Numerical demonstration of the semiclassical matrix element probability distribution between integrability and chaos

1994 J. Phys. A: Math. Gen. 27 L569

(http://iopscience.iop.org/0305-4470/27/16/002)

J. Phys. A: Math. Gen. 27 (1994) L569–L577. Printed in the UK

LETTER TO THE EDITOR

Numerical demonstration of the semiclassical matrix element probability distribution between integrability and chaos

Tomaž Prosen

Center for Applied Mathematics and Theoretical Physics, University of Maribor, Krekova 2, SLO-62000 Maribor, Slovenia

Received 3 May 1994

Abstract. In this letter I report on the first successful verification of the semiclassical matrix element probability distribution for the Hamiltonian systems between integrability and chaos. As for all the other statistical properties of quantum dynamical systems (e.g. level spacing distribution, phase space localization of eigenstates, etc) the semiclassical limit was found to converge extremely slowly. So a rather abstract dynamical system was used, namely the standard map on a torus, in order to clearly demonstrate the semiclassical regime.

The rapidly developing field of quantum chaos has so far answered many questions concerning statistical properties of quantum systems whose classical counterparts are chaotic (see, for example, Giannoni *et al* 1991, Gutzwiller 1990 or Eckhardt 1988). But less is known about the statistical properties of matrix elements of typical operators in the eigenbasis of a chaotic Hamiltonian (see, for example, Feingold and Peres 1986, Feingold *et al* 1989, Austin and Wilkinson 1993, Prosen and Robnik 1993b, and Prosen 1994—hereafter P94) and even less if the underlying Hamiltonian is between integrability and chaos (Alhassid and Feingold 1989, Prosen and Robnik 1993b, P94). There are two sets of universality classes of quantum fluctuations (of any physical quantity) which correspond to two extreme characters of classical motion, namely, integrable—regular, and ergodic—fully chaotic. For the latter—classically ergodic—case it was found that the quantum fluctuations can be modelled by the statistical ensembles of random matrices GOE/GUE/GSE (of random matrix theory RMT (see, for example, Mehta 1991))—conjecture of Bohigas *et al* 1984. The most frequently used Gaussian orthogonal ensemble (GOE) refers to the case where there is a time reversal symmetry (e.g. no magnetic field) or some other anti-unitary symmetry (Robnik and Berry 1986, Robnik 1986), and no spins are involved.

In a recent paper P94 I have verified the validity of RMT for describing the statistical properties of matrix elements of typical observables in an eigenbasis of chaotic Hamiltonian by means of (i) matrix element probability distribution (MEPD) $\mathcal{D}^{\omega}_{E}(A)$, where $\mathcal{D}^{\omega}_{E}(A)\,\mathrm{d}A$ is a probability that a randomly chosen matrix element $A_{kl} = \langle E_k|\hat{A}|E_l\rangle$, with energies E_k, E_l close to E and the transition frequency $\omega_{kl} = (E_k - E_l)/\hbar$ close to w† lies in the interval $[A - \mathrm{d}A/2, A + \mathrm{d}A/2]$, and (ii) more general multi-operator cross matrix

† For time-dependent, periodically driven systems the transition frequency is just the difference of the eigenphases of the Floquet propagator, $\omega_{kl} = \phi_k - \phi_l$, and the other argument E (energy) makes no sense and is omitted.

0305-4470/94/160569+09$19.50

element probability distribution (CMEPD) $\mathcal{D}_E^{\omega}(A, B, \ldots)$, where $\mathcal{D}_E^{\omega}(A, B \ldots)\mathrm{d}A\,\mathrm{d}B \ldots$ is a probability that randomly chosen n-tuple of matrix elements $A_{kl}, B_{kl} \ldots$ lie in the intervals $[A - \mathrm{d}A/2, A + \mathrm{d}A/2], [B - \mathrm{d}B/2, B + \mathrm{d}B/2] \ldots$. The notation in this letter follows exactly that of P94. In the classically ergodic case (with time reversal symmetry) typical operators are supposed to be represented by GOE matrices whose elements are Gaussian random variables with zero mean, so

$$\mathcal{D}^{a}_{\mathrm{GOE}}(A) = \frac{1}{\sqrt{2\pi}a} \exp\left(-\frac{A^2}{2a^2}\right) \tag{1}$$

$$\mathcal{D}^{M}_{\mathrm{GOE}}(A_1, \ldots, A_n) = \frac{1}{\sqrt{(2\pi)^n \det M}} \exp\left(-\tfrac{1}{2}\sum_{i,j=1}^{n} (\mathbf{M}^{-1})_{ij} A_i A_j\right). \tag{2}$$

where $\mathbf{M}$ is the so-called covariance matrix $M_{ij} = \langle A_i A_j \rangle = \int \mathrm{d}A_1 \ldots \mathrm{d}A_n\, A_i A_j \mathcal{D}^{M}_{\mathrm{GOE}}(A_1 \ldots A_n)$, since typical observables $\widehat{A}_i, i = 1 \ldots n$ need not be uncorrelated. For the other extreme of classically integrable systems we have

$$\mathcal{D}_{\mathrm{regular}}(A) = \delta(A) \qquad \mathcal{D}_{\mathrm{regular}}(A_1 \ldots A_n) = \delta(A_1) \cdots \delta(A_n) \tag{3}$$

in the semiclassical limit $\hbar \to 0$, as a consequence of selection rules which set most of the matrix elements to zero (Prosen and Robnik 1993c). Note that the convergence to the semiclassical limit (3) is not uniform but only point-wise, since non-semiclassical MEPD $\mathcal{D}_{\mathrm{regular}}(A)$ has typically slowly decaying tails, so higher moments $\langle A^{2m} \rangle$, $m \geqslant 2$ may remain different from zero or even become infinite in the semiclassical limit.

For the generic systems between integrability and chaos we use the *principle of uniform semiclassical condensation of eigenstates onto the classical invariant ergodic components in phase space which can be either integrable (invariant tori) or chaotic* (Robnik 1994). Then we also use the fact that the matrix element of any smooth observable between two states whose phase space (Wigner/Husimi) distribution functions have disjoint supports vanishes in the semiclassical limit (see appendix D of P94). Let us assume for simplicity that we have only one chaotic component† with relative phase space volume ρ_2 and all integrable components merged into a regular region with relative volume $\rho_1 = 1 - \rho_2$. The only non-zero matrix elements in the semiclassical limit are between two chaotic states (having the same support) with relative measure ρ_2^2, so using RMT

$$\mathcal{D}^{\omega}_{\mathrm{mixed}}(A) = (1 - \rho_2^2)\delta(A) + \rho_2^2 \mathcal{D}^{a(\omega)}_{\mathrm{GOE}}(A) \tag{4}$$

$$\mathcal{D}^{\omega}_{\mathrm{mixed}}(A_1 \ldots A_n) = (1 - \rho_2^2)\delta(A_1) \ldots \delta(A_n) + \rho_2^2 \mathcal{D}^{M(\omega)}_{\mathrm{GOE}}(A_1 \ldots A_n). \tag{5}$$

The variance $a^2(\omega)$ and the covariance matrix $M(\omega)$ can also be determined solely by the classical dynamics, i.e. as classical averages $\langle\rangle_C$ over the chaotic component C of the smoothed classical power spectra (see P94)

$$a^2(\omega) = \frac{\tau}{\sqrt{\pi}\hbar d \rho_2} \left\langle \left| \int_{-\infty}^{\infty} \mathrm{d}t\, a(t) \mathrm{e}^{\mathrm{i}\omega t - t^2/2\tau^2} \right|^2 \right\rangle_C \tag{6}$$

$$M_{kl}(\omega) = \frac{\tau}{\sqrt{\pi}\hbar d \rho_2} \left\langle \int_{-\infty}^{\infty} \mathrm{d}t\, a_k(t) \mathrm{e}^{\mathrm{i}\omega t - t^2/2\tau^2} \int_{-\infty}^{\infty} \mathrm{d}t\, a_l(t) \mathrm{e}^{-\mathrm{i}\omega t - t^2/2\tau^2} \right\rangle_C . \tag{7}$$

† This is usually a very good approximation since the next largest chaotic component is typically orders of magnitude smaller provided we are deep in the transition region far away from the pseudo-integrable (KAM) regime.

Signals $a_j(t)$ are the time evolutions of classical counterparts of $\widehat{A}_j$, d is the density of states, and the smoothing time τ should be as large as possible but not larger than the so-called *break time* $t_{\mathrm{break}} = 2\pi\hbar d$.

Let us now define our dynamical system. Its phase space is a compact two-dimensional torus $T_2 = \{(x, y); x, y \in [-\pi, \pi)\}$, where the periodic coordinates x and y will be referred to as position and momentum, respectively. The dynamics is given by consecutive applications of 'free motions' $U_{\mathrm{free}}(x, y) = (x + y, y)$ and 'kicks' $U_{\mathrm{kick}}(x, y) = (x, y - a\sin(x))$. The most useful is the symmetric representation of the evolution mapping U,

$$U = U_{\mathrm{kick}}^{1/2} \circ U_{\mathrm{free}} \circ U_{\mathrm{kick}}^{1/2} \tag{8}$$

which clearly exhibits the two symmetries of the compact version of the (Chirikov) standard map (8); namely the time reversal symmetry $T(x, y) = (x, -y)$, $T \circ U \circ T = U^{-1}$ and parity $P(x, y) = (-x, -y)$, $P \circ U \circ P = U$.

Since the classical phase space is compact, the quantum Hilbert space is finite-dimensional and its dimension n determines the dimensionless value of the effective Planck's constant $\hbar_{\mathrm{eff}} = 2\pi/n$. Let n be an even number $n = 2m$. The position and momentum eigenstates denoted by $|x_k\rangle$ and $|y_l\rangle$ can be defined through the relation $\langle x_k|y_l\rangle = n^{-1/2}\exp((\mathrm{i}n/2\pi)x_k y_l)$, where our choice $x_k = (2\pi/n)(k - \frac{1}{2})$, $y_l = (2\pi/n)(l - 1)$, $k, l = 1 \ldots n$, warrants the single-valuedness on the torus T_2. The quantization procedure is now almost obvious: the quantum unitary evolution propagator $\widehat{U}$ is decomposed to products of free motions $\widehat{U}_{\mathrm{free}}$ and kicks $\widehat{U}_{\mathrm{kick}}$ in precisely the same way as the classical one (8) where quantum analogues for the kick and the free motion are diagonal in position and momentum representation, respectively:

$$\begin{aligned}
\widehat{U}_{\mathrm{kick}} &= \sum_k \exp\left(\frac{\mathrm{i}n}{2\pi} a\cos(x_k)\right)|x_k\rangle\langle x_k| \\
\widehat{U}_{\mathrm{free}} &= \sum_l \exp\left(-\frac{\mathrm{i}n}{2\pi}\frac{y_l^2}{2}\right)|y_l\rangle\langle y_l|\,.
\end{aligned} \tag{9}$$

The phases of the diagonal elements in (9) are the classical generating functions, which generate the classical mapping (8), divided by $2\pi/n$. Therefore as $n \to \infty$ the quantum evolution approaches the classical dynamics. There exists a simple closed form expression for the propagator in position representation

$$\langle x_k|\widehat{U}|x_{k'}\rangle = \frac{1}{\sqrt{n}}\exp\left[\frac{\mathrm{i}n}{2\pi}\left(\tfrac{1}{2}(x_k - x_{k'})^2 + \tfrac{1}{2}a\cos(x_k) + \tfrac{1}{2}a\cos(x_{k'})\right)\right] \tag{10}$$

which is the discrete time analogue of the well known infinitesimal propagator $\exp[(\mathrm{i}/\hbar)((x - x')^2/2m\,\mathrm{d}t - (V(x) + V(x'))\mathrm{d}t/2)]$ for the general continuous Hamiltonian case. Using the symmetry under parity P one can further reduce n-dimensional unitary matrix $U_{kl} = \langle x_k|\widehat{U}|x_{k'}\rangle$ to two $(m = n/2)$-dimensional unitary matrices $U_{kl}^{\sigma} = \langle x_k\sigma|\widehat{U}|x_{k'}\sigma\rangle$ where $|x_k\sigma\rangle$ are parity preserving position eigenstates $|x_k\sigma\rangle = 2^{-1/2}(|x_k\rangle + \sigma|-x_k\rangle)$, $k = 1 \ldots m$ and $\sigma = \pm 1$ is a parity eigenvalue. Quantization can also be worked out for odd values of n but it is physically less transparent so I have used only even values of n in my numerical example.

I have diagonalized symmetric (due to time reversal) and unitary matrices U_{kl}^{σ} as far in the semiclassical limit $m \to \infty$ as possible giving the eigenphases ϕ_j^{σ} and the orthogonal set of eigenvectors $|\phi_k^{\sigma}\rangle$ having real components in position representation $\langle x_j\sigma|\phi_k^{\sigma}\rangle = \langle\phi_k^{\sigma}|x_j\sigma\rangle$. I have chosen the two simplest operators which are diagonal in position representation and are periodic functions of x, namely $\widehat{A} = \cos(\widehat{x})$ and $\widehat{B} = \cos(2\widehat{x})$. The matrix elements were calculated by means of the simple formulae

$$A^{\sigma}_{kl} = \sum_{j=1}^{m} \langle \phi^{\sigma}_{k} | x_j \sigma \rangle \cos(x_j) \langle x_j \sigma | \phi^{\sigma}_{l} \rangle \tag{11}$$

$$B^{\sigma}_{kl} = \sum_{j=1}^{m} \langle \phi^{\sigma}_{k} | x_j \sigma \rangle \cos(2x_j) \langle x_j \sigma | \phi^{\sigma}_{l} \rangle . \tag{12}$$

I have investigated the statistics of matrix elements for the quantum standard map (10) and operators $\widehat{A}$ and $\widehat{B}$ as high in the semiclassical limit $m \to \infty$ as possible. The compactified standard map is integrable for $a = 0$ and almost completely chaotic for $a \geqslant 7$. Since we are interested in the mixed regime, I will present the results for $a = 1.8$ where approximately three quarters of phase space is covered by a single connected chaotic component, $\rho_1 = 0.265$ $(1 \pm 0.8\%)$. As in the analogous semiclassical study of the level spacing statistics (Prosen and Robnik 1994a, b) I have found that in the non-semiclassical regime there exists a quasi-universal family of phenomenological MEPDs $\mathcal{D}_\alpha(A)$ where a delta-like spike is being formed at small A but has a long and accurate *exponential tail* at moderate and large A

$$\mathcal{D}_\alpha(A) \propto \exp(-\alpha|A|) \qquad \text{if} \quad \alpha|A| \geqslant 1 . \tag{13}$$

Best fitting exponential distribution (13) agrees excellently with numerics for sufficiently small m (see figure 1). This was also found (P94) in a completely different system, namely the Robnik's billiard, so it has analogous status as the family of Brody distributions for modelling the level spacing statistics (Prosen and Robnik 1993a, 1994a, b)†.

By increasing m one observes slow and continuous transition from linear–logarithmic behaviour $\log \mathcal{D}^{\omega}(A) = \mathcal{O}(A)$ to quadratic–logarithmic behaviour $\log \mathcal{D}^{\omega}(A) = \mathcal{O}(A^2)$, the latter being typical of the Gaussian part in (4) and (5), and only at $m \approx 8000$ the fit to the true semiclassical formulae (4) and (5) becomes significant (see figure 2). The average (with respect to ω) best fitting value of the parameter $\rho_1 = 0.272$ is by 2.6% larger than the classical value and is exactly the same as obtained from the analogous study of the level spacing distribution (Prosen and Robnik 1994a). In figure 3 I demonstrate the predicting power of the generalized Feingold–Peres formula (Prosen and Robnik 1993b, P94; see also Feingold and Peres 1986, Alhassid and Feingold 1989) for the classical estimate of the average square of magnitude of matrix elements (and of the correlation coefficients between matrix elements of different observables (P94)) as a function of the transition frequency (equations (6) and (7) with $\rho_2 = 1$ and $C =$ the whole phase space, or energy surface for autonomous systems). I have applied the semiclassical formulae (4) and (5) and determined the best-fitting parameters $\rho_1 = 1 - \rho_2, a, M$ as functions of the frequency ω and compared them with the corresponding classical values: $\rho_1(\omega)$ with the classical fractional volume of the regular component and $a(\omega), M(\omega)$ with the formulae (6) and (7). In both cases excellent agreement was found. I have also compared the relative moments $\mu_m(\omega) = \langle A^{2m}_{kl} \rangle^{\omega} / ((2m-1)!!(\langle A^2_{kl} \rangle^{\omega})^m)$ with their semiclassical values $\mu^{\mathrm{scl}}_m(A) = 1/\rho_2^{2(m-1)}$ (derived using (4)), provided that regular–regular MEPD $\mathcal{D}_{\mathrm{regular}}(A)$ decays sufficiently fast as $A \to \infty$. This need not be the case, especially in the regions

† Qualitatively similar distributions (sharp peak at small amplitudes and exponential tail at large amplitudes) were also obtained in the context of nuclear shell-model theory in (Whitehead *et al* 1978) and possibly in Verbaarschot and Brussaard (1979) although the reasons for the deviation from Porter-Thomas Gaussian are different in these two cases (selection rules and dependence upon mean energy of the basis–states) than in our case (mixed classical dynamics) so these distributions are not quantitatively applicable to our case.

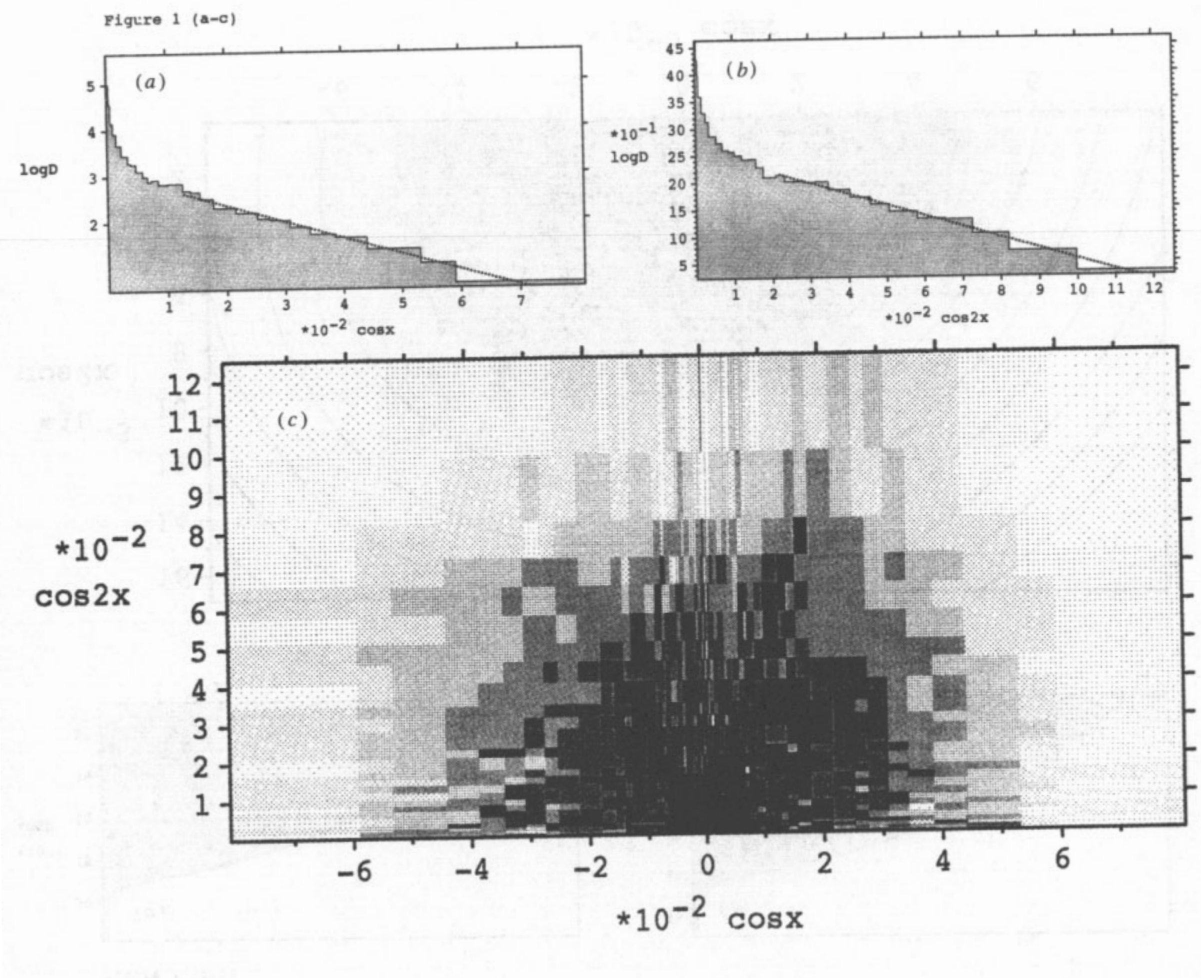

Figure 1. Demonstration of the linear behaviour of the logarithm of MEPD $\log \mathcal{D}^{\omega}$ for the kick parameter $a = 1.8$ and for operators (*a*) $\widehat{A} = \cos\widehat{x}$ and (*b*) $\widehat{B} = \cos 2\widehat{x}$ in the near-semiclassical regime; matrix elements for $m = 10\ldots100$ and transition frequencies in the interval $\omega \in [2\pi/10, 3\pi/10]$ were merged together in order to improve statistics. The dotted curves are the best-fitting exponentials (13). The CMEPD $\mathcal{D}^{\omega}(A, B)$ is also shown in (*c*) where neighbouring levels of greyness are by a constant factor of 1.7 apart.

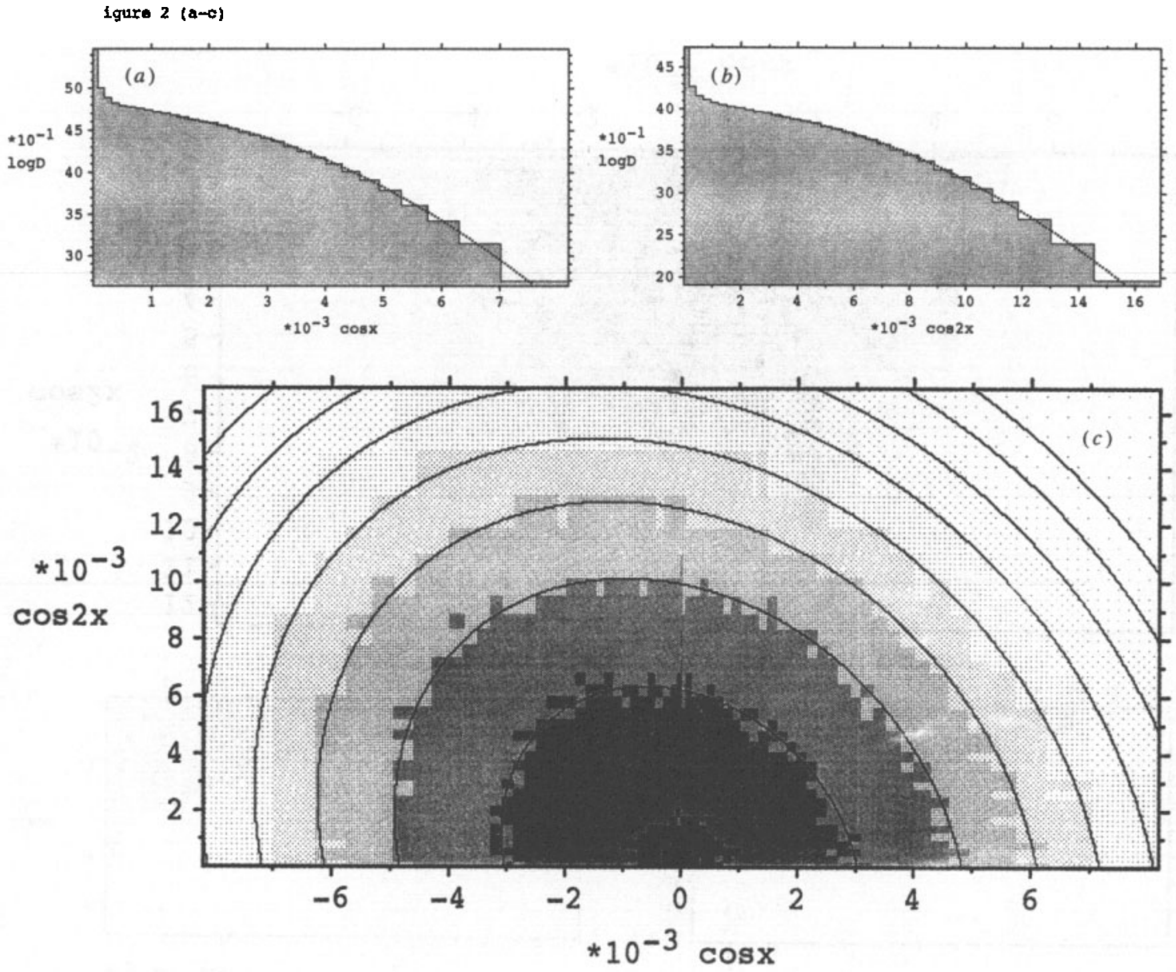

Figure 2. Similar presentation of logarithm of MEPD $\log \mathcal{D}^{\omega}$ for operators (*a*) $\cos\widehat{x}$ and (*b*) $\cos 2\widehat{x}$ at $a = 1.8$ as in figure 1, except that the semiclassical regime is much deeper now; $\approx 1.5 \times 10^6$ matrix elements for $m = 7991 \ldots 7995$ and transition frequencies in the interval $\omega \in [67\pi/200, 68\pi/200]$ were merged together. The dotted curves are the best fitting parabolas $\log \mathcal{D}^{\omega}(A) = \mathrm{const} - \frac{1}{2}A^2/a^2(\omega)$ to the semiclassical formula (4) and agree excellently with the data. The CMEPD $\mathcal{D}^{\omega}(A, B)$ shown in (c) with neighbouring levels of greyness by a factor of 1.7 apart is also compared with the best fitting semiclassical distribution (5) which is represented by contours which are lying at the same values as the boundaries between the levels of greyness (by factors of 1.7 apart). The match between these boundaries and contours confirms the semiclassical formulae for the cross statistics.

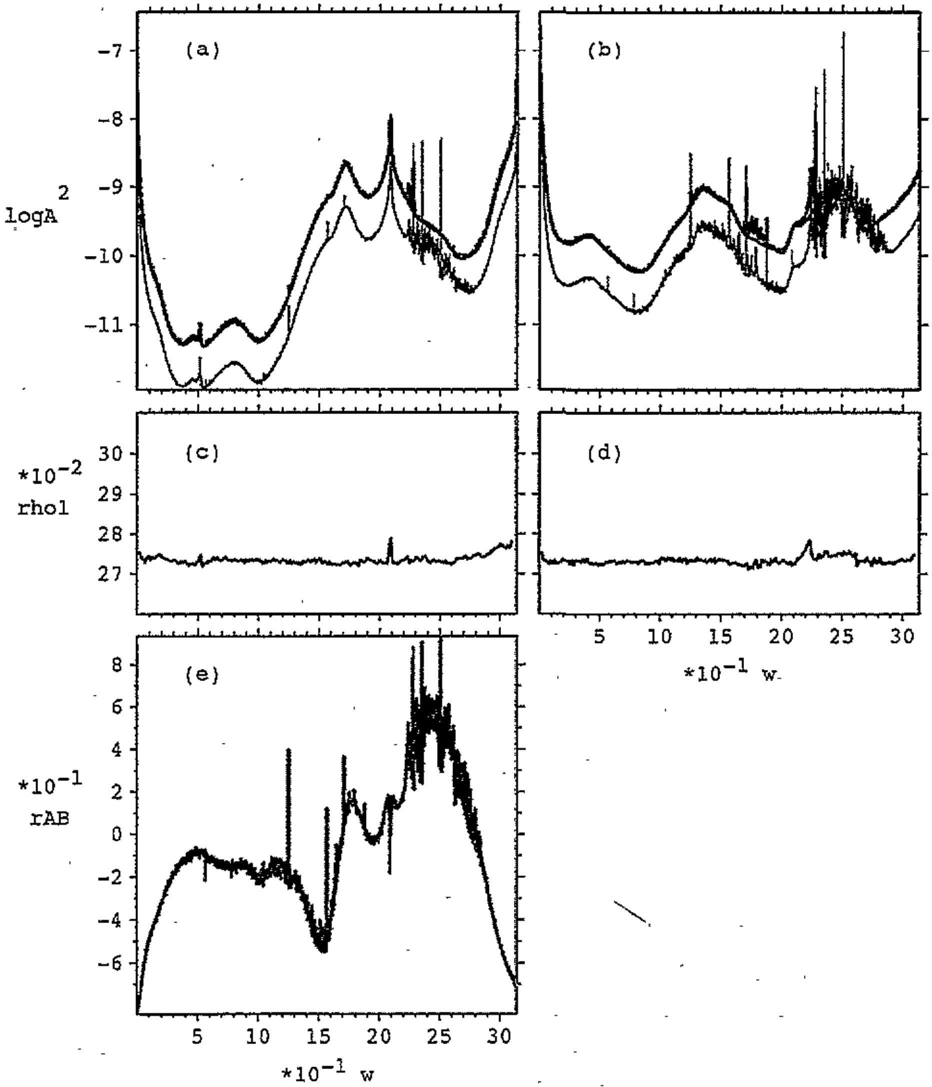

Figure 3. The logarithm of the average square of magnitude of matrix elements of operators (a), (c) $\cos\widehat{x}$ and (b), (d) $\cos 2\widehat{x}$ at the kick parameter $a = 1.8$ in the far semiclassical limit $m = 7991\ldots7995$. There are two sets of curves: the lower one refers to the quantal mean square ((a), (b) thin curves) compared with the classical prediction according to the formula (6) with $\rho_2 = 1$ and C being the entire phase space (shown in thin grey background curves). The upper set refers to the mean square of the chaotic–chaotic matrix elements ((a), (b) thick curves), which is obtained as parameter $a^2(\omega)$ by the best fit to the formula (4), compared to the classical prediction (6) with $\rho_2 = 0.73$ and C being the chaotic component in the phase space (shown in thick grey background curves). The other best fitting parameter $\rho_1(\omega)$ is given in (c), (d) as the function of transition frequency. The correlation coefficient $\langle A_{kl}B_{kl}\rangle / \sqrt{\langle A_{kl}^2\rangle\langle B_{kl}^2\rangle}$ is shown in (d). All quantum quantities in (a)–(e) agree with the corresponding classical expressions (given by (6,7) with smoothing time $\tau = 1000$, where $t_{\rm break} = m \approx 8000$) which are shown as background grey curves. Note that the spikes of the grey curves are just the classical resonances. The quantum $\rho_1(\omega)$ slightly fluctuates around the value 0.272 which deviates only by 2.6% from the classical value $\rho_1^{\rm cl} = 0.265$.

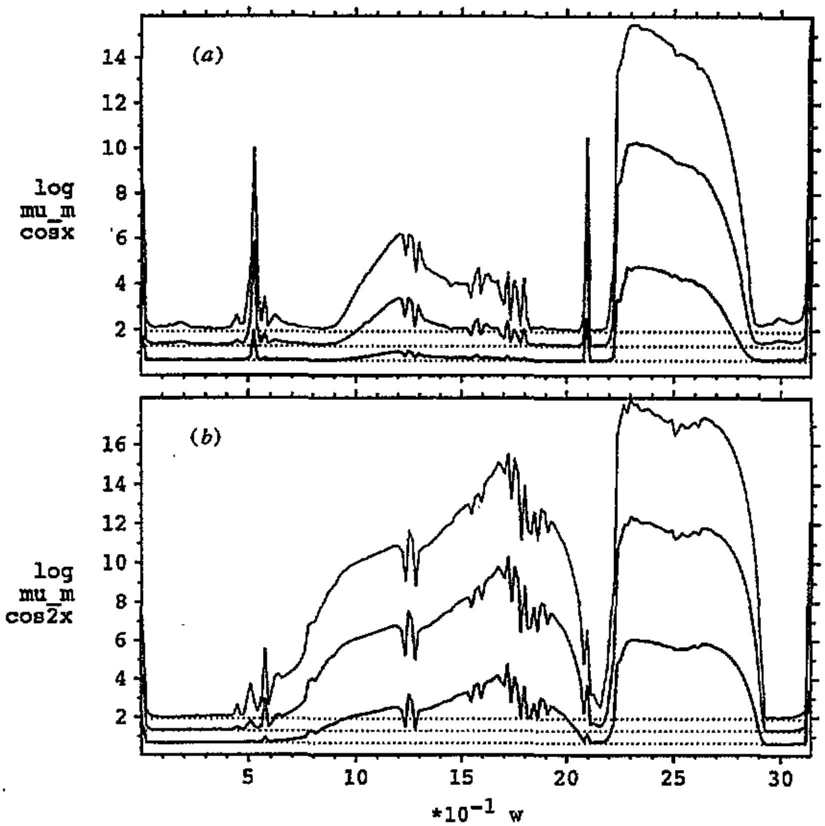

Figure 4. The logarithms of the relative moments $\mu_m(\omega) = \langle A_{kl}^{2m} \rangle^{\omega} / ((2m-1)!!(\langle A_{kl}^2 \rangle^{\omega})^m)$ ($m = 2, 3, 4$ for thick, medium and thin curve, respectively) of the operators (*a*) $\cos\hat{x}$ and (*b*) $\cos 2\hat{x}$ and at the kick parameter $a = 1.8$ in the far semiclassical limit $m = 7991 \ldots 7995$. The relative moments match with the corresponding semiclassical values, denoted by dotted lines, in the regions where there are no classical resonances (compare with figure 3).

where classical resonances are clustered (see figure 3) resulting in ordered series of strong quantum transitions. Indeed, in figure 4 we observe the agreement between the relative moments $\mu_m(\omega)$ and their semiclassical values in the ω-intervals where classical resonances are almost absent but in resonant regions $\mu_m(\omega)$ typically increase by orders of magnitude.

In this letter I have demonstrated the validity of the semiclassical formula for the (cross-)matrix element probability distribution (4), (5) in a one-dimensional compact quantum standard map, since sufficient depth into the semiclassical regime can, so far, only be reached in kicked one-dimensional systems. This also agrees with the results of analogous studies of the level spacing distribution (Prosen and Robnik 1994a, b), and the phase space localization of eigenstates (Prosen and Robnik 1994c), where it has been demonstrated *directly how the principle of uniform semiclassical condensation* (*Berry–Robnik approach*) of eigenstates onto the classical invariant ergodic components correlates with the validity of the various semiclassical formulae: for the energy level statistics (Berry and Robnik 1984), for the delta statistics (Seligman and Verbaarschot 1985) and for the (C)MEPD (P94).

I am grateful to Professor Marko Robnik for stimulating discussions, for enabling collaboration on related projects, and for reading the manuscript. The financial support by the Ministry of Science and Technology of the Republic of Slovenia is gratefully acknowledged.

References

Alhassid Y and Feingold M 1989 *Phys. Rev.* A **39** 374
Austin E and Wilkinson M 1992 *Europhys. Lett.* **20** 589
Berry M V and Robnik M 1984 *J. Phys. A: Math. Gen.* **17** 2413
Bohigas O, Giannoni M-J and Schmit C 1984 *Phys. Rev. Lett.* **52** 1
Eckhardt B 1988 *Phys. Rep.* **163** 205
Feingold M, Leitner D M and Piro O 1989 *Phys. Rev.* A **39** 6507
Feingold M and Peres A 1986 *Phys. Rev.* A **34** 591
Giannoni M-J, Voros A and Zinn-Justin J 1991 *Chaos and Quantum Physics* (Amsterdam: North-Holland)
Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (New York: Springer)
Mehta M L 1991 *Random Matrices* (San Diego, CA: Academic)
Prosen T 1994 *Ann. Phys., NY* at press
Prosen T and Robnik M 1993a *J. Phys. A: Math. Gen.* **26** 2371
——1993b *J. Phys. A: Math. Gen.* **26** L319
——1993c *J. Phys. A: Math. Gen.* **26** 1105
——1994a *J. Phys. A: Math. Gen.* **27** at press
——1994b *J. Phys. A: Math. Gen.* submitted
——1994c *J. Phys. A: Math. Gen.* submitted
Robnik M 1986 *Lecture Notes in Physics 263* (Berlin: Springer) p 120
——1994 Private communication
Robnik M and Berry M V 1986 *J. Phys. A: Math. Gen.* **19** 669
Seligman T H and Verbaarschot J J M 1985 *J. Phys. A: Math. Gen.* **18** 2227
Verbaarschot J J M and Brussaard P J 1979 *Phys. Lett.* **87B** 155
Whitehead R R, Watt A, Kelvin D and Conkie A 1978 *Phys. Lett.* **76B** 149