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LETTER TO THE EDITOR

Quantum surface-of-section method: demonstration of semiclassical Berry–Robnik energy level-spacing distribution in a generic two-dimensional Hamiltonian system

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Abstract. The recently developed *quantum surface-of-section method* is applied to a search for extremely high-lying energy levels in a simple but generic Hamiltonian system between *integrability and chaos, namely the semiseparable two-dimensional oscillator. Using the stretch* of 13 445 consecutive levels with the sequential number around 1.8×10^7 (eighteen million) we have clearly demonstrated the validity of the semiclassical Berry–Robnik level-spacing distribution while at 1000 times smaller sequential quantum numbers we find the very persistent quasi-universal phenomenon of power-law level repulsion which is globally very well described by the phenomenological Brody distribution. This is the first statistically significant numerical confirmation of the Berry–Robnik surmise in an *autonomous* two-dimensional Hamiltonian system.

The study of energy-level statistics of generic quantum Hamiltonian systems whose classical dynamics is between integrability and full chaos continues to be a challenging problem [18–20]. Until very recently there were incompatible results concerning the so-called *level-spacing distribution* $P(S)$ where $P(S)\,\mathrm{d}S$ is the probability that a randomly chosen spacing between two adjacent energy levels lies between $S-\mathrm{d}S/2$ and $S+\mathrm{d}S/2$. Berry and Robnik [3] derived the semiclassical level-spacing distribution $P^{\mathrm{BR}}(S)$ assuming the *principle of uniform semiclassical condensation* [2, 23, 15, 10, 20] of eigenstates onto classical invariant components (which can be either regular (tori) or irregular (chaotic)) and the statistical independence of the level subsequences belonging to various disjoint classical invariant components. (Regular levels associated with quantized invariant tori may be merged together giving the well known Poisson distribution $P_{\mathrm{Poisson}}(S) = \mathrm{e}^{-S}$.) Using the factorization of gap distributions $E(S) = \int_S^\infty \mathrm{d}\sigma\,(\sigma - S)P(\sigma)$ upon statistically independent superposition of spectra one may write

$$E^{\mathrm{BR}}_{\rho_1}(S) = E^{\mathrm{Poisson}}(\rho_1 S)E^{\mathrm{GOE}}(\rho_2 S) \tag{1}$$

for the simplest case of only one chaotic component with relative measure ρ_2 and regular components with total relative measure $\rho_1 = 1-\rho_2$. The Berry–Robnik distribution does not exhibit *level repulsion*, since $P^{\mathrm{BR}}_{\rho_1}(0) = 1-\rho_2^2 \neq 0$. On the other hand there has been a vast

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amount of phenomenological evidence [20] in favour of the so-called *fractional power-law level repulsion* which is very well described globally by the Brody [6] distribution

$$P_\beta^{\mathrm{B}}(S) = aS^\beta \exp\left(-bS^{\beta+1}\right) \qquad a = (\beta+1)b \qquad b = [\Gamma(1+(\beta+1)^{-1})]^{\beta+1} \tag{2}$$

which is characterized by the non-integer exponent β, $P(S \to 0) \propto S^\beta$. The Brody distribution is purely phenomenological and analytically the simplest globalization of the power-law level repulsion and it is not supported by any rigorous theoretical argument. Numerical spectra which contain even up to several tens of thousands of energy levels of quantum Hamiltonian systems with mixed classical dynamics typically still exhibit the phenomenon of fractional level repulsion, with statistically significant global fit by the Brody distribution [20]†. In such cases there was a remaining puzzle as to how the level-spacing distribution converges to the semiclassical Berry–Robnik distribution as one increases the sequential quantum number or decreases the value of effective $\hbar$. However, recently we have succeeded in demonstrating the ultimate semiclassical Berry–Robnik level-spacing distribution in a rather abstract one-dimensional time-dependent dynamical system, namely the standard map on a torus, and showed the smooth transition from Brody-like to Berry–Robnik distribution as $\hbar$ decreases [19, 20] (see also [12]). The transition was described excellently by the two-parameter (ρ_1, β) Berry–Robnik–Brody model in which we substitute the GOE model for the chaotic part $E^{\mathrm{GOE}}(\rho_2 S)$ in the Berry–Robnik formula (1) by the Brody model $E_\beta^{\mathrm{B}}(\rho_2 S)$ with some exponent β. The major goal of this letter is to demonstrate this scenario in a *generic two-dimensional autonomous Hamiltonian system.*

Another goal of this letter is to demonstrate the practical power of the recently developed *quantum surface-of-section method* [11, 13, 24] (which has been motivated by the semiclassical version developed in [4] and extensively numerically investigated in [8]) and whose most thorough and complete presentation so far is given in [14]. We shall use the reactance matrix formulation of the quantization condition which has practical advantages over the scattering matrix formulation in the case of semiseparable systems [14, section 2.7]. Here we give a brief and hence rather heuristic description of the method for the quantum Hamiltonians $\hat{H}$ in two-dimensional configuration space (CS) with coordinates (x, y) where the line $y = 0$ represents the *configurational surface of section* (CSOS) while we use Dirichlet boundary conditions on the boundary lines $y = b_\uparrow > 0$ and $y = -b_\downarrow < 0$. Let $\Psi_{\sigma n}(x, y, E)$ be the solutions of the Schrödinger equation $\hat{H}\Psi_{\sigma n}(x, y, E) = E\Psi_{\sigma n}(x, y, E)$ on the upper $(y > 0, \sigma = \uparrow = +)$/lower $(y < 0, \sigma = \downarrow = -)$ side of CS which satisfy the boundary conditions $\Psi_{\sigma n}(x, 0, E) = u_n(x)$, $\Psi_{\sigma n}(x, \sigma b_\sigma, E) = 0$, and $u_n(x)$ is some complete set of functions for the *small* Hilbert space of L^2 functions over one-dimensional CSOS, e.g. the eigenfunction of the *reduced* Hamiltonian $\check{H}' = \hat{H}|_{y=0}$, $\check{H}' u_n(x) = E_n' u_n(x)$.The full eigenfunction $\Psi(x, y, E)$ of $\hat{H}$ can be expanded in terms of partial eigenfunctions $\Psi_{\sigma n}(x, y, E)$ on both sides as $\Psi(x, y, E) = \sum_n c_{\sigma n} |k_n(E)|^{-1/2} \Psi_{\sigma n}(x, y, E)$, where $\sigma = \mathrm{sign}(y)$ while the square roots of the *wavenumbers* $k_n = \hbar^{-1}\sqrt{2m(E - E_n')}$ provide a useful normalization. In order for $\Psi(x, y, E)$ to be a non-trivial eigenfunction on the entire CS it should be continuously differentiable on CSOS (at $y = 0$). Using the completeness of the set $u_n(x)$ the requirement for continuity gives $c_{\uparrow n} = c_{\downarrow n}$, whereas requiring continuity of the normal derivative yields the singularity condition for the *real-symmetric reactance matrix*

† Theoretical arguments [3, 22] suggest that level repulsion should be linear $P(S \to) \propto S$ for very small spacings $S <$ exp(−constant/$\hbar$) but this linear regime has not been observed so far (not even in the present work) since such small spacings cannot/can hardly be calculated and their number in a typical numerical spectrum is so small that they cannot significantly affect level-spacing statistics.

$\tilde{\mathbf{R}} = \tilde{\mathbf{R}}_\uparrow + \tilde{\mathbf{R}}_\downarrow$,

$$\tilde{\mathbf{R}}_{\sigma nl}(E) = \sigma |k_n(E)k_l(E)|^{-1/2} \int \mathrm{d}x\, \Psi_{\sigma n}(x, 0, E)\partial_y \Psi_{\sigma l}(x, 0, E) \tag{3}$$

$$\det \tilde{\mathbf{R}}(E) = 0\,. \tag{4}$$

This equation is equivalent to the more physical but numerically less effective (due to complex non-symmetric arithmetic) quantization condition $\det(1 - \mathbf{T}_\downarrow(E)\mathbf{T}_\uparrow(E)) = 0$ [11, 13, 24, 14] in terms of generalized (*non-unitary*) scattering matrices $\mathbf{T}_\sigma(E)$ of the two scattering problems (obtained by cutting off one half of the CS along CSOS and attaching the waveguide (flat in the y-direction) instead) which have a finite number N_o of propagating (open), and infinitely many evanescent (closed) modes $\mathrm{e}^{\pm \mathrm{i}k_n(E)y}u_n(x)$, for $k_n^2(E) > 0$, and $k_n^2(E) < 0$, respectively. The scattering matrices are related to (*non-real*) reactance matrices by $\mathbf{T}_\sigma = (1 + \mathrm{i}\mathbf{R}_\sigma)(1 - \mathrm{i}\mathbf{R}_\sigma)^{-1}$, where the latter are made real by a simple diagonal transformation $\tilde{\mathbf{R}}_\sigma = \mathbf{D}\mathbf{R}_\sigma\mathbf{D}$, where $\mathbf{D} = \mathrm{diag}(1, 1 \ldots N_o\ times \ldots 1, \sqrt{\mathrm{i}}, \sqrt{\mathrm{i}} \ldots)$.

We have applied this method to a semiseparable system which is separable above/below CSOS but not separable on the whole CS, namely to a two-dimensional semiseparable oscillator (SSO) with the Hamiltonian

$$\hat{H} = -\tfrac{1}{2}\hbar^2(\partial_y^2 + \partial_x^2) + \tfrac{1}{2}(x - \tfrac{1}{2}\mathrm{sign}(y)a)^2 \qquad -b_\downarrow \leqslant y \leqslant b_\uparrow \tag{5}$$

with the parameters a, b_σ and $\hbar$. SSO has a scaling symmetry $(a, b_\sigma, \hbar, E) \to (\alpha a, \alpha b_\sigma, \alpha^2\hbar, \alpha^2 E)$. SSO is geometrically a rather special system but dynamically it is completely generic (like periodically kicked systems). The reduced Hamiltonian is just a simple one-dimensional harmonic oscillator $-\frac{1}{2}\hbar^2\partial_x^2 + \frac{1}{2}x^2$ with eigenfunctions $u_n(x) = (\sqrt{\pi\hbar}2^n n!)^{-1/2}\exp(-x^2/2\hbar)H_n(x/\sqrt{\hbar})$ and eigenenergies $E'_n = (n + \frac{1}{2})\hbar$ determining the wavenumbers $k_n(E) = \hbar^{-1}\sqrt{2E - (2n+1)\hbar}$, $n = 0, 1 \ldots$. It is easy to derive an explicit expression for the reactance matrices for SSO

$$\tilde{\mathbf{R}}_\uparrow(E) = \mathbf{J}(E)\mathbf{O}\mathbf{C}_\uparrow(E)\mathbf{O}^T\mathbf{J}(E) \qquad \tilde{\mathbf{R}}_\downarrow(E) = \mathbf{J}(E)\mathbf{O}^T\mathbf{C}_\downarrow(E)\mathbf{O}\mathbf{J}(E) \tag{6}$$

where $\mathbf{J}(E)$ and $\mathbf{C}_\sigma(E)$ are *real diagonal matrices*

$$\mathbf{J}_{nl}(E) = \delta_{nl}|k_n(E)|^{-1/2} \qquad \mathbf{C}_{\sigma nl}(E) = -\delta_{nl}k_n(E)\cot(k_n(E)b_\sigma) \tag{7}$$

and $\mathbf{O}$ is the *real orthogonal shift matrix*

$$\mathbf{O}_{nl} = \int \mathrm{d}x\, u_n(x)u_l(x + \tfrac{1}{2}a) \tag{8}$$

whose matrix elements can be calculated via the *numerically stable* symmetric recursion

$$\mathbf{O}_{n,0} = \frac{1}{\sqrt{n!}}\exp\left(-\frac{a^2}{16\hbar}\right) \qquad \mathbf{O}_{0,l} = \frac{(-1)^l}{\sqrt{l!}}\exp\left(-\frac{a^2}{16\hbar}\right)$$

$$\mathbf{O}_{n,l} = \frac{1}{2}\left(\sqrt{\frac{n}{l}} + \sqrt{\frac{l}{n}}\right)\mathbf{O}_{n-1,l-1} + \frac{a}{\sqrt{32\hbar n}}\mathbf{O}_{n-1,l} - \frac{a}{\sqrt{32\hbar l}}\mathbf{O}_{n,l-1}\,.$$

It is important how we truncate these infinitely-dimensional matrices for the numerical calculation. One has to consider all the $N_o = \mathrm{round}(E/\hbar)$ open modes plus as many N_c closed modes so that the numerical results (roots of (4)) converge. I have used semiclassical arguments (the SOS (x, p_x) phase space supports of coherent state representation of the states $u_n(x), n = 0, \ldots, N_o + N_c - 1$ should cover the supports of the states $u_l(x + \frac{1}{2}a), l = 0, \ldots, N_o - 1$) to estimate the minimal number of closed modes

$$N_c \approx \left(\frac{2a}{\sqrt{2E}} + \frac{a^2}{2E}\right)N_o\,. \tag{9}$$

The dimension of matrices $N = N_o + N_c$ is thus usually (for small a) only a little larger than the number of open modes N_o.

It is also very important to stress that the shift matrix and therefore also the reactance matrices are *effectively banded.* I have obtained a semiclassical formula for their bandwidths using an overlap condition for the coherent state representation of the SOS states $u_n(x)$ and $u_l(x + \frac{1}{2}a)$

$$\text{bandwidth}(\tilde{\mathbf{R}}_\sigma(E)) = 2\,\text{bandwidth}(\mathbf{O}) \approx \frac{a}{\hbar}\sqrt{2E}\,. \tag{10}$$

Note that the function $f(E) = \det \tilde{\mathbf{R}}(E)$ has singularities (poles) at the points E where for some n, $k_n(E)b_\sigma$ is a multiple of π. But between the two successive poles $f(E)$ is a smooth (even analytic) real function of real energy E. I have devised an algorithm for calculation of almost all levels—zeros of $f(E)$ within a given interval $[E_i, E_f]$ which only needs to evaluate $f(E)$ about 25 times per mean-level-spacing while it typically misses less than 0.5% of all levels. The control over missed levels is, in general, a very difficult problem. The number of all energy levels below a given energy E, $\mathcal{N}(E)$ can be estimated by means of the Thomas–Fermi rule

$$\mathcal{N}(E) \approx \mathcal{N}^{\text{TF}}(E) = \frac{b_\uparrow + b_\downarrow}{3\pi\hbar^2}(2E)^{3/2} = \mathcal{O}(N^2)\,. \tag{11}$$

But this formula is generally not very helpful even if the next semiclassical corrections are negligible since the fluctuation of the number of levels in an interval $[E_i, E_f]$ is proportional to $\sqrt{\mathcal{N}(E_f) - \mathcal{N}(E_i)}$ except in the extreme case of fully chaotic systems where the spectra are much stiffer and the fluctuation is proportional to $\log[\mathcal{N}(E_f) - \mathcal{N}(E_i)]$ so that Thomas–Fermi rule can be used to detect even a single missing level [5, 1].

We have chosen the following values of the parameters for our numerical demonstration: $a = 0.03, b_\uparrow = 5.0, b_\downarrow = 10.0$ and $E = 0.5$, while for quantal calculations we take the energy to be in a narrow interval around $E = 0.5$. For illustration we plot the classical SOS $(x, p_x, y = 0)$ in figure 1. There is only one dominating chaotic component with relative measure $\rho_2 = 0.709 \pm 0.001$ and the regular region still with some very small chaotic components with the complementary total relative measure $\rho_1 = 1 - \rho_2 = 0.291 \pm 0.001$. For the quantal calculations we have chosen two different values of $\hbar = 0.01$ and $\hbar = 0.0003$ which correspond to the sequential numbers $\mathcal{N} \approx 16\,000$ and $\mathcal{N} \approx 17\,684\,000$, respectively.

In the first case ($\hbar = 0.01, \mathcal{N} \approx 1.6 \times 10^4$) we have calculated 14 231 levels in the interval $0.35 < E < 0.65$. We have performed a χ^2 test and obtained a *statistically significant* fit of $P(S)$ by the Brody distribution with $\beta = 0.142 \pm 0.002$, $\chi^2_{\text{B}} = 5320$ and a *non-significant* Berry–Robnik fit with $\rho_1 = 0.548$, $\chi^2_{\text{BR}} = 130\,000$ (see figure 2). The phenomenological Brody distribution globally and locally captures the numerical data, e.g. for 973 small spacings in the range $0 < S < 0.1$ the local best fit by the Brody model is highly significant and gives the level repulsion exponent $\beta = 0.140 \pm 0.005$ in perfect agreement with the global value. In order to present the most detailed information we plot a cumulative level-spacing distribution $W(S) = \int_0^S \mathrm{d}\sigma\, P(\sigma)$ and the deviation of the numerical U-function [18] $U(W(S)) = (2/\pi)\arccos(\sqrt{1 - W(S)})$ from the best-fit Berry–Robnik U-function $U(W^{\text{BR}}(S))$ versus $W(S)$ which has the nice property that the estimated statistical error $\delta U = 1/\pi\sqrt{N}$ and the density of numerical points along the abscissa are constant. In spite of the already very high sequential number this is still an example of the so-called near-semiclassical regime characterized by the fractional power-law level repulsion.

In the second case ($\hbar = 0.0003, \mathcal{N} \approx 1.8 \times 10^7$) we have calculated 13 445 levels on the interval $0.499\,85 < E < 0.500\,105$ and found a *significant* fit by the

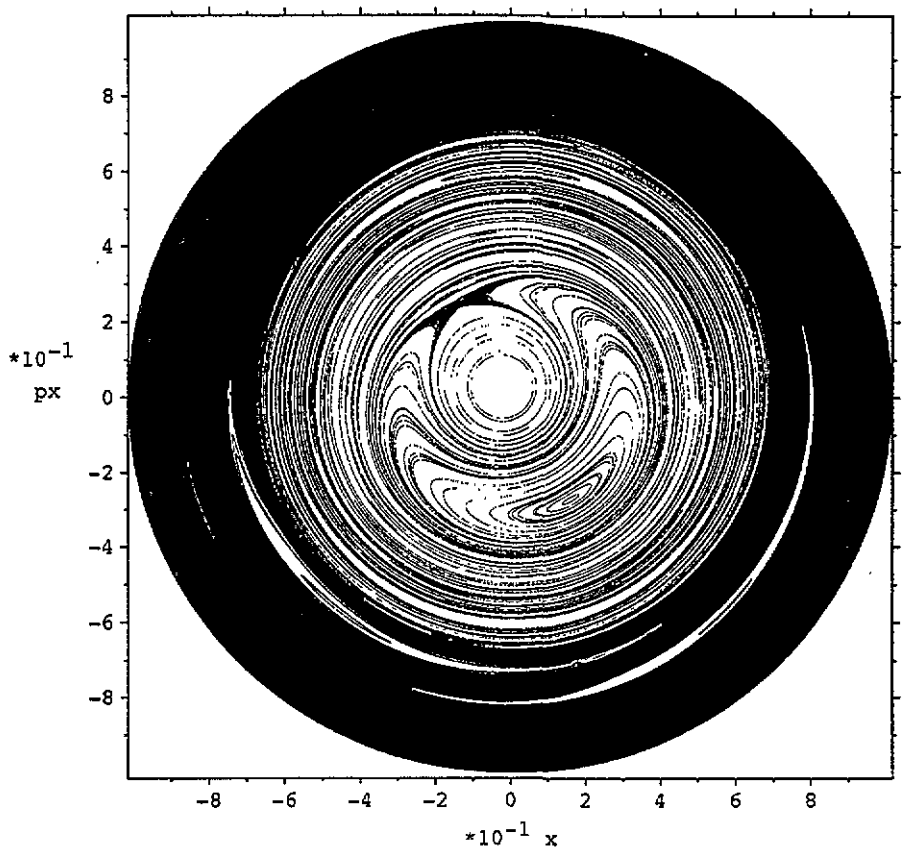

Figure 1. Classical surface of section $y = 0$ with coordinates x and p_x of the semiseparable oscillator: $a = 0.03, b_\uparrow = 5.0, b_\downarrow = 10.0$ and $E = 0.5$. 250 orbits with 40 000 crossings of SOS each are shown.

semiclassical Berry–Robnik formula (see figure 3) with the *correct* value of regular volume $\rho_1 = 0.286 \pm 0.005$, $\chi^2_{\mathrm{BR}} = 12\,150$ while the Brody fit becomes highly non-significant, $\beta = 0.367$, $\chi^2_{\mathrm{B}} = 249\,000$. Thus we have demonstrated the so-called far-semiclassical regime with the quantum value of ρ_1 which agrees excellently with the classical regular volume (the small deviation is within error bars). The fit to the combined Berry–Robnik–Brody model *does not* significantly improve $\chi^2 = 11\,950$ while it substitutes the GOE model for the chaotic part by the Brody model with $\beta \approx 0.85$.

Large square-root number fluctuations prevent the determination of the number of missed levels by using the Thomas–Fermi rule (although higher-order semiclassical corrections are negligible in this regime). One can compare the number of levels $\mathcal{N}(E)$ with the number of levels $\mathcal{N}_0(E)$ or $\mathcal{N}_\infty(E)$ for the two nearby integrable–separable cases (with the same b_σ but with $a = 0$ (single-box limit) or $a \to \infty$ (two-box limit), respectively) since the leading-order semiclassics (Thomas–Fermi rule) does not depend upon defect a. $\mathcal{N}_0(E)$ and $\mathcal{N}_\infty(E)$ can be easily calculated numerically and *large-scale* fluctuations of $\mathcal{N}(E) - \mathcal{N}_{0,\infty}(E)$ turn out to be much smaller than the fluctuations of $\mathcal{N}(E) - \mathcal{N}^{\mathrm{TF}}(E)$ suggesting that we have missed *less* than 20 levels out of 14 231 at $\hbar = 0.01$ (figure 2) and 40–80 levels out of 13 445 at $\hbar = 0.0003$ (figure 3). Note that in the first case ($\hbar = 0.01$) there were much fewer almost

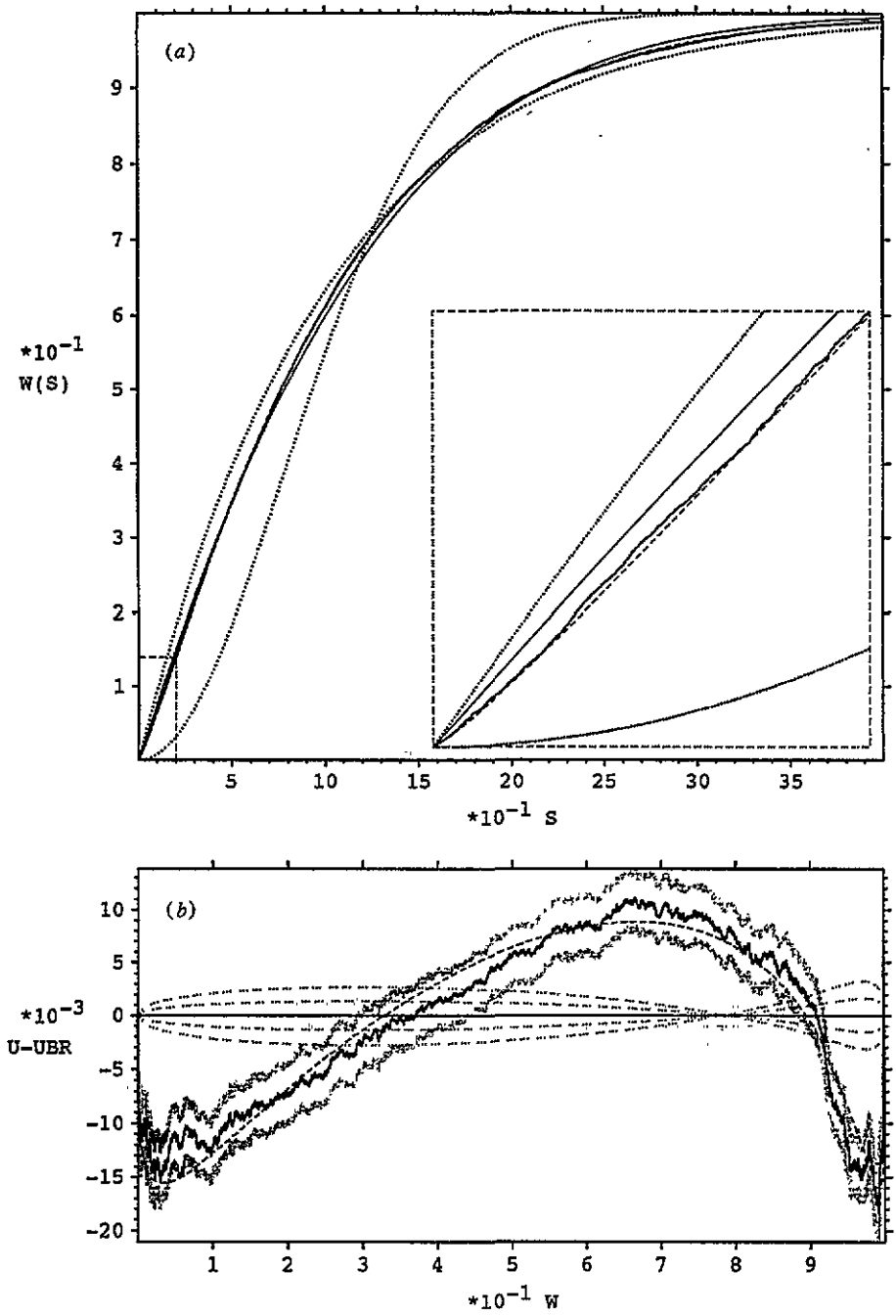

Figure 2. (a) Cumulative level-spacing distribution $W(S)$ and (b) deviation of its U-function from the best-fit Berry–Robnik distribution for 14 231 consecutive levels of SSO at $a = 0.03, b_\uparrow = 5.0, b_\downarrow = 10.0, 0.35 < E < 0.65$ and $\hbar = 0.01$. Thick full curves (a) and (b) (within $\pm$ one sigma error band (b)) represent numerical data, the thin full curve (a) is a best-fit Berry–Robnik distribution with $\rho_1 = 0.548$ whereas the broken curves (a),(b) are the best-fit Brody distribution with $\beta = 0.142$. The dotted curves (a) represent the limiting Poisson and GOE distributions whereas the broken dotted curves (b) represent the nearby Berry–Robnik curves with $\rho_1 = 0.548 \pm 0.01, \pm 0.02$.

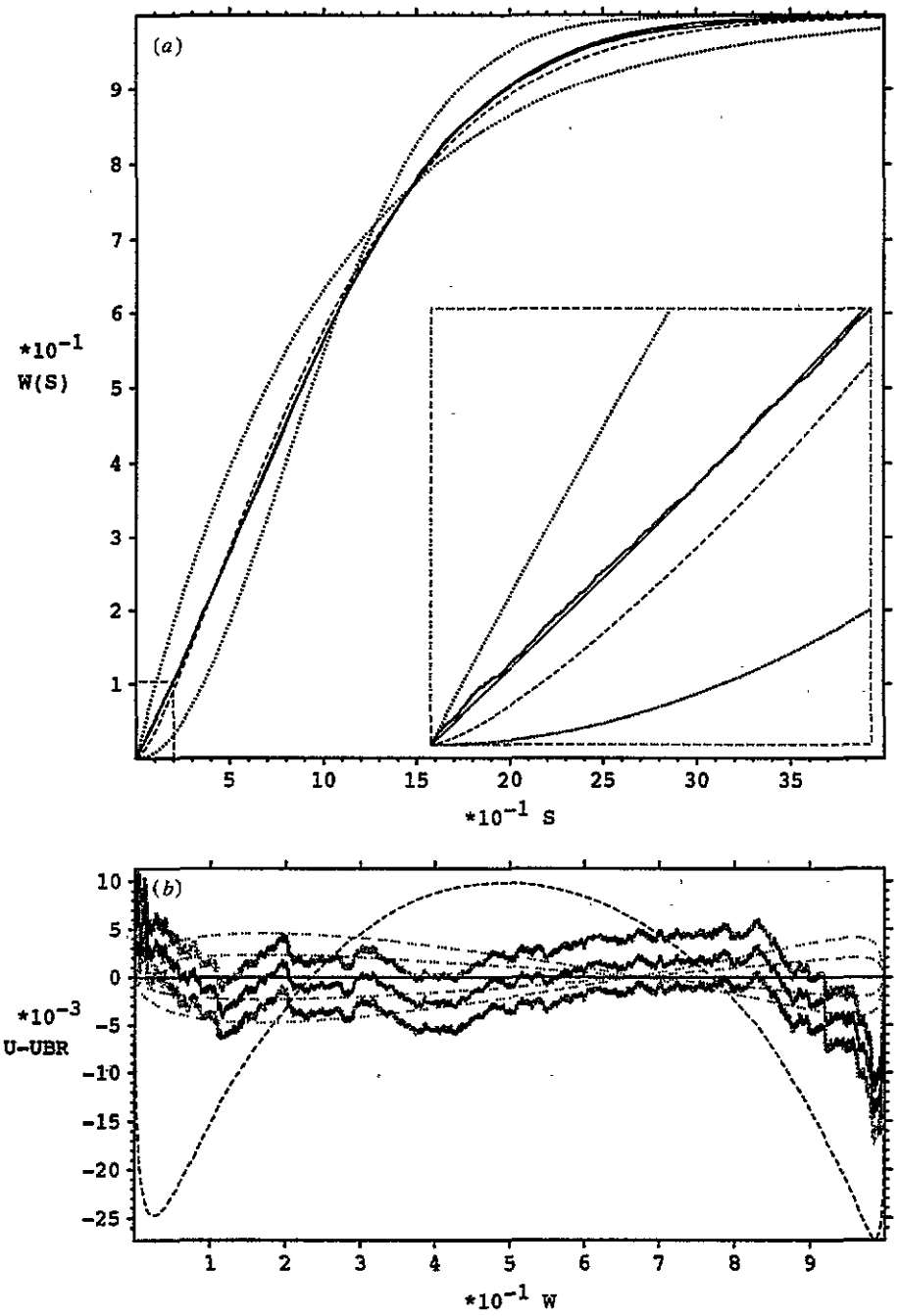

Figure 3. The same as in figure 2 but now at $\hbar = 0.0003$ for 13 445 levels in the interval $0.499\,85 < E < 0.500\,105$ in the true (far) semiclassical regime (see text). The Berry–Robnik distribution with $\rho_1 = 0.287$ is now statistically significant and for an illustration of the accuracy of the fitted ρ_1 we also provide Berry–Robnik curves for $\rho_1 = 0.287 \pm 0.01, \pm 0.02$ (broken dotted curves (*b*)).

degenerate pairs of levels (and therefore less missed levels) due to the level repulsion.

In conclusion I should emphasize that the present letter presents a clear demonstration of the semiclassical Berry–Robnik level-spacing distribution in a generic two-dimensional autonomous Hamiltonian system between integrability and chaos, i.e. a semiseparable oscillator. This would not be possible without application of the quantum surface-of-section method which enabled us to calculate 13 445 consecutive levels with sequential numbers $\mathcal{N} \approx 1.8 \times 10^7$ within a week of Convex 3680 CPU time. For this system, the quantum surface-of-section method requires $\mathcal{O}(a^2\mathcal{N}^{3/2})$ FPO/level. In forthcoming publications [16] I will discuss in detail the energy spectra, quantum eigenstates, and quantum SOS evolution by the quantum SOS method in the semiseparable oscillator, and [17] apply the quantum SOS method to a more realistic example, namely the diamagnetic Kepler problem [9, 7, 21].

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