PHYSICAL REVIEW E **68**, 065205(R) (2003)

Low-rank perturbations and the spectral statistics of pseudointegrable billiards

Thomas Gorin*
Theoretische Quantendynamik, Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, D-79104 Freiburg, Germany

Jan Wiersig
Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee, D-28359 Bremen, Germany

(Received 18 March 2003; published 24 December 2003)

We present an efficient method to solve Schrödinger's equation for perturbations of low rank. The method is ideally suited for systems with short range interactions or quantum billiards. It involves a secular equation of low dimension, which directly returns the level counting function. For illustration, we calculate the number variance for two pseudointegrable quantum billiards: the barrier billiard and a right triangle billiard. In this way, we obtain precise estimates for the level compressibility in the semiclassical (high energy) limit. In both cases, our results confirm recent theoretical predictions, based on periodic orbit summation, disregarding diffractive orbits.

DOI: 10.1103/PhysRevE.68.065205 PACS number(s): 05.45.Mt, 02.70.−c, 03.65.Ge

Consider a bound quantum system with Hamiltonian $H=H_0+W$, where the eigenbasis of H_0 is known, and the perturbation W is non-negative (nonpositive) and of low rank. Then, our method allows to obtain the level counting function, by solving an eigenvalue problem of the dimension which is equal to the rank of the perturbation. This possibility is an important further development of the first implementation in Ref. [1]. The class of systems which fulfill the above requirements is large. Quite evidently, few particle systems with short range residual interactions, e.g., Ref. [2], fall into this category. Quantum billiards can also be considered. To see this, choose for H_0 an integrable billiard $\mathcal{B}_0$, which encloses the billiard $\mathcal{B}$ of interest. Then, the boundary can be modeled by a potential with a one-dimensional δ-shaped profile, which is of low rank in the Hilbert space of H_0. As a result, the spectrum of H contains the desired eigenvalues of $\mathcal{B}$ and those of its complement $\mathcal{B}_0-\mathcal{B}$. They can be separated with the help of an appropriate observable, and in some cases, e.g., the Sinai billiard, and the examples considered below, the separation is given beforehand.

We illustrate our method with two examples, the barrier billiard [3], and the right triangle billiard [4] with acute angle $\pi/5$. Both examples are two-dimensional, pseudointegrable polygon billiards [4,5]. While pseudointegrable systems have enough constants of motion to assure local integrability, singularities in the Hamiltonian flow allow invariant surfaces with genus larger than one. This introduces some kind of randomness into the classical dynamics, though the Lyapunov exponent is equal to zero, everywhere. The nonstandard topology of the invariant surfaces leads to an algebraic dispersion of nearby trajectories [6].

In the spirit of quantum-classical correspondence, there have been numerous efforts to study the implications of pseudointegrability on the quantum spectrum [1,5,7–10]. In Refs. [8,11] it is conjectured that the statistical properties of pseudointegrable billiards are intermediate between Poisson statistics, typically related to integrable systems [12], and the statistics of the Gaussian orthogonal ensemble [13], related to fully chaotic (time reversal invariant) systems. The so-called "intermediate statistics" has also been observed in disordered, mesoscopic systems at the metal-insulator transition [14], for systems with interacting electrons [15], and for incommensurate double-walled carbon nanotubes [16].

A suitable measure for intermediate spectral statistics is the level compressibility $\chi=\lim_{L\to\infty}\Sigma^2(L)/L$, where $\Sigma^2(L)$ is the number variance [13] for energy intervals of length L (measured in units of the average level spacing). Note that χ coincides with the value of the spectral two-point form factor in the limit of small times. Recently, analytical results for χ became available for a certain class of right triangle billiards [17], as well as for the barrier billiard [10]. These results are based on the diagonal approximation and on the assumption that diffractive orbits do not contribute. In particular the latter assumption is questionable because diffraction is an important mechanism in the development of intermediate statistics. Unfortunately, numerical studies could not confirm those results with the desirable clarity, since the convergence to the semiclassical limit is very slow. For example in the case of the barrier billiard one obtains $\chi\approx 0.34$ in the region between level number 400 000 and 420 000, while the semiclassical prediction is $\chi=1/2$ [10].

As shown below, our method is almost ideally suited for the calculation of the number variance for large L. Therefore, we are able to calculate the level compressibility at much higher energies and with better statistics. In the case of the barrier billiard, for example, we calculate number variances in the region of absolute level number $\mathcal{N}>1.6\times 10^7$ within an energy interval which contains about 10^5 levels.

Here we only sketch the general method (a detailed presentation will be published elsewhere). Assume, that the Hamiltonian H can be approximated by a projection on an appropriately chosen N-dimensional Hilbert space, $N<\infty$. Assume further that its matrix representation is of the following form:

$$H=H_0+\eta\, V\, V^{\dagger}. \tag{1}$$

*Electronic address: Thomas.Gorin@physik.uni-freiburg.de

Here V is a $N\times M$ matrix with mutually orthogonal column vectors, $M<N$, and η is a positive parameter. Such a representation can be obtained, for instance, by diagonalizing a non-negative perturbation of small rank M. Then, in general, the spectrum of H consists of a trivial component S_0, contained in the spectrum of H_0, and a nontrivial, disjoint component S_1. The eigenvalues in S_1 are roots of the secular equation

$$\det[1-\eta K(E)]=0, \quad K(E)=V^\dagger \frac{1}{E-H_0}V, \tag{2}$$

where $\dim[K(E)]=M$ [1]. Equation (2) can be considered as an eigenvalue equation $K(E)\vec{x}=\delta\vec{x}$, where one of the eigenvalues must be equal to η^{-1}.

Differentiating $K(E)$ with respect to the energy gives a negative definite matrix. This shows that the eigenvalues of $K(E)$ are monotonously decreasing. The eigenvalues of H_0 coincide with the positions of the poles of $K(E)$. Therefore, each time the energy moves across a pole, a new eigenvalue of $K(E)$ appears at $+\infty$. The eigenvalue decreases with energy, until it reaches the value $1/\eta$. At this point the secular equation (2) has a root. Beyond this point, the eigenvalue continues to decrease, until it disappears at $-\infty$. This behavior gives rise to the following *sum rule*: Let $n_0(n_1)$ denote the number of eigenvalues of K, larger than $1/\eta$, at $E=E_0(E_1)$, and let N_p denote the number of poles and N_r the number of roots of $\det[K(E)]$ in the interval (E_0,E_1). Then it holds

$$n_0+N_p-N_r=n_1. \tag{3}$$

This relation can be used to bracket the eigenvalues in S_1, before using a standard root searching algorithm to obtain the desired accuracy. In this case, Eq. (3) assures that no eigenvalues are overlooked. However, if only long range correlations are of interest, one can do even better. It may then be sufficient to calculate the level counting function at the points of a previously defined grid, with possibly quite large spacings.

To calculate the spectrum of the barrier billiard [10], we choose as H_0 the Hamiltonian of a rectangle billiard with sides of length a and b. With the origin of a Cartesian coordinate system fixed at one of the corners, the normalized eigenfunctions are

$$\Psi_{mn}(x,y)=2(ab)^{-1/2}\sin(\pi mx/a)\sin(\pi ny/b), \tag{4}$$

while $\varepsilon_{mn}=[(m/a)^2+(n/b)^2]\pi^2/2$ are the corresponding eigenvalues. We use units, in which the mass and Planck's constant $\hbar$ are both equal to one. The perturbation consists of an additional boundary segment inside the billiard, connecting the points $(a_0,0)$ and (a_0,c). It is modeled by a potential well with δ-shaped profile

$$H=H_0+\eta W, \quad W=(a/2)\delta(x-a_0)\theta(c-y), \tag{5}$$

where $\delta(x)$ is the usual δ function, and $\theta(y)$ is the unit step function. As η increases from 0 to ∞, the spectrum of H changes from the spectrum of the rectangle billiard to the spectrum of the barrier billiard. In what follows we set $a_0=a/2, c=b/2$, where $a=2\pi^{3/2}/3$ and $b=6/\pi^{1/2}$. In this way, we obtain the same spectrum as in Ref. [10]. In this case the trivial component S_0 of the spectrum corresponds to states Ψ_{mn} with a node line at $x=a/2$. In order to obtain the nontrivial component alone, we require the eigenstates to be reflection symmetric with respect to that line. In other words, we consider the spectrum of a new rectangle billiard with sides $a/2$ and b, which has Dirichlet boundaries everywhere, except for the boundary segment between the points $(a/2,b/2)$ and $(a/2,b)$, which is a von Neumann boundary.

To obtain the decomposition $W=VV^T$, we calculate all eigenvectors of W which correspond to nonzero eigenvalues. This is rather simple because W is separable in the x and y modes of the eigenfunctions of H_0

$$V_{mn}^{(\alpha)}=s(m)\tilde{A}_n^{(\alpha)}, \quad s(m)=\sin(\pi m/2), \tag{6}$$

$$\tilde{A}_{2n}^{(\alpha)}=\frac{\delta_{n\alpha}}{\sqrt{2}}, \quad \tilde{A}_{2n-1}^{(\alpha)}=\frac{\sqrt{2}\alpha}{\pi}\frac{(-)^{\alpha+n}}{\alpha^2-(n-1/2)^2}. \tag{7}$$

For the matrix elements of $K(E)$ we get

$$K_{\alpha\beta}(E)=\sum_{mn}\frac{V_{mn}^{(\alpha)}V_{mn}^{(\beta)}}{E-\varepsilon_{mn}}=\sum_{mn}\tilde{A}_n^{(\alpha)}\tilde{A}_n^{(\beta)}\frac{s(m)^2}{E-\varepsilon_{mn}}. \tag{8}$$

Taking the limit $m\to\infty$, we can evaluate the sum over m analytically

$$K_{\alpha\beta}(E)=\frac{a^2}{2\pi}\sum_n \tilde{A}_n^{(\alpha)}\tilde{A}_n^{(\beta)}G_n(E), \tag{9}$$

with $G_n(E)=-\tan(\pi z_n/2)/z_n$. Here, z_n is the effective quantum number for H_0 at given energy E, i.e., $(z_n\pi/a)^2+(n\pi/b)^2=2E$. Note that $G_n(E)$ remains real, even for imaginary z_n. We may introduce the orthogonal matrix $A_{nm}=\sqrt{2}\tilde{A}_{2m-1}^{(n)}$, and truncating the sum in Eq. (9) at $n=M$, we obtain

$$K(E)=\frac{a^2}{4\pi}(A\,G^{\mathrm{odd}}A^T+G^{\mathrm{even}}), \tag{10}$$

with $G^{\mathrm{odd}}=\mathrm{diag}[G_{2n-1}(E)]$, and $G^{\mathrm{even}}=\mathrm{diag}[G_{2n}(E)]$. Multiplying Eq. (10) from left and/or right by A^T and/or A, one can construct the variants: $L=A^TK$, $K'=A^TKA$, and $L'=KA$. All of them can be used to find the eigenvalues of the barrier billiard. However, the matrices $K(E)$ and $K'(E)$ are real and symmetric, and hence easy to diagonalize. Finally, due to faster numerical convergence, we opted for $K'(E)$.

In what follows, we aim at a precise, numerical estimate for the level compressibility, which can be compared to the analytical results obtained in Refs. [10,11]. To this end, we compute the level counting function on a finite grid $\mathcal{N}_0, L_{\mathrm{tot}}, L_{\mathrm{st}}$ of consecutive intervals of length L_{st}, starting at $\mathcal{N}_0$ and ending at $\mathcal{N}_0+L_{\mathrm{tot}}$. The grid is defined on the unfolded energy axis, where the average level spacing is equal to one. It is then mapped onto the physical energy axis, by

TABLE I. Data sets for the barrier billiard.

(A)	(B)	(C)	(D)
$\mathcal{N}_0=8\times10^5$	2×10^6	8×10^6	1.6×10^7
$L_{\rm tot}=10^5$	1.4×10^5	10^5	10^5

TABLE II. Data sets for the right triangle billiard ($\alpha=\pi/5$).

$(T1)$	$(T2)$	$(T3)$
$\mathcal{N}_0=4\times10^5$	10^6	4×10^6
$L_{\rm tot}=4\times10^4$	10^5	10^5

inverting Weyl's law [18]: $4\pi\mathcal{N}(E)=ab\,E-(a+b)\sqrt{2E}+\pi/4$. We count the number of levels in each interval, using Eq. (3). The data sets, listed in Table I, are produced in this way. They are used to calculate the number variance $\Sigma^2(L)$ at integer multiples of $L_{\rm st}=10$.

The number variance $\Sigma^2(L)$ saturates at $L\approx L_{\rm max}$, which is related to the inverse period of the shortest (nondiffractive) periodic orbit [19]. For our barrier billiard

$$L_{\rm max}=\sqrt{2\pi\mathcal{N}_0\,b/a}=\sqrt{18\mathcal{N}_0/\pi}. \tag{11}$$

Therefore, the ratio $\Sigma^2(L)/L$ being constant at $1\ll L\ll L_{\rm max}$ starts to decrease when L approaches $L_{\rm max}$. We expect that $\Sigma^2(L)/L$ plotted versus $L/L_{\rm max}$ depends only weakly on $L_{\rm max}$, and hence on $\mathcal{N}_0$. We call this function the *scaled number variance*:

$$g(x)=\Sigma^2(L_{\rm max}x)/(L_{\rm max}x). \tag{12}$$

For integrable and pseudointegrable systems, it is expected that the ratio $\Sigma^2(L)/L$ becomes constant as L is increased. In practice, convergence is quite fast, and it turned out that $L\approx10$ is sufficient for our purposes. The semiclassical limit $\mathcal{N}_0\to\infty$ is the really difficult one. There, the level compressibility must be estimated by extrapolation, $\chi=\lim_{x\to0}g(x)$.

Figure 1 shows the scaled number variance for the data sets given in Table I. For the error bars, we estimated that the relative error is approximately equal to $1.6\sqrt{L/L_{\rm tot}}$. To obtain this value, we computed the variance of the distribution of different partial averages, fitting them with a normal distribution. Note that $L_{\rm tot}/L$ gives the number of independent level counts in the energy range considered. Figure 1 explains the discrepancy between the numerical estimate for the level compressibility obtained in Ref. [10], and the theoretical expectation. For $x>0.01$ the scaled number variance looks perfectly linear, and one is easily lead to assume that the linear behavior continues down to the point $x=0$. However, for $x<0.01$, the slope changes drastically, and a second linear regime appears. There, the scaled number variance $g(x)$ approaches the theoretical prediction $\chi=1/2$ as $x\to0$. In order to put our findings on a quantitative basis, we consider the following phenomenological parametrization:

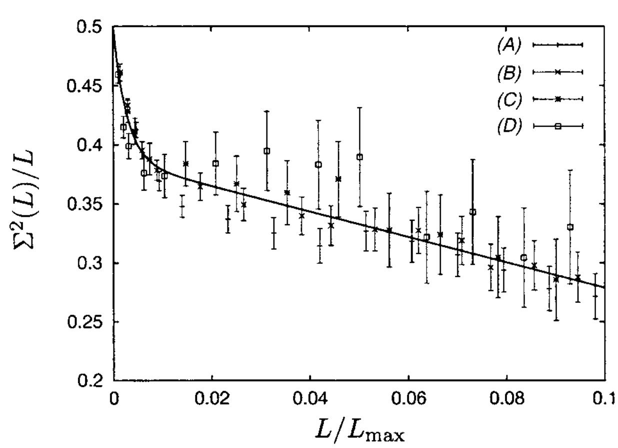

FIG. 1. The scaled number variance $\Sigma^2(L)/L$ vs $x=L/L_{\rm max}$ for the data sets in Table I. For clarity, only some of the data points are plotted. The thick solid line gives the fit function $g(x)$ with parameters as given in Eq. (14).

$$g(x)=a_2-a_1x+(a_0-a_2)\exp(-a_3x). \tag{13}$$

Its form is such that both linear regimes are reproduced. While $a_0=g(0)$ gives the best estimate for χ in the semiclassical limit, a_2 would be the result in the absence of data points with $x<0.01$. For the fit, all data sets in Table I are taken into account, up to $x=0.2$. Beyond this point (which is outside the interval shown in Fig. 1) the parametrization (13) breaks down. Using the nonlinear least squares Marquardt-Levenberg algorithm [20], we obtain the following estimates:

$$a_0=0.5008(91),\quad a_1=1.077(18),$$

$$a_2=0.3866(17),\quad a_3=364(39), \tag{14}$$

with a reduced χ^2 value of $\chi^2_{\rm fit}/f\approx0.54$ (the number of degrees of freedom is $f=305$).

With a_0, we have finally obtained a precise numerical estimate for the level compressibility in the semiclassical limit. It agrees within a relative error of roughly 2% with the theoretical result $\chi=1/2$. In addition, the moderate value for $\chi^2_{\rm fit}$ is quite remarkable. It gives some support to the assumption that within the statistical error, the scaled number variance is independent of the energy region (for $x\lesssim0.2$).

In what follows, we repeat the numerical analysis for the $\pi/5$-right triangle billiard. For this system, the matrix $K(E)$ has been calculated in Ref. [1]. The length scale $L_{\rm max}$, for the saturation of the number variance, is here about 2.6 times smaller than for the barrier billiard

$$L_{\rm max}=\sqrt{2\pi\mathcal{N}_0/(8\sin2\alpha)}\qquad\alpha=\pi/5, \tag{15}$$

We calculated three data sets in different energy regions, as listed in Table II ($L_{\rm st}=10$, as before). With all data sets, we fit the scaled number variance $g(x)$ using the parametrization (13), excluding again all data points with $x>0.2$. The resulting estimates are

$$a_0=0.5385(57),\quad a_1=0.958(37),$$

$$a_2=0.4154(54),\quad a_3=46.2(5.4), \tag{16}$$

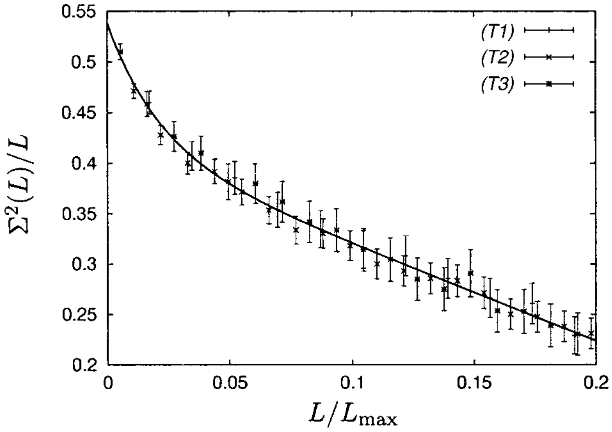

FIG. 2. The scaled number variance for the data sets in Table II. Only a subset of the data points is plotted. The solid line gives the fit $g(x)$ with parameters as given in Eq. (16).

with a reduced χ^2 value of $\chi^2_{\rm fit}/f \approx 0.20$ ($f=61$). The numerical results for $g(x)$, and the fit with Eq. (13), are plotted in Fig. 2. For the error bars, we have checked that the same approximation holds as in the case of the barrier billiard. The absolute errors are smaller here, because the data sets are taken at lower energies. As in Fig. 1, we find two linear regimes with different slopes. However, the initial slope is less steep, and the transition occurs somewhat later, at $x \approx 0.04$. Thus, the overall change in the graph is less pronounced. Though the agreement of the extrapolated value for $g(0)$ with the theoretical expectation $\chi=5/9$ [17] is not perfect, our estimate is very close to it. Note that the error estimates in Eq. (16) are also based on statistical data. In particular in the case of a_0, there are only relatively few relevant data points, which leads to rather large uncertainties.

We advanced the technique, recently proposed in Ref. [1], to solve the Schrödinger equation for perturbations of low rank. As a new result, we derived a *sum rule*, which allows to obtain the level counting function directly from the secular equation. Systems involving short range interactions and general quantum billiards may be good candidates for future applications. In this paper, we considered two pseudointegrable billiards: the barrier billiard and the $\pi/5$-right triangle billiard. In spite of their apparent simplicity, the spectral statistics is only hardly understood. We performed extensive numerical calculations for the number variance $\Sigma^2(L), L \gg 1$ in energy regions up to $\mathcal{N} > 1.6\times 10^7$ (for the barrier billiard) and $\mathcal{N} > 4\times 10^6$ (for the right triangle billiard). With the help of the scaled number variance, we obtained very precise estimates for the level compressibility. In contrast to earlier numerical studies, they largely confirm the analytical results. This shows that diffraction is not the basic mechanism leading to intermediate statistics.

T.G. thanks L. Kaplan and T. Papenbrock for stimulating discussions at the Centro Internacional de Ciencas in Cuernavaca, Mexico, and the EU Human Potential Program Contract No. HPRN-CT-2000-00156 for financial support.

[1] T. Gorin, J. Phys. A **34**, 8281 (2001).
[2] B. Davoudi, M. Polini, R. Asgari, and M.P. Tosi, Phys. Rev. B **66**, 075110 (2002); L.G.G.V. Dias da Silva and M.A.M. de Aguiar, *ibid.* **66**, 165309 (2002).
[3] J.H. Hannay and R.J. McCraw, J. Phys. A **23**, 887 (1990).
[4] E. Gutkin, Physica D **19**, 311 (1986); J. Stat. Phys. **83**, 7 (1996).
[5] P.J. Richens and M.V. Berry, Physica D **2**, 495 (1981).
[6] G.M. Zaslavsky, Phys. Rep. **371**, 461 (2002).
[7] B. Grémaud and S.R. Jain, J. Phys. A **31**, L637 (1998).
[8] E.B. Bogomolny, U. Gerland, and C. Schmit, Phys. Rev. E **59**, R1315 (1999).
[9] G. Casati and T. Prosen (unpublished).
[10] J. Wiersig, Phys. Rev. E **65**, 046217 (2002).
[11] E. Bogomolny, U. Gerland, and C. Schmit, Eur. Phys. J. B **19**, 121 (2001).
[12] M.V. Berry and M. Tabor, Proc. R. Soc. London, Ser. A **356**, 375 (1977).
[13] M. Mehta, *Random Matrices and the Statistical Theory of Energy Levels* (Academic Press, New York, 1991).
[14] B. Shklovskii *et al.*, Phys. Rev. B **47**, 11 487 (1993).
[15] X. Waintal, D. Weinmann, and J. Pichard, Eur. Phys. J. B **7**, 451 (1999).
[16] K.-H. Ahn, Y.H. Kim, J. Wiersig, and K.J. Chang, Phys. Rev. Lett. **90**, 026601 (2003).
[17] E. Bogomolny, O. Giraud, and C. Schmit, Commun. Math. Phys. **222**, 327 (2001).
[18] M. Brack and R.K. Bhaduri, *Semiclassical Physics* (Addison Wesley, New York, 1997).
[19] M.V. Berry, Proc. R. Soc. London, Ser. A **400**, 229 (1985).
[20] Gnuplot 3.7, patchlevel 1 (1999).