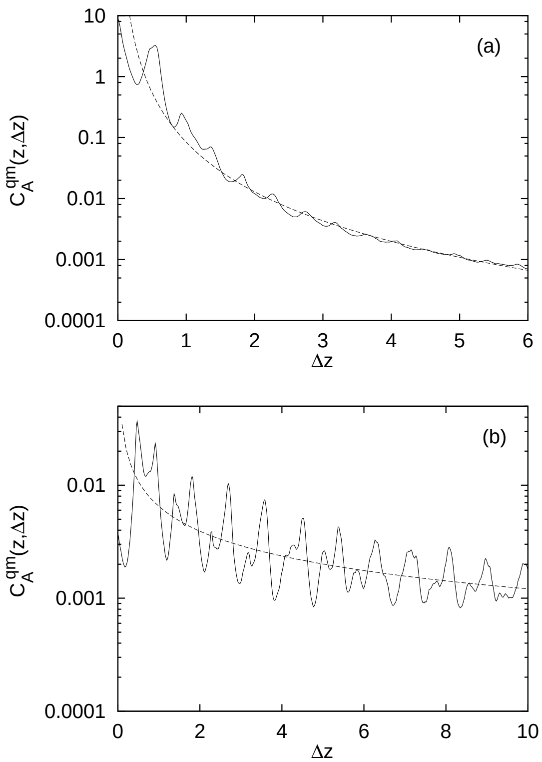

FIG. 1. Quantum variances $C_A^{\rm qm}(z,\Delta z)$ at $z = 30$, with smoothing parameters $\eta = 5$, $\Delta\eta = 0.02$. (a) Transition operator $\hat{A} = Z$, (b) $\hat{A} = 1/\hat{P}^2$. Dashed lines: Smooth fits $C_A^{\rm qm}(z,\Delta z) \sim (\Delta z)^{-\nu}$ with $\nu = 2.7$ in (a) and $\nu = 0.73$ in (b).

a Lorentzian broadening with widths $\eta = 5$ and $\Delta\eta = 0.02$ of the δ-functions in (3) and figure 1. Detailed results for various broadening widths and the relations of the dominant contribution (Weyl term) of C_A to the classical autocorrelation function have been presented by Boosé et al. [7]. The variances show large fluctuations superimposed on a smooth behaviour $\overline{C_A^{\rm qm}}(z,\Delta z) \sim (\Delta z)^{-\nu}$ (dashed lines in figure 1) with $\nu = 2.7$ for $\hat{A} = Z$ and $\nu = 0.73$ for $\hat{A} = 1/\hat{P}^2$.

With the general behaviour of the variances $C_A^{\rm qm}(z,\Delta z)$ for our system at hand it is possible to unfold the matrix elements to constant variance $\overline{\sigma} = 1$,

$$x = \frac{1}{\sqrt{\overline{C_A^{\rm qm}}(z,\Delta z)}} \langle m|\hat{A}|n\rangle \ . \tag{4}$$

Note that we use the smoothed behaviour of the variances only for unfolding, the fluctuations of $C_A^{\rm qm}(z,\Delta z)$ depend on the broadening width $\Delta\eta$ of the δ-function in (3) (see [7]). The rescaled and unfolded matrix elements x are now regarded as random variables and the fluctuations of the squares of the unfolded matrix elements

$$y = |x|^2 = \frac{1}{\overline{C_A^{\rm qm}}(z,\Delta z)} \, |\langle m|\hat{A}|n\rangle|^2 \tag{5}$$

are compared with the Porter-Thomas distribution

$$P(y) = \frac{1}{\sqrt{2\pi y}} e^{-y/2} \ . \tag{6}$$

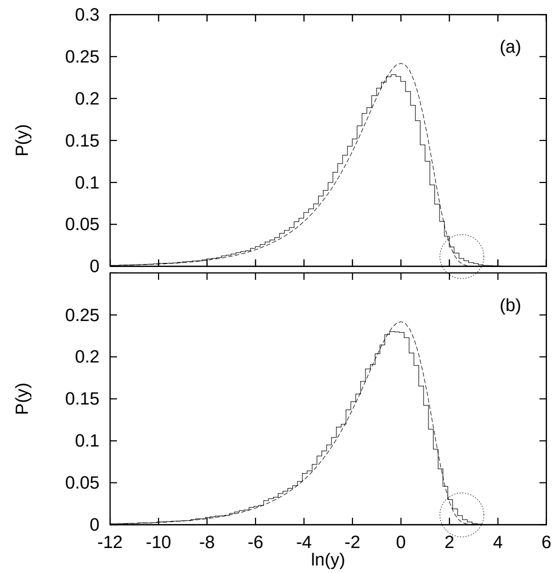

FIG. 2. Distribution $P(y)$ of the generalized intensities y of the operator (a) $\hat{A} = Z$; (b) $\hat{A} = 1/\hat{P}^2$. The range of analyzed transitions is given by $6 \leq \Delta z \leq 12$. The circles mark deviations from the Porter-Thomas distribution at large intensities (note the logarithmic scale for y). The fluctuations are not fully covered by the Porter-Thomas distribution.

In figure 2 we present our results for the distribution $P(y)$ of the squared matrix elements (generalized intensities). The histograms show an overall agreement with the prediction of random matrix theory, but significant deviations from the Porter-Thomas distribution (dashed curve) can be detected, in particular, in the region of large intensities, y ($\log y > 2$), marked by circles.

3. Effect of scars

The main result of this paper is that these deviations can be traced back to the scarring [13] of the wave functions involved in these matrix elements. As mentioned above, at the scaled energy considered, $\varepsilon = -0.1$, all orbits are unstable, also the parallel orbit, but the latter turns stable at the slightly higher energy $\varepsilon = -0.099873$, and therefore its Liapunov exponent at $\varepsilon = -0.1$ is relatively small. Moreover, no other orbit is found to turn stable in the vicinity of $\varepsilon = -0.1$. orbit becomes stable at slightly higher energy $\varepsilon = -0.099873$. Thus the parallel orbit is the only candidate for a localization (scarring) of wave functions along the classical path. To put this observation on a quantitative basis we calculated the "scar strengths"

$$I_n^r = \int_r \Psi_n^2(\nu,\mu)\,(\nu^2+\mu^2)\,\nu\,\mu\,ds \qquad (7)$$

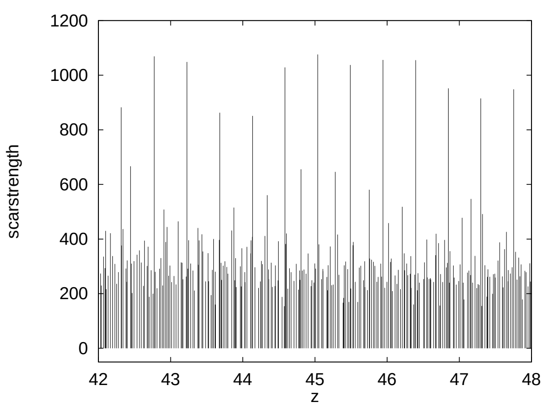

FIG. 3. Scar strengths of wave functions along the orbit parallel to the magnetic field axis as a function of the eigenvalue z.

(Wintgen and Hönig [12]) of wave functions along different periodic orbits r of the hydrogen atom in a magnetic field in semiparabolic coordinates μ, ν. This quantity provides a measure as to whether or not some periodic orbit significantly scars a given wave function. We have analyzed the scar strength of wave functions with respect to the periodic orbit parallel to the field and have found a sequence of strongly scarred states with spacings $\Delta z = 1/\tilde{S}^r = 0.447$ given by the scaled action $\tilde{S}^r = 2.236$ of the parallel orbit. The scar strengths of wave functions with eigenvalues $42 < z < 48$ are presented in figure 3. Scarring features of similar strength have not been observed for any other periodic orbit at scaled energy $\varepsilon = -0.1$.

We are now in a position to demonstrate that matrix elements involving states scarred by the parallel orbit are responsible for the deviations observed in the distribution of y from random matrix predictions. By excluding all matrix elements between transitions where at least one of the states is scarred (with scar strength $I_n^r >\sim 500$) we obtain generalized intensities with the contribution of scars filtered out.

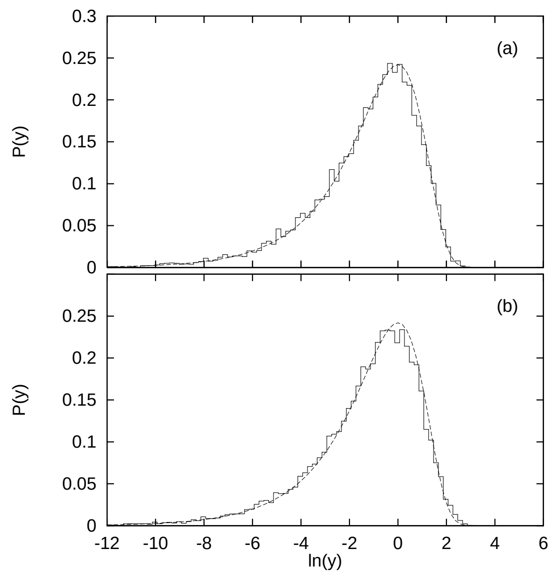

FIG. 4. Same as Fig. 2 but with the contribution of scarred states to the matrix elements removed. Now the histograms are covered by the Porter-Thomas distribution (dashed curves) also at large values of y.

Figure 4 shows our results for the distribution of the generalized intensities in that case. The discrepancies at large values of y have disappeared, which is strong evidence that the scarring of the wave functions by the parallel orbit was responsible for the deviations of the fluctuations of the generalized intensities from the Porter-Thomas distribution. Note that the distributions for both operators $\hat{A} = Z$ and $\hat{A} = 1/\hat{P}^2$ are affected by scarred wave functions in a similar way (figure 2) even though the variances of matrix elements $C_A^{\mathrm{qm}}(z, \Delta z)$ strongly depend on the choice of the transition operator (cf. figure 1).

In conclusion, we have presented clear evidence for the effects of scars on the statistical properties of quantum systems with chaotic classical counterparts. Our findings confirm earlier conjectures by Heller [13] as to the necessity of appropriately taking into account the effect of the scarring of eigenfunctions in the statistical analysis of matrix elements and transition probabilities.

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