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LETTER TO THE EDITOR

Failure of semiclassical methods to predict individual energy levels

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Abstract. We argue that semiclassical methods quite generally cannot predict the individual energy levels not even in the semiclassical limit of small but finite $\hbar$ and when the number of energy levels goes to infinity. By this we mean that the average relative error of the semiclassical eigenvalues in units of the mean level spacing typically increases indefinitely as the energy goes to infinity or is at least bounded from below. This we show for the case of the integrable circular billiard and the one-dimensional potential $U_0/\cos^2(\alpha x)$ by comparing the torus quantized semiclassical eigenenergies with the exact results. Since all the various semiclassical methods such as Gutzwiller's and Bogomolny's are reduced to the torus quantization in integrable cases we believe that our conclusion is generally valid. We have theoretical arguments and strong numerical evidence (for the case of the circular billiard) that nevertheless the statistical properties of the exact energy spectra are correctly reproduced by the semiclassical approximations. It is numerically found that the energy level spacing distribution and the spectral rigidity for the exact spectrum and for the semiclassical spectrum are in excellent agreement even for finite spectra where they both deviate from the limiting Poissonian behaviour, so we suggest that the non-universal approach to the limiting energy level statistics is also correctly described by the semiclassical theory. We discuss the validity of the semiclassical methods in the light of our negative and positive findings. In addition we find the surprising result for the previously mentioned special cases that the error distribution of the semiclassical approximation is stationary, i.e. it is independent of the energy.

In the course of the development of quantum chaos (see e.g. reviews by Berry (1983), Bohigas and Giannoni (1984), Robnik (1985), Eckhardt (1988) and by Gutzwiller (1990)) there has recently been much renewed interest in semiclassical methods of approximating the energy eigenvalues and the eigenstates of the Schrödinger operators. In classically integrable cases we have the well known torus quantization (EBK quantization) which is based essentially on the seminal work by Einstein (1917) and put in its final form by Maslov (1972). But in the general case we do not have invariant tori, so the torus quantization cannot be applied. However, there is the general approach developed by Gutzwiller (1967, 1969, 1970, 1971), which is based on the semiclassical expansion of the density of states in terms of classical periodic orbits, which can formally be applied in non-integrable Hamiltonian systems including the fully chaotic systems (ergodic systems). For reviews see Berry and

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Mount (1972), Berry (1983), Eckhardt (1988) and Gutzwiller (1990). This so-called semiclassical trace formula has the mathematical difficulty of being a divergent series. Considerable effort has recently been spent in trying to overcome this difficulty by a suitable resummation method based on mathematical principles (Sieber and Steiner 1990, Aurich *et al* 1992, Cvitanović and Eckhardt 1991, Berry and Keating 1990) and on physical ideas by introducing the quantum analogue of the surface of section method in the semiclassical limit (Bogomolny 1990). Even with these mathematical improvements in overcoming the divergence problems it is difficult or almost impossible to assess the error of the semiclassical eigenenergies as predicted by the trace formula, especially of high lying levels which are of interest in our work. The few cases where the trace formula is accidentally exact are, in fact, exceptions (e.g. geodesic motion on the constant negative curvature surface). For a non-trivial example of an ergodic system (anisotropic Kepler problem) the lowest 18 levels have been compared with the exact results by Gutzwiller (1980), and the quality of the approximation is hardly better than the crudest possible semiclassical quantization, namely the Thomas–Fermi rule. But it is well known (Berry and Tabor 1976) that in classically integrable cases the Gutzwiller formula is precisely equivalent to the torus quantization. Therefore those integrable systems which can be worked out explicitly can be used to test the accuracy of the semiclassical methods in predicting the individual energy levels. It should be emphasized that here we think of the error as measured in units of the mean energy level spacing. The results are believed to be typical of the quality of the semiclassical approximations.

We will demonstrate this point explicitly in two cases: the circular billiard and the one-dimensional potential $U_0/\cos^2(\alpha x)$.

The exact energy eigenvalues $E^{\rm ex}_{mn}$ of the unit circular billiard (in suitably chosen units $\hbar^2/2m = 1$) are just the squares of the zeros of Bessel functions, $J_m(\sqrt{E^{\rm ex}_{mn}}) = 0$, and we have numerically calculated the first 50 000 levels with the absolute precision 10^{-9}, implying the relative error in units of the mean level spacing equal to 10^{-10}. The claimed accuracy has been carefully checked by verifying one of the well known recursion relations for the Bessel functions. On the other hand the semiclassical torus quantization result for the eigenvalues $E^{\rm sc}_{mn}$ can be easily obtained both directly (Robnik 1984a), and also by working out the quantization formula of Bogomolny (1990) as was shown in Prosen (1993),

$$\sqrt{E^{\rm sc}_{mn} - m^2} - |m| \cos^{-1}\left(|m|/\sqrt{E^{\rm sc}_{mn}}\right) = (n + 3/4)\pi \tag{1}$$

where $n = 0, 1, 2\ldots$ is the radial quantum number and $m = 0, \pm 1, \pm 2\ldots$ is the angular momentum quantum number, so that for $m \neq 0$ we have doubly degeneracy.

Both even-parity spectra ($m \geqslant 0$), the exact one and the semiclassical, have been unfolded (Bohigas and Giannoni 1984) by using the Weyl formula (with perimeter corrections) for the even-parity spectral staircase $N(E)$ (Prosen and Robnik 1992),

$$N(E) = \frac{1}{8}E - \frac{\pi - 2}{4\pi}\sqrt{E} - \frac{1}{24} \tag{2}$$

and these unfolded spectra (henceforth denoted by the same symbols) have been used to calculate the error $E^{\rm ex} - E^{\rm sc}$. The results are presented in figures 1, 2 and 3. The pointwise-computed error presented in figure 1 shows some systematics but the sequence of largest errors clearly increases strictly monotonically. In figure 2 we

demonstrate that the average error, root-mean-square error and the maximal error (the average and the maximum is taken over 800 levels) increase indefinitely. We have also calculated the distribution of the logarithms of the errors for four consecutive stretches each consisting of roughly 5000 levels, and figure 3 gives clear evidence for the stationarity of such distribution, for all four curves are almost identical. Since the average error tends to infinity with increasing energy this distribution cannot have a finite first moment. This reliable numerical evidence forces one to draw the unavoidable conclusion that the semiclassical approximation definitely cannot predict the individual energy levels not even in the asymptotic limit when energy goes to infinity. (Note that this conclusion is independent of $\hbar$ due to the scaling property of energy eigenvalues with $\hbar$ for the billiards.)

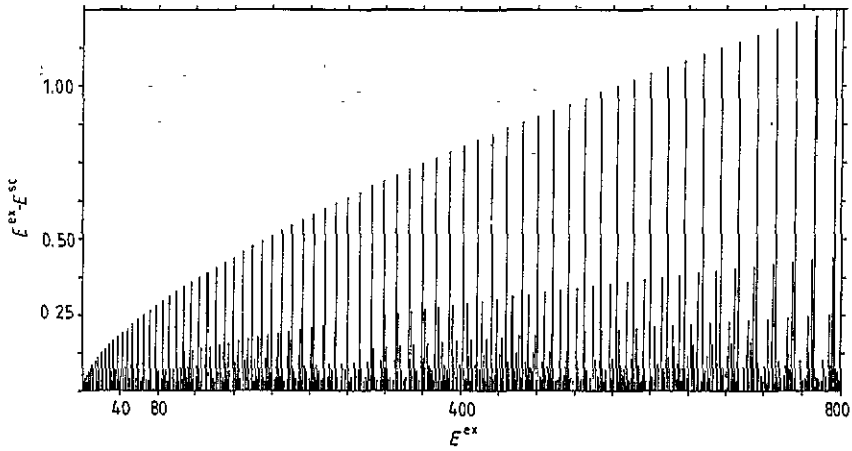

Figure 1. The pointwise-calculated error $E^{ex} - E^{sc}$ of the unfolded energy spectra plotted against E^{ex} for the first 800 levels.

This disappointing discovery is a strong statement and one would like to test it by another independent approach. The best chance of having the highest possible accuracy for the semiclassical individual levels is given by the one-dimensional systems, where the Sturm–Liouville theorem (Courant and Hilbert 1968, Loudon 1959) prohibits degeneracies (for the usual Schrödinger operators of the type 'kinetic energy plus potential') and thus implies local regularity of spectra (locally we have picket-fence-like spectra) by suppressing the spectral fluctuations. Therefore it is natural to make such a test for the case of an exactly soluble potential which can also be worked out in a closed form when applying the torus quantization. We have chosen the one-dimensional Hamiltonian, $H = (p^2/2m) + (U_0/\cos^2(\alpha x))$. Its exact and semiclassical eigenvalues are (see Landau and Lifshitz 1977)

$$E_n^{ex} = A(n + \tfrac{1}{2} + \tfrac{1}{2}\sqrt{1 + B^2})^2 \tag{3}$$

$$E_n^{sc} = A(n + \tfrac{1}{2} + \tfrac{1}{2}B)^2 \tag{4}$$

$$A = \frac{\hbar^2\alpha^2}{2m} \qquad B = \frac{\sqrt{8mU_0}}{\hbar\alpha} \qquad n = 0, 1, 2\ldots. \tag{5}$$

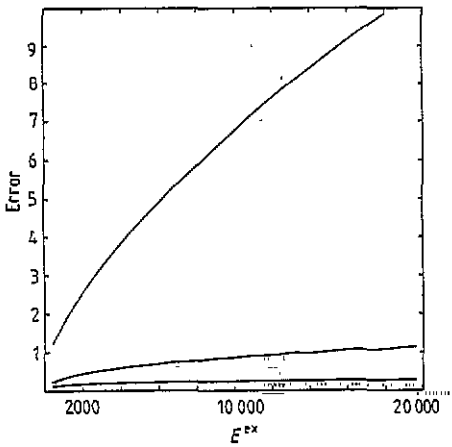

Figure 2. The maximum error (top curve), the root-mean-square error (middle one) and the average error (bottom curve) plotted against the unfolded energy E^{ex}. The average and the maximum are taken over the spectral stretches of 800 levels, and the plot is extended over the lowest 20 000 levels.

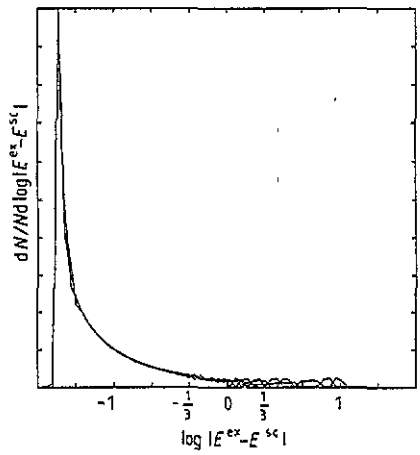

Figure 3. We plot the distributions $d\log N/d\log|E^{ex} - E^{sc}|$ over four consecutive spectral stretches each consisting of roughly 5000 levels. Note that they are essentially identical and therefore independent of the energy.

The error measured in units of the mean level spacing $\Delta E_n = E^{ex}_{n+1} - E^{ex}_n$ reads

$$\frac{E^{ex}_n - E^{sc}_n}{\Delta E_n} = \frac{\frac{1}{4} + (n+\frac{1}{2})(\sqrt{1+B^2} - B)}{2n+2+\sqrt{1+B^2}} = \begin{cases} \frac{1}{2}(\sqrt{1+B^2} - B) & n \to \infty \\ \frac{1}{2}(n+\frac{1}{2})/B^2 & B \to \infty. \end{cases} \quad (6)$$

Note that the limit $B \to \infty$ is equivalent to the limit $\hbar \to 0$ since $B \propto 1/\hbar$. The asymptotics (6) clearly shows that even for arbitrarily small but finite $\hbar$ ($1 \ll B < \infty$) the relative error becomes constant and equal to $\frac{1}{2}(\sqrt{1+B^2} - B) \approx 1/4B$, which is realized when $n \gg B$. So again, the relative error is bounded from below.

In spite of this severe deficiency in the semiclassical approximations we have reason to expect that the statistical properties of the energy spectra are nevertheless

correctly described. There are elaborate theoretical arguments by Berry and Tabor (1977) that classically integrable systems should have Poissonian statistics which can also be understood in a simple way by the remark that the existence of two or more quantum numbers implies effectively random superposition of infinitely many number sequences. In the case of classically ergodic (or more chaotic) systems there is no general argument, but we have Berry's (1985) semiclassical result on spectral rigidity (delta statistics) based on Gutzwiller's approach, showing that in the semiclassical limit delta statistics do indeed behave universally in agreement with the random matrix theories (Bohigas and Giannoni 1984).

In our case of the circular billiard we have numerically explored the energy level spacing distribution $P(S)$ and delta statistics $\Delta(L)$ using the lowest 50 000 even parity levels. As for $P(S)$ we indeed find convergence towards Poisson distribution. However, we find in addition something very surprising: even the deviations of $P(S)$ from e^{-S} are excellently described by the semiclassical levels and are thus obviously well determined by the dynamics of the system rather than being statistical noise. (The χ^2 test confirms that the deviations are statistically significant since they are within several (3 to 5) sigmas.) In order to exhibit these deviations in a most uniform and efficient way we have used the technique introduced in Prosen and Robnik (1992). We define the following quantities: The cumulative spacing distribution $W(S) = \int_0^S \mathrm{d}x P(x)$, the cumulative Poisson distribution $W_0(S) = 1 - e^{-S}$ and the so-called U-function $U(W) = (2/\pi)\cos^{-1}\sqrt{1-W}$. The latter has the property that the estimated statistical error is constant for all level spacings, $\delta U = 1/(\pi\sqrt{N})$. In figures 4(*a*)–(*c*) we plot $U(W(S)) - U(W_0(S))$ versus $W_0(S)$, which warrants uniform density of experimental points on the abscissa. The agreement between the exact and semiclassical curves is really striking.

In figure 5 we plot the delta statistics $\Delta(L)$ and we observe that the two curves, the exact and the semiclassical, are practically indistinguishable. At small L they do indeed behave in the Poissonian way $L/15$ but the transition towards the non-universal regime is surprisingly fast and smooth in contrast to what would be expected by Berry's (1985) theory of spectral rigidity. For example, the observed saturation sets in at $L = L_{\max} \approx 250$, whilst Berry's semiclassical estimate yields $L_{\max} \approx 500$.

Our general conclusion is that a reliable assessment of the accuracy of the semiclassical approximations for individual eigenenergies is a very delicate matter, and that quite generally the semiclassical methods fail to predict the energy levels within vanishing fraction of the mean level spacing even in the asymptotic region where according to the common folklore they are supposed to be exact. Amazingly, sometimes the semiclassical approximation is excellent even for low-lying levels including the ground state where it is supposed not to be applicable. One example for the Hénon–Heiles system can be found in Robnik (1984b). And as is well known the semiclassical approximation is incidentally exact in cases where the classical action is a quadratic function of the coordinates and if, in addition, certain conditions are satisfied. However, we have given arguments and numerical results supporting the firm common belief that the statistical properties of the exact quantum spectra are correctly reproduced by the semiclassical levels—a result which still calls for further theoretical investigation. It should be emphasized that this is true even for the deviation of statistics (for finite spectral stretches) from their limiting universal semiclassical behaviour. As for the systems in the transition region between integrability and chaos (KAM systems) we should mention that the limiting semiclassical distributions are

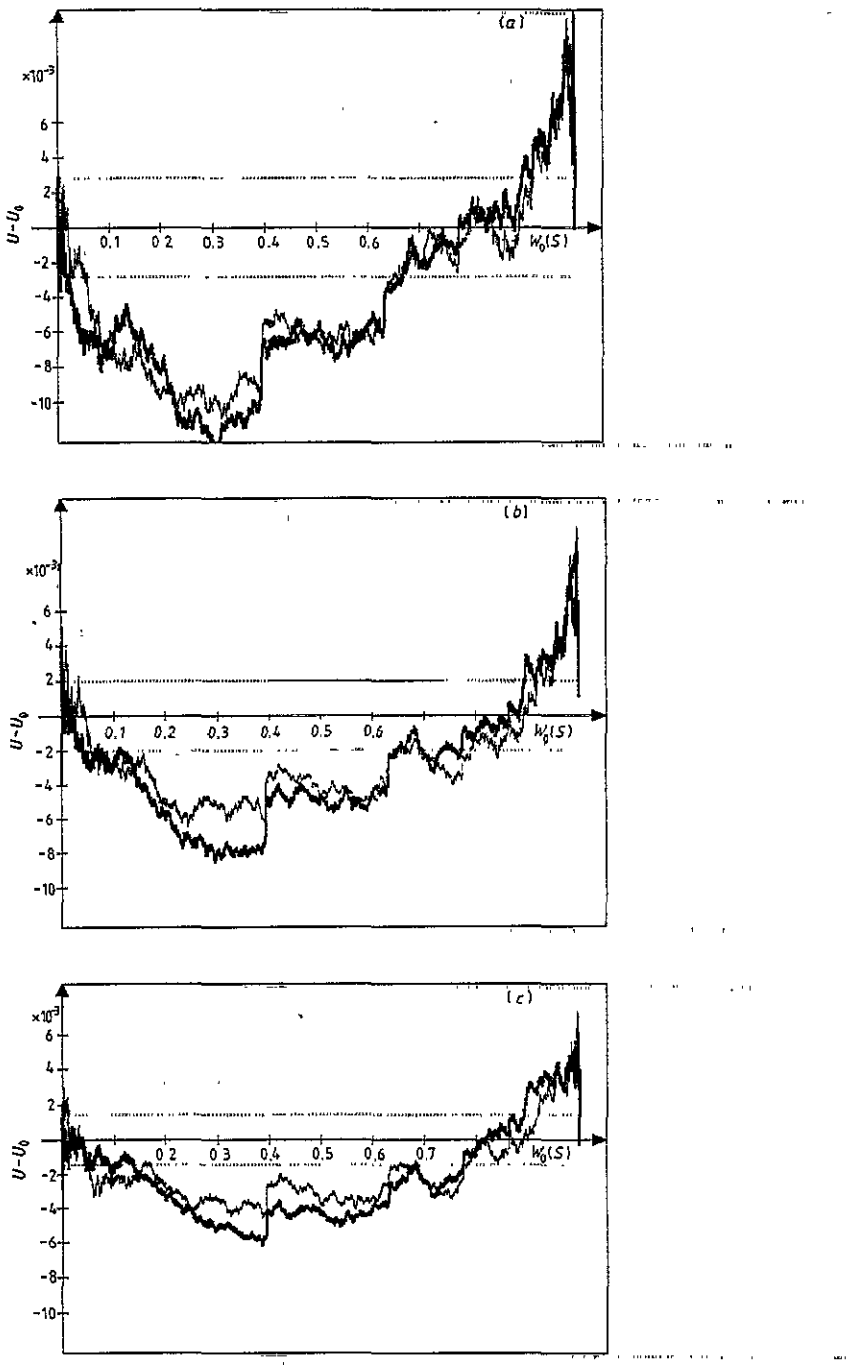

Figure 4. We plot $U(W(S)) - U(W_0(S))$ against $W_0(S)$ for the lowest 12 500 levels (*a*), 25 000 levels (*b*) and 50 000 levels (*c*). The thick curves represent the exact data, whilst the thin curves refer to the semiclassical eigenvalues. The dotted lines indicate the theoretically expected one-sigma error. Note that deviations from the Poissonian line (abscissa) are significant and the exact and the semiclassical curves are in surprising agreement. Also, the curves converge to the Poissonian line with increasing number of levels.

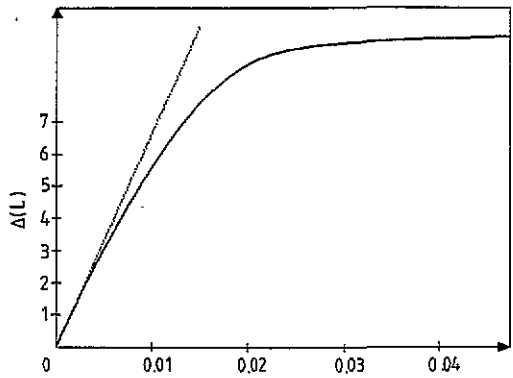

Figure 5. We plot the delta statistics $\Delta(L)$ using the semiclassical and the exact data for the lowest 50 000 levels, where the two curves are indistinguishable. Note that the transition from the Poissonian behaviour $L/15$ (the dotted line) is fast and smooth and the observed L_{max} at which the saturation sets in is roughly 250.

correctly described by the Berry–Robnik (1984) type approach (see also Seligman and Verbaarschot 1985, Prosen and Robnik 1992). Despite its deficiency in describing the individual levels, the semiclassical method is of fundamental importance in understanding the variety of qualitative behaviour of systems in quantum chaos. Similar conclusions are expected about the semiclassical description of eigenstates.

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