Semiclassical singularities from bifurcating orbits

Christopher Manderfeld\textsuperscript{1} and Henning Schomerus\textsuperscript{2}

\textsuperscript{1} Fachbereich Physik, Universit"at–Gesamthochschule Essen, 45 117 Essen, Germany
\textsuperscript{2} Instituut-Lorentz, Universiteit Leiden, P. O. Box 9506, 2300 RA Leiden, The Netherlands

Received: date / Revised version: date

Abstract. We study how the singular behaviour of classical systems at bifurcations is reflected by their quantum counterpart. The semiclassical contributions of individual periodic orbits to trace formulae of Gutzwiller type are known to diverge when orbits bifurcate, a situation characteristic for systems with a mixed phase space. This singular behaviour is reflected by the quantum system in the semiclassical limit, in which the individual contributions remain valid closer to a bifurcation, while the true collective amplitude at the bifurcation increases with some inverse power of Planck’s constant (with an exponent depending on the type of bifurcation). We illustrate the interplay between the two competing limits (closeness to a bifurcation and smallness of $\hbar$) numerically for a generic dynamical system, the kicked top.

PACS. 05.45.Mt Semiclassical Chaos (Quantum Chaos) – 03.65.Sq Semiclassical theories and applications

1 Introduction

The semiclassical approach allows to obtain spectral information about quantum systems from properties of classical periodic orbits. The most famous example of this quantum-classical correspondence is Gutzwiller’s trace formula for completely chaotic (hyperbolic) autonomous systems \footnote{1}, which expresses the density of states as a sum of contributions from periodic orbits. In such systems, the Lyapunov exponents of all periodic orbits are positive, and their semiclassical amplitudes $A \propto (\sin \lambda/2)^{-1}$ are finite. This is not true for systems with a mixed phase space, which accommodate also elliptic orbits with amplitude $A \propto (\sin \omega/2)^{-1}$. The quantity $\omega = r\omega_0$, known as the stability angle, increases linearly under $r$ repetitions of the orbit, and either by a suitable choice of $r$ or of an external control parameter the amplitude $A$ can become arbitrarily large. The contribution of an individual orbit eventually diverges when $\omega/2\pi$ is an integer. Normal-form theory\footnote{2} shows that this is precisely the condition for a bifurcation, the coalescence of two or more periodic orbits. Catastrophe theory\footnote{3} further reveals that the divergence comes from an illegitimate stationary-phase approximation, and provides us with uniform approximations (collective contributions of the bifurcating orbits) that regularise the singular behaviour\footnote{4,5,6,7,8,9,10}. The ensuing true semiclassical amplitude is finite at $\hbar \neq 0$, even directly at the bifurcation. It is clear, however, that an individual contribution of Gutzwiller type must be valid in the strict semiclassical limit, as soon as one does not sit precisely on a bifurcation (fixed distance $\varepsilon$ to a bifurcation in parameter space, $\hbar \to 0$). Analyticity at given $\hbar$ and varying $\varepsilon$ entails then that the true amplitude at the bifurcation ($\varepsilon = 0$) must diverge as $\hbar \to 0$, with a power law $\sim \hbar^{-\nu}$ as it happens to be\footnote{7}. Some consequences of this peculiar singularity have been studied recently in the context of spectral fluctuations\footnote{11}. A complete solution of this intricate problem is emerging\footnote{12}, but it is complicated because one has to consider also more complex bifurcations of higher codimension which are classically non-generic, but are nevertheless relevant in the quantum realm.

In this work we investigate the interplay of the two competing limits $\hbar \to 0$, $\varepsilon \to 0$, focusing on periodically driven systems with one degree of freedom. All results are relevant for autonomous systems with two degrees of freedom as well. For a representative system, the kicked top, we find that bifurcations often interfere even when they are separated in phase space. This adds additional complexity to the problem at hand. We use a filtering technique to extract contributions of bifurcating orbits and find that their amplitude corresponds well to the theoretical predictions.

The paper is organised as follows: In Section\textsuperscript{2} we describe how the exponents $\nu$ for the most commonly encountered bifurcations are derived. In Section\textsuperscript{3} we present numerical results for the kicked top. Section\textsuperscript{4} contains our conclusions.

2 Semiclassical contributions at bifurcations

Periodically driven systems are stroboscopically described by a unitary Floquet operator $F$. Spectral information about this operator is most conveniently extracted from the traces $\text{tr} F^n$, where $n$ plays the role of discretised time.
The analogue of Gutzwiller’s trace formula has been derived by Tabor [1,3], who found the relation

\[ \text{tr} F^n = \sum_{p, q, \ldots} \frac{n_0}{|2 - \text{tr} M|^{1/2}} \exp \left( i J S - i \mu \frac{\pi}{2} \right), \tag{1} \]

between the traces and the periodic orbits of the corresponding chaotic classical map. For convenience we denote here the inverse Planck’s constant by \( h^{-1} = J \). The sum is made up of all orbits of primitive (first return) period \( n_0 \) with \( n = n_0 r, r \) an integer. The \( r \)th return of an orbit is characterised by the action \( S = r S_0 \), trace of the monodromy matrix (linearised map) \( M = M_0^\mu \), and the Maslov index \( \mu = r \mu_0 \) (which for elliptic orbits satisfies a slightly more involved composition law under repetitions).

Eq. (1) is valid for completely chaotic systems. For hyperbolic orbits, the eigenvalues of the monodromy matrix \( M_0 \) are \( e^{\pm \omega_0} \), while elliptic orbits have unimodular eigenvalues \( e^{\pm i \omega_0} \). In both cases the expressions for the semiclassical amplitudes \( A \propto |2 - \text{tr} M|^{-1/2} \) given in the introduction follow immediately. As advertised, the semiclassical amplitude \( A \) of an individual orbit diverges when \( \omega_0 = 2\pi n/m \), with \( n, m \) integers (taken relatively prime).

The type of bifurcation depends on \( m \), with \( m = 1 \) the tangent bifurcation, \( m = 2 \) the period-doubling bifurcation, \( m = 3 \) the period-tripling bifurcation, and so forth. Close to a bifurcation one should replace contributions of individual orbits by collective contributions in the trace formula, of the form

\[ A = \frac{J}{2\pi} \int_0^{\infty} dI \int_0^{2\pi} d\phi \Psi(I, \phi) \exp[iJ\Phi(I, \phi)], \tag{2} \]

with the ‘amplitude function’ \( \Psi \) and the ‘phase function’ \( \Phi \) both depending on the type of bifurcation under consideration. Here we have used canonical polar coordinates \( I, \phi \), which parametrise the phase space of the classical map as

\[ p = \sqrt{2I} \sin \phi, \quad q = \sqrt{2I} \cos \phi, \tag{3} \]

giving for the differentials \( dp \, dq = dI \, d\phi \). The phase function is a local approximation to the generating functions \( S(q', p) \) of the classical map \( (q, p) \rightarrow (q', p') \). Right at the bifurcation the amplitude function reduces to \( \Psi = 1 \), while the phase function is given by simple normal forms. For generic bifurcations we have

\[ \Phi = S_0 - \varepsilon q - a q^3 - b p^2 \quad (m = 1), \]
\[ \Phi = S_0 - \varepsilon q - a q^3 - b p^2 \quad (m = 2), \]
\[ \Phi = S_0 - \varepsilon I - a I^{3/2} \cos 3\phi \quad (m = 3), \]
\[ \Phi = S_0 - \varepsilon I - a I^{3/2} - b I^2 \cos 4\phi \quad (m = 4). \tag{4} \]

Here \( \varepsilon \) is the bifurcation parameter (bifurcations take place at \( \varepsilon = 0 \)), while \( S_0, a, b \) can be regarded as constants. At the bifurcation (\( \varepsilon = 0 \)) we can rescale the integration variables \( q, p \) for \( m = 1, 2 \) or \( I \) for \( m \geq 3 \), such that the combination \( J \Phi \) appearing in the exponent of Eq. (3) becomes independent of \( J \). What remains is a \( J \)-dependent prefactor in front of a \( J \)-independent integral. We find \( A \propto J^\nu \) with

\[ \nu = 1/6 \quad (m = 1), \quad \nu = 1/3 \quad (m = 3), \quad \nu = 1/2 \quad (m \geq 4). \tag{5} \]

For \( \varepsilon \neq 0 \) the integral remains \( J \)-independent if one also rescales the bifurcation parameter according to \( \varepsilon' = \varepsilon J^m \)

\[ \mu = 2/3 \quad (m = 1), \quad \mu = 1/2 \quad (m = 2), \quad \mu = 1/2 \quad (m = 4). \tag{6} \]

These exponents determine the semiclassical range of the bifurcations in parameter space.

The case \( m = 3 \) is special in the sense that period-tripling bifurcations are usually accompanied by a tangent bifurcation, so close in parameter space that the semiclassical contribution given above loses validity for accessible values of \( J \). This gives the unique opportunity to test also predictions for a bifurcation of higher codimension. The normal form is

\[ \Phi(I, \phi') = S_0 - \varepsilon I - a I^{3/2} \cos 3\phi - b I^2. \tag{7} \]

The tangent bifurcation takes place at \( \varepsilon = \frac{9a^2}{4b^2} \), while the period-tripling bifurcation occurs at \( \varepsilon = 0 \). For \( \varepsilon = a = 0 \) one has to consider an integral of the form

\[ J \int_0^{\infty} dI \int_0^{2\pi} d\phi \exp[iJ I^2] \propto J^{1/2}, \tag{8} \]

and obtains \( \nu = 1/2 \). For \( \varepsilon, a \neq 0 \) we obtain the two scaling parameters \( \mu_{\varepsilon} = 1/2 \) and \( \mu_a = 1/4 \) that characterise the semiclassical range of the bifurcation in parameter space.

### 3 Numerical results

We now wish to investigate how the semiclassical singularities at bifurcations emerge for a representative dynamical system, the periodically kicked top [4], which has proven useful in testing semiclassical results before. The dynamics consists of a sequence of rotations and torsions, with Floquet operator

\[ F = \exp \left( -i \frac{k_1}{2j + 1} \hat{J}_z^2 - i\alpha_1 \hat{J}_z \right) \exp \left( -i\beta \hat{J}_y \right) \]
\[ \times \exp \left( -i \frac{k_2}{2j + 1} \hat{J}_z^2 - i\alpha_2 \hat{J}_z \right). \tag{9} \]

The angular momentum operators \( \hat{J}_{x,y,z} \) obey the commutator relation \( [\hat{J}_i, \hat{J}_j] = i \varepsilon_{ijk} \hat{J}_k \). Since the square of the angular momentum \( \hat{J}^2 = j(j + 1) \) is conserved the phase space is the unit sphere. The role of the inverse Planck’s constant is played by \( J = j + \frac{1}{2} \), which is equal to one half of the Hilbert space dimension. The semiclassical limit is reached by sending \( J \rightarrow \infty \). We fix the rotation parameters \( \alpha_1 = 0.8, \beta = 1, \alpha_2 = 0.3 \), and use the torsion
strengths $k_1 \equiv k$ and $k_2 = k/10$ to control the degree of chaos of the classical map. The system is integrable for $k = 0$ and displays well-developed chaos from $k \approx 5$.

The quantum-mechanical evaluation of $F$ is described in Ref. [14]. We computed the traces of the Floquet operator and separated the contributions of different (clusters of) orbits by evaluating the action spectrum (a Fourier transformation of the trace with respect to the inverse Planck’s constant) [15],

$$T^{(n)}(S) = \frac{1}{j_{\text{max}} - j_{\text{min}} + 1} \sum_{j = j_{\text{min}}}^{j_{\text{max}}} \text{tr} F^n(j) e^{-i(j + \frac{1}{2})S},$$  

where the difference $j_{\text{max}} - j_{\text{min}}$ determines the resolution in $S$ ($j_{\text{min}} = 1$, $j_{\text{max}} = 100$). The results for parameters close to different types of bifurcations are shown in Fig. 1.

The contribution at given $j$ of orbits pertaining to a given peak can be obtained by an inverse Fourier transformation,

$$A \propto \int_{S_{\text{Bif}} - \frac{\Delta S}{2}}^{S_{\text{Bif}} + \frac{\Delta S}{2}} \text{d}S \left( \sum_{j' = j_{\text{min}}}^{j_{\text{max}}} \text{tr} F^n(j') e^{-i(j' + \frac{1}{2})S} \right) e^{i(j + \frac{1}{2})S}$$  

$$= 2 \sum_{j' = j_{\text{min}}}^{j_{\text{max}}} \text{tr} F^n(j') e^{i(j - j')S_{\text{Bif}}} \sin \left[ (j - j') \Delta S / 2 \right] / (j - j'),$$  

where the integral over actions $S$ is restricted to an interval $\Delta S$ around the centre $S_{\text{Bif}}$ of the peak. This eliminates contributions of other periodic orbits.

It is convenient to tune the control parameter $k$ slightly away from the bifurcation to the value that maximises the contribution of the bifurcating orbits to $\text{tr} F^n$. The
parameter $k$ of the maximum approaches the true bifurcation point with the exponent $\nu$, Eq. (6). The maximal contribution is of the same order of magnitude as the contribution at the bifurcation, but it is less sensitive to changes in the parameters. Most importantly, this procedure does not require any classical information (like the precise parameter value of the bifurcation) and is hence genuinely quantum mechanical. We extract the exponents $\nu$ from logarithmic plots of the maximal $|A|$ versus $\nu$, shown in Fig. 2. In all cases we find good agreement with the theoretical predictions. For a tangent bifurcation at $k \approx 2.5$ the observed exponent is $\nu \approx 0.1866$ (theoretically, $\nu = 1/6$). Two different period-doubling bifurcations appear at $k \approx 2.8$ and produce overlapping peaks in the action spectrum. We separated them by changing $\alpha_1$ to $\alpha_1 = 1.39$, moving in that way one of the period-doubling bifurcations to $k \approx 2.1$. The exponent for this bifurcation is $\nu \approx 0.2636$ (theoretically, $\nu = 1/4$). Back to the original value $\alpha_1 = 0.8$, we find for the period-quadrupling bifurcation at $k \approx 1.0$ the exponent $\nu \approx 0.5734$ (theoretically, $\nu = 1/2$).

As mentioned above, for all known dynamical systems period-tripling bifurcations are typically accompanied by a tangent bifurcation, so close in parameter space that one has to treat the situation as a bifurcation of higher codimension. For the kicked top, an angular momentum of about $J \approx 10^5$ would be needed for separating the orbits in the ‘period-tripling+tangent’ bifurcation at $k \approx 1.85$. The same is true for a similar sequence of bifurcations at $k \approx 1.97$. For the much smaller values of $J$ that we use here we hence have the unique opportunity to test the exponent for a case of higher codimension. As before, the result $\nu \approx 0.5327$ (for the bifurcations at $k \approx 1.85$) is close to the theoretical expectation $\nu = 1/2$.

### 4 Conclusions

We have studied the asymptotic behaviour for $\hbar \to 0$ of periodic-orbit contributions to semiclassical trace formulae, around points in parameter space where orbits bifurcate. For the most common types of bifurcations the theoretically predicted power-law divergence $\propto \hbar^{-\nu}$ was tested numerically for a representative dynamical system, the kicked top, giving good agreement for the exponents $\nu$.

In the semiclassical limit the contribution of non-bifurcating orbits reaches a constant value $|A| = \mathcal{O}(|\hbar|^0)$, corresponding to $\nu = 0$. It follows from Eq. (2) that the exponent for bifurcating orbits falls into the range $0 < \nu < 1$. As a consequence, the semiclassical contribution of bifurcating orbits is dominant when parameters are close enough to the bifurcation point. On first sight this seems to require a careful tuning of the parameters. From the perspective of spectral statistics, however, a careful tuning often turns out to be unnecessary [11,12]: The period $n$ of orbits that contribute to the spectrum increases in the semiclassical limit as well, and one enters a competition between the weight of bifurcations in parameter space (given by the exponents $\nu$ and $\mu$) and the proliferation of their number with increasing $n$. Some quantities are dominated by bifurcating orbits even when the proliferation is not taken into account. The final outcome of this competition is not clear at the moment and certainly deserves further investigation.

This work was supported by the Sonderforschungsbereich 237 of the Deutsche Forschungsgemeinschaft and the Dutch Science Foundation NWO/FOM.

### References

1. M. C. Gutzwiller, J. Math. Phys. **12**, 343 (1971).
2. K. R. Meyer, Trans. Am. Math. Soc. **149**, 95 (1970).
3. T. Poston and I. N. Stewart, *Catastrophe Theory and its Applications* (Pitman, London, 1978).
4. A. M. Ozorio de Almeida and J. H. Hannay, J. Phys. A **20**, 5873 (1987).
5. A. M. Ozorio de Almeida, Hamiltonian Systems: Chaos and Quantisation (Cambridge University, Cambridge, 1988).
6. M. Kuś, F. Haake, and D. Delande, Phys. Rev. Lett. **71**, 2167 (1993).
7. H. Schomerus and M. Sieber, J. Phys. A **30**, 4537 (1997).
8. M. Sieber and H. Schomerus, J. Phys. A **31**, 165 (1998).
9. H. Schomerus, Europhys. Lett. **38**, 423 (1997).
10. H. Schomerus, J. Phys. A **31**, 4167 (1998).
11. M. V. Berry, J. P. Keating, and S. D. Prado, J. Phys. A **31**, 1245 (1998).
12. M. V. Berry, to appear in *New Directions in Quantum Chaos*, edited by G. Casati, I. Guarneri, and U. Smilansky (IOS, Amsterdam, 1999).
13. M. Tabor, Physica D **6**, 195 (1993).
14. P. A. Braun, P. Gerwinski, F. Haake, and H. Schomerus, Z. Phys. B **100**, 115 (1996).
15. U. Eichmann, K. Richter, D. Wintgen, and W. Sander, Phys. Rev. Lett. **61**, 2438 (1988).