Abteilung Theoretische Physik

Universität Ulm

Semiclassical approximations and periodic orbit expansions in chaotic and mixed systems

Habilitationsschrift

vorgelegt an der Fakultät für Naturwissenschaften

der Universität Ulm

von

Dr. rer. nat. Martin Sieber

Mai 1998

Contents

Summary

The correspondence between a quantum system and its classical limit is closely connected to the periodic orbits of the system. They characterize the oscillations in quantum spectra since the Fourier components of the density of energy levels are determined in the semiclassical limit by periodic orbits. We present here a collection of articles that examine various properties of semiclassical approximations in terms of periodic orbits. The form of these approximations depends on the nature of the classical motion. Several applications are discussed.

In the first part we consider chaotic systems in which the approximation is given by Gutzwiller's periodic orbit theory. The original formulation in terms of the spectral density is not necessarily the most convenient form for calculating semiclassical energies and we present a different method that uses the spectral staircase. Another efficient technique involves the spectral determinant that can be semiclassically expressed in terms of combinations of periodic orbits, so-called pseudo-orbits. We examine the convergence properties of this sum and reproduce them by a statistical model. Berry and Keating derived a resummation of the pseudo-orbit sum and expressed it in terms of a finite number of orbits. This approximation is tested in detail by checking the amplitude as well as the zeros of the determinant. It requires to carry out a regularization of the determinant so that it can be accurately determined from a finite number of energies. We further present a method by which, in billiard systems, particular contributions in semiclassical approximations can be isolated and studied separately. This is achieved by choosing parameter-dependent mixed boundary conditions. Finally, we present a method for deriving periodic-orbit contributions in three-dimensional billiard systems that yields a simple algorithm for determining the stability matrix and the Maslov index of the orbits.

The second part deals with applications of semiclassical approximations in chaotic systems in connection with statistics of energy levels. There is much evidence that the statistical distributions of the energy levels can be described by random matrix theory. By using the trace formula we show that this property has to be reflected by properties of the periodic orbits. It leads to the prediction of generalized action correlations that can be observed numerically. We further semiclassically calculate deviations from random matrix results in the stadium billiard whose origin is the family of bouncing ball orbits and which have been observed in a microwave experiment. We further discuss the sensitivity of semiclassical approximations for the spectral form factor on the definition of the averaging procedure.

Most two-dimensional conservative systems are not chaotic but have a mixed phase space dynamics that can show regular as well as chaotic behaviour. These systems are much less accessible to a semiclassical approximation than either chaotic or integrable systems since the periodic orbits in these systems form clusters and bifurcate when a parameter of the system is varied. A semiclassical treatment requires a collective treatment of these orbits. We derive uniform approximations for all generic cases of orbit bifurcations that occur in two-dimensional systems. We consider also an example of an integrable system in which bifurcations occur and discuss how the uniform approximations have to be modified when the system is perturbed.

Another class of systems in which semiclassical approximations have to be modified are systems in which diffraction occurs, for example billiard systems with corners. In these systems so-called diffractive orbits that run into the corners yield additional semiclassical

contributions. We derive a uniform approximation for diffractive orbits that run into one corner. This approximation avoids the divergences of previous treatments by Keller's geometrical theory of diffraction.

In the last part we apply semiclassical methods to a problem in nuclear physics, the well-known asymmetric mass distribution of the fission fragments that arise in the fission of many actinide nuclei. This asymmetric mass distributions can be reproduced, for example, in shell correction calculations with realistic shell-model potentials. We show that there is a simple semiclassical explanation for this asymmetry. It can be related to the constancy of the actions of the shortest periodic orbits.

We note that references of the form [Px] where x is a number refer to the publications that are included in this collection.

1 Introduction

Semiclassical methods are essential tools for the investigation of highly excited quantum systems. They describe the correct analytical behaviour of wave functions, energy levels, scattering resonances, etc. in the short-wavelength limit where $\hbar$ is small in comparison to relevant action functions of the corresponding classical system. Being expressed in terms of classical quantities they are a natural mean for studying how characteristic properties of a classical system are reflected in the corresponding quantum system. This is one of the central questions in quantum chaology, the study of quantum properties of chaotic or, more general, non-integrable systems. Conversely, semiclassical approximations often allow a simple understanding of the nature of quantum fluctuations that are observed in experiments or in numerical calculations by relating them to properties of classical trajectories. They have led to physical insight into a variety of quantum phenomena in different areas as e. g. atomic, molecular, nuclear or cluster physics.

Semiclassical methods are very powerful in one-dimensional systems where they can be applied, in form of the WKB-approximation, to accurately calculate energies and wave functions of highly excited states that would be difficult to determine by directly solving the Schrödinger equation (see e. g. the review [1]). These methods can be extended to higher-dimensional systems in cases in which the motion is integrable (or near-integrable). There they take the form of the EBK-conditions. For general higher-dimensional systems, however, semiclassical approximations have a different characteristic. For chaotic systems Gutzwiller obtained an approximation for energy levels that is usually expressed in terms of the so-called trace formula for the level density [2, 3, 4]

$$\begin{aligned} d(E) &= \sum_n \delta(E - E_n) \\ &\approx \bar{d}(E) + \frac{1}{\pi\hbar} \sum_\gamma \frac{T_\gamma(E)}{r_\gamma \sqrt{|\det(M_\gamma - 1)|}} \cos\left(\frac{S_\gamma(E)}{\hbar} - \frac{\pi}{2}\nu_\gamma\right) . \end{aligned} \tag{1}$$

Here the energies E_n are the solutions of the stationary Schrödinger equation. The approximation for the level density involves the smooth function $\bar{d}(E)$ describing the average level density which in leading semiclassical order is given by the Thomas-Fermi approximation for $d(E)$. The sum over γ runs over all periodic orbits of the classical system, including repetitions, and it involves classical properties of these orbits: the period T_γ, action S_γ, stability matrix M_γ, Maslov index ν_γ, and repetition number r_γ.

It is implicitly assumed in the derivation of the trace formula (1) that the classical motion is chaotic. This is because the semiclassical contributions of the periodic orbits are derived by assuming that they are isolated. This is strictly valid only if they are unstable. In the vicinity of stable periodic orbits there are always other periodic orbits which are related to the stable orbit and its repetitions through bifurcations as the energy (or a parameter) of the system is changed, a point to be discussed in more detail in the following.

In comparison to EBK-quantization conditions the semiclassical condition (1) for the energy levels is more indirect. Whereas the EBK-conditions require the solution of a system of coupled equations, the quantized levels in (1) arise as peaks through the constructive interference of oscillatory terms that are determined by the periodic orbits. These orbits are in general not known analytically but have to be determined numerically. Moreover, the number of these orbits increases exponentially with their period. However, the

structure underlying (1) is more general than that of the EBK-conditions and it allows generalizations also to larger classes of systems. It can be shown in general, that the leading order contributions to the level density are determined by the periodic orbits of the classical system. This follows from the fact that the level density can be semiclassically expressed in terms of oscillatory integrals with stationary points that correspond to periodic orbits. Depending on whether the classical motion is chaotic, integrable or mixed these orbits are isolated, appear in families or form more complicated clusters. For integrable systems the corresponding trace formulas have been derived in [5, 6]. More general symmetries have been treated in [7, 8].

Properties of the trace formula (1) have been examined under various aspects, one of the early motivations being to find a method for the determination of high-lying energies that is applicable to chaotic systems. The main obstacle for this is the exponential proliferation of the number of periodic orbits. As a consequence of this proliferation, the sum over periodic orbits in (1) is divergent for real values of the energy. In order to apply the trace formula in a controlled way it has to be brought into a convergent form, as can be done, for example, by an analytical folding of the formula with appropriate smoothing functions [9, 10]. But even with an trace formula that involves only absolutely convergent sums the determination of higher lying energies requires an exponentially increasing numerical effort. For that reason there has been a large effort to understand in detail the analytical and general properties of the trace formula in order to find more efficient quantization conditions. For this purpose different approaches have been applied, involving the study of motion on Riemann surfaces with constant negative curvature for which the trace formula is an exact relation (see e. g. [11]), using analogies to trace formulas for the Riemann zeta function (see e. g. [12]), applying the scattering approach to the quantization of billiard systems [13, 14, 15], the Fredholm theory for integral equations in billiard problems [16, 17, 18, 19], or the cumulant expansion for scattering problems [20]. Very efficient have been approaches in which the quantum levels are determined by the zeros of a function, for example involving the spectral staircase [P1], or the spectral determinant [21] which has been treated by curvature expansions [22, 23, 24], as Dirichlet series [25] or has been resummed and expressed in terms of a finite number of periodic orbits [26, 27]. These methods have led to a clear reduction of the numerical effort that is required for the semiclassical determination of energy levels.

Despite this progress there remains the basic problem that the numerical effort for the calculation of higher-lying energies increases exponentially. There is a different semiclassical method that avoids this problem. This is Bogomolny's transfer operator approach [17]. It involves the evaluation of determinants of matrices whose elements are expressed in terms of classical trajectories. However, also this method does not necessarily require less numerical effort than a direct solution of the Schrödinger equation, and when it is used for analyzing semiclassical spectra, it reduces to the Gutzwiller trace formula.

Since the trace formula does not facilitate the determination of high-lying energy levels its significance lies to a large extend in theoretical applications for analyzing fluctuations in the spectra of chaotic systems. It is one of the few analytical instruments that is available for this purpose. One of the central findings in quantum chaology has been the observation that the statistical distributions of energy levels of chaotic systems have universal properties that agree with those of the eigenvalues of random matrices [28, 29], whereas the levels of integrable systems show a Poissonian distribution [30]. By using the trace formula this agreement could be explained in certain regimes [31] that have

been recently extended [32]. Furthermore, deviations from the universal behaviour for long-range correlations can be explained in terms of the short periodic orbits in a system [31, 33].

Another area where periodic-orbit approximations are powerful are applications that involve only a few of the shortest periodic orbits. This is the case in systems in which the contributions of long periodic orbits are suppressed, for example by temperature effects in mesoscopic systems or by pairing correlation corrections to mean-field approximations in interacting multi-fermion systems. Examples for applications in this area are the semiclassical description of ground state deformations of atomic nuclei [34] or metallic clusters [35], the prediction of supershells in metallic clusters [4, 36], conductivity oscillations in antidot lattices [37, 38] or oscillations of the magnetic susceptibility in ballistic mesoscopic systems [39]. For an overview see [40].

Due to the central role of the trace formula for studying the correspondence between classical and quantum properties of a system, one tries to generalize it so that it can be applied to larger classes of systems. One such class consists of systems in which diffractive effects are important, for example billiard systems with corners or concave boundaries. Diffractive effects play also a role in systems like the resonant tunneling diode (see the cusp-orbits in [41]) or for core-effects in non-hydrogenic Rydberg atoms [42]. In these systems diffraction leads to additional contributions in the trace formula in form of diffractive or creeping orbits. The semiclassical contributions of these orbits have been derived within the framework of Keller's geometrical theory of diffraction in [43, 44, 45]. This theory is, however, not sufficient for a complete description of the diffractive contributions and it has to be modified by uniform approximations near so-called optical boundaries where it is divergent (see [46, 47],[P9]).

The largest class of conservative systems are mixed systems in which the motion can be regular as well as chaotic depending on the initial conditions. With respect to periodic orbits a characteristic difference between mixed, integrable and chaotic systems is the presence of stable periodic orbits in mixed systems, whereas in chaotic systems the orbits are typically unstable and in integrable systems marginally stable. Stable periodic orbits have the property that they bifurcate if the energy or an external parameter is changed, i. e. they coalesce with other periodic orbits. For a semiclassical approximation this has the consequence that in the vicinity of a bifurcation the participating periodic orbits cannot be treated isolated. Instead they give joint semiclassical contributions to the level density which have been treated by uniform approximations [48],[P10,P11,P12]. This allows to apply semiclassical approximations in cases in which mainly the contributions of the shortest periodic orbits are needed. The inclusion of long periodic orbits would require the joint treatment of large clusters of periodic orbits that are involved in several subsequent bifurcations (for two subsequent bifurcations see [49, 50, 51]).

The present work is a collection of articles that examine various aspects of semiclassical periodic orbit expansions that have been addressed above. These articles are ordered in four sections.

The first section deals with general properties and applications of the trace formula for chaotic systems. It discusses different forms of the semiclassical quantization condition and its convergence properties, and analyzes individual contributions to the trace formula. In particular, a semiclassical quantization condition is proposed in terms of the spectral staircase. The convergence properties of a representation of the spectral determinant in terms of combinations of periodic orbits is examined and explained by a statistical

model. A detailed test of the resummation formula of Berry and Keating for the spectral determinant is carried out that checks not only the positions of the zeros but also the amplitude of the determinant. Furthermore, a method is developed for isolating particular contributions to trace formulas allowing in this way a much more detailed analysis of semiclassical contributions, and a method for calculating semiclassical contributions in three-dimensional billiard systems is developed.

The second section contains applications of semiclassical trace formulas in connection with spectral statistics. The periodic orbits of a chaotic system must satisfy certain conditions in order that the energy levels of the quantum system show universal statistical distributions. This follows by using the trace formula, and it leads to the prediction of generalized correlations between the actions of periodic orbits that are also observed numerically. Furthermore, the influence of the bouncing ball orbits on the energy spectrum in the stadium billiard is investigated semiclassically and used for analyzing the outcome of a microwave experiment. A further topic in this section are subtle properties of semiclassical approximations for the spectral form factor.

The third section treats extensions of semiclassical periodic orbits approximations to systems with diffraction and mixed systems. For billiard systems with corners a uniform approximation is derived for diffractive orbits that run once into a corner. Such uniform approximations are necessary, for example, if one aims at a semiclassical understanding of the spectral properties of pseudo-integrable systems. For the semiclassical treatment of mixed systems uniform approximations are derived for all generic bifurcations that occur in two-dimensional conservative systems or one-dimensional area-preserving maps. Furthermore, periodic orbit approximations are derived for an integrable system in which bifurcations occur, the ellipse billiard, and for a non-integrable perturbation of it.

Finally, the fourth section contains an application of periodic orbit approximations, including a uniform approximation for a cusp bifurcation, in order to describe shell-corrections for a nuclear model. In this way a simple physical explanation is obtained for the asymmetric fission of actinide nuclei.

2 Semiclassical methods in chaotic systems

2.1 A novel rule for quantizing chaos

One of the main goals in the study of quantum systems with a chaotic classical limit has been to find effective semiclassical techniques for calculating quantum energies of bounded systems, or quasi-energies of time-periodic systems. Almost all methods that have been employed for this purpose are based on Gutzwiller's periodic orbit theory [2, 3], they differ in the way in which the information about the quantum levels is extracted from the periodic orbits.

The direct application of the trace formula for the level density, with a sum over periodic orbits up to some maximal period T^*, typically gives a good approximation for the first levels. For higher-lying levels it fails since an increase of the cut-off period T^* leads to the development of larger and larger spurious oscillations which are a sign of the sum's divergence. This divergence is a consequence of the form in which the theory is formulated, namely in terms of a distribution, the level density, which itself diverges at the energies. By folding the density with a smoothing function one can derive well-defined trace formulas that contain only absolutely convergent series [9, 10].

The main question then is to find semiclassical methods which require the least number of periodic orbits for the determination of a certain number of levels. In [P1] a semiclassical quantization condition was proposed that proved to be very efficient in comparison with other methods. It is based on the spectral staircase function $N(E)$ that jumps by one at every eigenvalue of the Schrödinger equation (or by its multiplicity in case of a degenerate level). The quantization condition has the form $N_{\rm sc}(E) = n - 1/2$, $N_{\rm sc}(E)$ being the semiclassical approximation to $N(E)$, and it is equivalent to

$$\cos(\pi N_{\rm sc}(E)) = 0 \; . \tag{2}$$

Again, by a smoothing of the staircase the periodic orbit sum can be brought into an absolutely convergent form but applications show that this is often not necessary.

There are several explanations for the fact that the condition (2) works often better than other methods in numerical applications. One expects in general that quantization conditions in terms of the zeros of a function are more efficient than those in terms of the peaks of a function. A heuristic argument for this is the following. In order to resolve two adjacent maxima of a function, one has to include in its Fourier representation at least all its Fourier components up to those which oscillate once between the maxima. For periodic orbits this implies a cut-off at the Heisenberg time $T_H = 2\pi\hbar\bar{d}(E)$, where $\bar{d}(E)$ is the mean level density. In contrast to this, two adjacent zeros of a function can already be resolved by including the Fourier components up to half this value, since an oscillating function has to perform only half an oscillation between two zeros. A second reason in favour of (2) is that for $N_{\rm sc}(E) = n-1/2$ to work well it is not necessary that the whole spectral staircase is approximated well by $N_{\rm sc}(E)$, it suffices if $N_{\rm sc}(E)$ goes through the middle of the steps. Numerical applications in [P1] show that $N_{\rm sc}(E)$ often has this property even at energies where the semiclassical curve is not able to reproduce the steps of $N(E)$. Furthermore, in contrast to other quantization conditions that are formulated in terms of the zeros of a function, like the dynamical zeta function that is discussed in the next section, equation (2) does not require the evaluation of pseudo orbits and thus needs less numerical effort.

The condition $N_{\rm sc}(E) = n - 1/2$ has also been used in analytical evaluations. Bogomolny and Keating applied it in semiclassical evaluations of spectral statistics in order to obtain a discrete quantum spectrum from a finite number of periodic orbits [32]. In this way they derived the leading order oscillatory behaviour of the two-level correlation function $R_2(x)$ for large values of x.

2.2 Crossing the entropy barrier of dynamical zeta functions

The Riemann zeta function serves often as a guide for the development of semiclassical theories in chaotic systems. There is a strong similarity between the identity that relates the non-trivial zeros of the Riemann zeta function to the prime numbers, and the Gutzwiller trace formula which relates the eigenvalues of a Hamiltonian to the classical periodic orbits [52]. This and the fact that much more is known about prime numbers than about the periodic orbits of a typical chaotic system often provides hints as how to progress with the general semiclassical theory (see e. g. [12]).

For a chaotic system the analogue of the Riemann zeta function is the dynamical zeta function [21] or, for the motion on certain Riemann surfaces with constant negative curvature, the Selberg zeta function (see e. g. [53]). The former appears in semiclassical approximations for spectral determinants, and its zeros correspond to the semiclassical energy levels. There are several reasons for the interest in this function. Firstly, as discussed above one is interested in quantization conditions in terms of the zeros of a function. Secondly, there is a powerful method for calculating the zeros of the Riemann zeta function, the Riemann-Siegel formula, that can be generalized to dynamical zeta functions [26, 27]. Thirdly, there is an exact quantum analogue to the dynamical zeta function in the case of billiard systems. This is the Fredholm determinant that is obtained from a boundary integral equation which determines the quantum energies of the billiard system [16, 17, 18, 19].

The dynamical zeta function is defined by a product over all periodic orbits of a system, the so-called Euler product, in the region where this product converges. It is known that this region does not contain the locations where its zeros are, respectively the zeros of its analytical continuation [21]. Alternatively, by expanding the product, the zeta function can be expressed by a series over combinations of periodic orbits, so-called pseudo-orbits. The sum over pseudo-orbits in general has better convergence properties than the product over periodic orbits, and it forms the basis for resummation techniques like the Riemann-Siegel like formulas [27, 54], for direct quantizations [25], or for cycle expansions [22, 23, 24]. The article [P 2] examines in detail the convergence properties of the pseudo-orbit sum, in particular whether it is convergent on the real energy axis where the eigenvalues of the Schrödinger equation are located.

The analysis of the convergence properties of the pseudo-orbit sum rests on the property of the pseudo-orbit sum that it has, for scaling systems, the form of a generalized Dirichlet series. For billiard systems or the geodesic motion on Riemann surfaces of constant negative curvature that are considered in [P 2] the argument of the Dirichlet series is the wave number $k = \sqrt{2mE}/\hbar$. The convergence properties of such series are well known. A Dirichlet series converges absolutely in a half-plane $\mathbf{Im}\, k > \sigma_a$ and conditionally in a half-plane $\mathbf{Im}\, k > \sigma_c$ with $\sigma_c \leq \sigma_a$. The abscissa of absolute and conditional convergence, σ_a and σ_c, can be expressed as the limit of a function of the amplitudes and exponents in the Dirichlet series, and this provides a means to determine them.

It can be shown that σ_a is given by $\sigma_a = \tau - \bar{\lambda}/2$ where τ is the topological entropy that describes the exponential proliferation of the number of periodic orbits, and $\bar{\lambda}$ is an averaged Lyapunov exponent. In bounded systems where $\tau = \bar{\lambda}$ is expected to hold, this implies that the series is not absolutely convergence for real values of k where the quantum energies are located. The effect that the non-vanishing topological entropy prevents an absolute convergence of the pseudo-orbit sum for real k is denoted by the entropy barrier. The abscissa of conditional convergence σ_c depends further on the statistical properties of the Maslov indices and of the degeneracies of the periodic orbits. They lead to a novel parameter that we denoted the third entropy δ in [P2] which determines the difference between the abscissa of absolute and conditional convergence $\delta = \sigma_a - \sigma_c$. The size of δ decides whether the Dirichlet series is convergent for real k.

An estimate for δ is obtained in [P2] by a simple statistical model for the amplitudes in the Dirichlet series. It is assumed that they are randomly distributed according to some probability density with zero mean. Under this assumption and by applying the central limit theorem one obtains an estimate for δ in the form $\delta = (\tau - \alpha)/2$, where α describes a possible exponential increase of the multiplicities of lengths of pseudo orbits. Such an exponential increase for the multiplicities of pseudo orbits can already occur if the periodic orbits have a constant mean multiplicity. The statistical model thus predicts that in a typical bounded system with $\tau = \bar{\lambda}$ one can have at most $\sigma_c = 0$, meaning that the limit of the region of conditional convergence is exactly the real k-axis, but this is only possible if $\alpha = 0$, as for example in a generic chaotic system without symmetries and without time-reversal symmetry.

The predictions of the statistical model were tested on four hyperbolic systems in [P2]. For three of them the numerical results were in good agreement with the model, only for Artin's billiard there were distinct deviations. This system is of a rather special type, it belongs to the class of arithmetic systems, and it shows correlations between the amplitudes in the Dirichlet series so that the conditions of the statistical model are not fulfilled.

2.3 Calculation of spectral determinants

The dynamical zeta function is a semiclassical approximation to a spectral determinant $\Delta(E)$ that has zeros at the eigenvalues of the Hamiltonian. A fundamental property of this spectral determinant is that it satisfies a functional equation. This functional equation follows from the self-adjointness of the Hamilton operator, and it can be used in order to extend semiclassical periodic orbit expansions to regions where the orbit sums are divergent. The dynamical zeta function, i. e. the semiclassical approximation to $\Delta(E)$, satisfies the functional equation only in leading semiclassical order, but by imposing it as an exact equality, Berry and Keating derived a resummation of the pseudo-orbit series for the dynamical zeta function by a contour integral method [27]. For billiard systems this resummed series has the following form

$$\xi(k) = \zeta(k)\mathrm{e}^{-i\pi\bar{N}(k)} \simeq \xi_0(k,l) + \sum_{m=3}^{\infty} \xi_m(k,l) \; . \tag{3}$$

Here $\zeta(k)$ is the zeta function as a function of the wavenumber k, and $\bar{N}(k)$ is the mean spectral staircase. The functions $\xi_m(k,l)$ are all given by sums over pseudo-orbits which

are smoothly cut-off at half the Heisenberg time T_H, and l is a free parameter of the representation. The m-series is an asymptotic series whose first terms converge very rapidly if the parameter l is chosen appropriately, so that only few terms have to be taken into account. By far the most important term is $\xi_0(k,l)$.

The cut-off of the pseudo-orbit sums in (3) is not an approximation. The contributions of the long orbits are still present, they are resummed in terms of the short orbits. This is reflected by the fact that $\xi_0(k,l)$ is roughly twice the real part of the original Dirichlet series, cut-off at half the Heisenberg time. This shows that (3) is not simply obtained by a cut-off of the original series.

The object of the article [P3] is a detailed investigation of the Riemann-Siegel-type formula (3) on the example of a strongly chaotic system, the hyperbola billiard (see [55]). This system is well suited for this purpose, since a large number of periodic orbits is known completely up to some maximal length of the trajectories $l_{\max}$, altogether more than 100 000 orbits. Furthermore, the unusual form of the asymptotic series for the mean spectral staircase of this unbounded billiard system allows the investigation of the correction terms $\xi_m(k,l)$, $m \geq 3$, in (3). In bounded billiard systems these terms vanish.

A detailed test of the orbit resummation underlying the formula (3) has to compare not only the position of the zeros of the function ξ with the quantum energies, but also the amplitude of ξ with that of the spectral determinant $\Delta(E)$, since the resummation process shows up most clearly in the factor 2 by which the pseudo-orbit contributions to ξ differ from those to the original Dirichlet series. The main obstacle in doing this lies in the quantum calculation, since the representation of $\Delta(E)$ by a product over energy levels converges very slowly. This problem was circumvented in [P3] by defining a new determinant $\Delta_X(E)$ that is completely specified by all energies $E_n \leq X$, and by deriving a semiclassical approximation for this new quantity. For energies $E < X$ it is expressed again in terms of the dynamical zeta function.

The comparison of the quantum result with the semiclassical one shows a remarkable good agreement for the amplitudes as well as for the position of the zeros. This provides a confirmation of the resummation ideas underlying equation (3). The error in the semiclassical energies was approximately three percent of the mean spacing between the levels. Alternative evaluations of the zeta function by the original Dirichlet series and by the Euler product give also good approximations to the spectral determinant, however not quite as good as the resummed series. Both these semiclassical curves show fluctuations about the quantum result. For the Euler product it is a sign of its divergence, for the Dirichlet series the results are not conclusive, since it is not clear whether the amplitude of the fluctuations increases with an increasing number of orbits. The fluctuations could also be explained by the sharp cut-off of the sum over pseudo-orbits.

2.4 Billiards with mixed boundary conditions

Billiard systems have been introduced in the study of dynamical systems, since they show the typical qualitative features of general Hamiltonian systems, while they are much more easy to treat formally. The quantum analogues of classical billiards have the same advantages. There are powerful techniques like the boundary integral method for solving the Schrödinger equation [56, 57, 58], and for a semiclassical analysis one can often determine a large number of periodic orbits by simple Newtonian methods (see [59]).

The quantization of a given classical billiard system is not unique. There is the freedom

to choose the boundary conditions, restricted to the condition that they lead to a self-adjoint Hamilton operator. In general, one can require that a linear combination of the wave function and its normal derivative vanishes on the boundary $\partial\mathcal{B}$

$$\kappa(\vec{r})\,\psi(\vec{r}) + \partial_{\hat{n}}\,\psi(\vec{r}) = 0\ , \qquad \vec{r} \in \partial\mathcal{B}\ . \tag{4}$$

The large freedom of choosing the (positive) function $\kappa(\vec{r})$ offers the possibility to study semiclassical approximations in a much more refined way than is possible when restricting to one realization of a quantum billiard. This was the motivation for studying mixed boundary conditions in [P4]. Before we address this point in more detail we discuss some of the results of [P4].

In the first part of the article the semiclassical theory for billiards with mixed boundary conditions is developed for piecewise constant functions $\kappa(\vec{r})$. This includes the derivation of the smooth and the oscillatory parts of the spectral density. Both are obtained by several different methods, applicable either to integrable, to chaotic or to general systems. The smooth part of the level density was obtained, for example, by modifications of the methods of Stewartson and Waechter [60] and of Balian and Bloch [61], and the oscillatory part was derived by using the scattering approach to the semiclassical quantization of billiard systems [13, 14, 15], and by the KKR-method for the Sinai billiard [62]. For the smooth part one finds that the leading area term is independent of the boundary conditions, as expected, whereas the higher-order corrections depend on the function $\kappa(\vec{r})$. Explicit expressions are given for the length term, the curvature term and a 90° corner term. The oscillatory contributions in the trace formula contain, in comparison to Dirichlet boundary conditions, an additional phase of the form

$$2\sum_{i=1}^{n} \arctan\left(\frac{k}{\kappa(\vec{r}_i)}\cos\theta_i\right)\ , \tag{5}$$

where the sum runs over the n points of reflection of a periodic orbit and $k\cos\theta_i$ is the component of the momentum normal to the boundary at the i-th reflection point. Expression (5) interpolates between the two values 0 and $n\pi$ for the Dirichlet and Neumann cases, respectively.

The important point in (5) is that the phase factor depends only on the value of $\kappa(\vec{r})$ at the points of reflection. If $\kappa(\vec{r})$ is changed on a part of the boundary then only those periodic orbits are effected that are reflected at least once in this region. This property allows to isolate particular periodic-orbit contributions to the semiclassical trace formula, for example by taking the difference between two spectral densities corresponding to two functions $\kappa(\vec{r})$ that differ only on a part of the boundary.

In [P4] this method was applied to eliminate the non-generic "bouncing ball"-contributions from the trace formula for two-dimensional Sinai billiards. This was achieved by applying mixed boundary conditions with a constant value of κ on the disk of the Sinai billiard and varying the value of κ. By taking the derivative of the spectral density with respect to κ one is left with a trace formula that contains only the generic contributions of all unstable periodic orbits. Taking the derivative of the spectral density has the additional advantage, that also non-generic diffractive contributions of orbits that are tangent to the disk are removed (at least in leading order). The elimination of non-generic contributions is even more important in higher dimensions where bouncing ball families contribute in a higher order of $1/\hbar$, and the number of different bouncing ball families increases

strongly. The examination of the semiclassical accuracy in the three-dimensional Sinai billiard in [63, 64] would not have been possible without removing bouncing ball and tangent contributions.

There are various possibilities for further applications of mixed boundary conditions that extract partial contributions to trace formulas. The method can be convenient if one is interested in semiclassical contributions from certain regions in coordinate space, if one examines semiclassical contributions to scarred wave functions, or if one wants to study correlations between actions of periodic orbits in more detail (see section 3.1). So far only few of these possibilities have been exploited.

There is a further motivation for studying mixed boundary conditions. A central characteristic of quantum systems with a chaotic classical limit are the universal properties of the level statistics. This universality is not restricted to correlations within the spectra of single systems, it can also be observed in the dependence of a system on an external parameter (see e. g. [65, 66, 67]). For example, the form in which the correlations between two spectra for different parameter values decay as the parameter difference is increased is characteristic for the type of the corresponding classical motion and the symmetries of the systems. Mixed boundary conditions allow to define a parameter dependence that effects only the quantum system and not its classical limit. This implies that semiclassical approximations involve the same set of periodic orbits for all parameter values, and this strongly simplifies a semiclassical study. In this respect systems with mixed boundary conditions play the same role for the study of the parameter dependence of a system as scaling systems do for the energy dependence. Billiard systems with a flux line have similar properties. In contrast to billiards with mixed boundary conditions, however, they are systems without time-reversal symmetry or with slightly broken time-reversal symmetry, and the flux line leads to additional diffractive contributions to the trace formula in case it goes through the billiard domain.

2.5 The trace formula for three-dimensional billiard systems

In the study of autonomous dynamical systems and their quantized versions many concepts have been developed on basis of the insight that has been gained from the study of simple model systems. These models are chosen with the point of view that they should be both simple and in some sense typical. For this reason most of the studies have been performed on two-dimensional systems, since these are the simplest conservative systems in which chaotic motion can take place, and they are numerically much less demanding than higher-dimensional systems. Nevertheless, two-dimensional systems have rather special properties in comparison to higher-dimensional ones. In two dimensions invariant tori separate different regions on the energy surface in phase space whereas in higher dimensions Arnold diffusion takes place. Also the periodic orbits in two-dimensional systems don't have the full general form, since loxodromic orbits occur only if the dimension is larger than two. In order to study more realistic models one has to go to three dimensions, and, as in two dimensions, convenient models are again billiard systems.

The article [P5] is a semiclassical study of three-dimensional billiard systems. It contains a derivation of semiclassical contributions of isolated periodic orbits, and of families of periodic orbits in axially symmetric billiard systems. It gives for the first time a practical method for calculating the stability matrix and the Maslov index of a periodic orbit in three dimensions in terms of partial stability matrices for single reflections, the mo-

tion between reflections, and rotations of the local coordinate system. We discuss in the following the relation of this work to previous work.

Semiclassical approximations in three-dimensional billiard systems have been derived before by Balian and Bloch [61, 68, 4]. They performed a systematic investigation of semiclassical contributions of periodic orbits for various geometrical configurations. Their results are expressed in terms of the $2n \times 2n$-matrix of second derivatives of the orbit length with respect to a change of the n points of reflections. This matrix determines both, the stability and the Maslov index of an orbit. Although Balian and Bloch completely specify the semiclassical approximation, their formalism is not convenient for practical calculations, since it requires a large effort to determine the $2n \times 2n$-matrix for every periodic orbit. Instead it is preferable to express the result in the usual Gutzwiller form, i. e. in terms of the 4×4-stability matrix M, and to give an explicit method how to calculate M and the Maslov index.

For two-dimensional systems the periodic orbit contributions have been derived in the Gutzwiller form. Harayama and Shudo obtained them starting from a boundary integral equation[18]. The derivation involved the reduction of n-dimensional matrices where again n is the number of reflections of an orbit. (That the index in their trace formula is identical to the usual Maslov index was shown in [69].) For the two-dimensional problem of the scattering on m disks Wirzba derived the Gutzwiller form directly from the Balian/Bloch-result [20]. In his case the orbits did not have conjugate points and the index in the trace formula was twice the number of reflections.

Both methods require the reduction of large matrices. In higher dimensions this would be a very elaborate task. In [P5] we applied a different method which doesn't involve large matrices, and we derived the Gutzwiller form from an iterative method that follows the trajectory from reflection point to reflection point. This procedure automatically yields a method for determining the stability matrix and the index of an orbit, and it is straightforward to show that this index is identical to the Maslov index. The same method has been used in [P9] for deriving the semiclassical contributions of diffractive orbits in two dimensions.

3 Semiclassical methods and spectral statistics

3.1 Correlations in the actions of periodic orbits

There is a great amount of numerical evidence that the energy levels of a generic chaotic system, when unfolded to a mean spacing of one, have the same statistical distribution as the eigenvalues of random matrices, chosen from appropriate ensembles (see e. g. [29]). Recent analytical work has made a large step in explaining this agreement [70, 32, 31]. It is now possible to obtain from semiclassical considerations the full leading-order random matrix result, i. e. the leading oscillatory and smooth behaviour, for the two-level correlation function $R_2(x)$ as $x \to \infty$ [32]. Despite this progress a complete derivation of the full level distribution is still lacking. This would require a much finer knowledge about the statistical properties of periodic orbits, including the distributions of their actions, periods, stabilities and Maslov indices, than is presently available.

The article [P6] followed an opposite strategy. It assumed that we know that the spectral statistics of a chaotic system follow random matrix theory in the semiclassical limit. Based on this assumption it examined what predictions the semiclassical theory makes about the statistical properties of periodic orbits. The result is an explicit, universal expression for a classical distribution function for the periodic orbits which has the form of a weighted action correlation function. For systems as e. g. the geodesic motion on some compact Riemannian surfaces with constant negative curvature, this distribution function is a pure action correlation, and it predicts a tendency towards action repulsion, i. e. a lowered probability for two periodic orbits with approximately the same period to have a small action difference. In general, the correlation function includes weight factors depending on the stabilities and Maslov indices of the orbits.

The remarkable point about this result is that these classical correlations have been previously unnoticed and they were obtained purely from observed quantum properties of the system, and by applying a semiclassical approximation. Numerical tests on chaotic systems in [P6] showed that these action correlations are indeed present. Further evidence is provided by the Riemann zeta function for which the action correlation function describes the correlations between pairs of prime numbers. It is shown that the results of [P6] are consistent with the Hardy-Littlewood conjecture on the pairwise distribution of primes.

It is still an open question, how these classical correlations can be explained from purely classical considerations. Detailed numerical examinations in [71] indicate that the correlations occur mainly between orbits that share some common properties, e. g. have the same number of bounces in a billiard system, or, if a classification of the periodic orbits by a symbolic code is possible, share some common features in the code words. Similar results can be obtained by considering the response of a system to a small perturbation. One finds that the action correlations occur mainly between periodic orbits that are similarly affected by a perturbation [72].

If classical correlations between periodic orbits could indeed be derived from classical arguments this would strongly enlarge the scope of semiclassical approximations. It would allow also direct evaluations of off-diagonal contributions in sums over periodic orbits.

3.2 Non-universal spectral statistics in the quantized stadium billiard

Billiard systems are not merely convenient theoretical models, they can also be realized in experiments [73, 74, 75, 76, 77]. These experiments are macroscopic and use the equivalence of the Schrödinger equation for billiard systems with the Helmholtz equation for electromagnetic waves in order to model quantum billiards by microwave cavities. If the cavities are chosen as flat quasi two-dimensional systems then also the boundary conditions for the lowest states agree with Dirichlet boundary conditions and one can obtain by a measurement the spectrum of two-dimensional quantum billiards up to some maximal energy that is determined by the height of the cavity. The experimental group of Prof. Achim Richter in Darmstadt performed measurements on one of the standard examples of a chaotic system, a desymmetrized stadium billiard [76]. When the measured spectrum was analyzed and the spectral correlations were determined in form of the spectral rigidity the outcome was distinctly different from the characteristics that are expected for a generic chaotic system.

The spectral rigidity $\Delta_3(L)$ is a two-level statistic that measures how well the spectral staircase of a system can be approximated by a straight line. If it is calculated from a finite portion of the spectrum of a chaotic system, then one expects to reproduce the results of random matrix theory (RMT), if L is not too large. For long range-correlations (large L) $\Delta_3(L)$ typically shows a smaller increase than the logarithmic form of the RMT curve and finally saturates at a constant value. This saturation is predicted by the semiclassical theory of Berry [31] and is related to the shortest periodic orbits of the system.

In contrast to this the $\Delta_3(L)$-statistic of the stadium billiard shows a strong increase beyond the RMT curve. This deviation was the original motivation for the article [P7]. It was soon clear that the cause for the deviations was the non-generic family of bouncing ball orbits in the stadium billiard. In [P7] these deviations were described quantitatively. The semiclassical contributions of bouncing ball trajectories to the spectral density were derived, and with this result the influence of these orbits on the spectral rigidity was calculated. The final result states that the bouncing ball orbits yield an additional contribution to the spectral rigidity that has to be added to the semiclassical expression for the rigidity of a generic chaotic system. The results of [P7] were used for the analysis of the data in [76].

From another point of view, the existence of additional terms in the trace formula that are of higher power in $1/\hbar$ than the contributions of isolated orbits were the reason for the additive contribution to $\Delta_3(L)$. Similar results were obtained recently in [78] for bifurcating periodic orbits that likewise yield an additive contribution to the number variance, or, equivalently, to the spectral rigidity. Here the difference in the power of $1/\hbar$ between isolated periodic orbit and bifurcating periodic orbit contributions is given by the singularity index of the bifurcation.

In [P7] further non-generic semiclassical contributions in the stadium billiard were derived, that are due to the borders of the family of bouncing ball orbits, and to edge orbits, that run along a part of the boundary. The full trace formula was applied for a Fourier analysis of the measured spectrum of the microwave cavity. Overall there was a good agreement between semiclassics and experiment, which confirms that microwave cavities are an appropriate means for carrying out experiments in quantum chaos.

3.3 An exponentially increasing semiclassical spectral form factor

The simplest statistical distributions of energy levels which show universal behaviour are two-level statistics. They can be measured by different distribution functions like the two-level correlation function, the two-level form factor, or the spectral rigidity. These statistical measures emphasize different aspects of the fluctuations in the spectrum, but they are all equivalent.

For semiclassical investigations the most easily accessible measure is the spectral form factor $K(\tau)$, the Fourier transform of the two-level correlation function. Its argument τ is directly related to the period T of the orbits that contribute semiclassically by $\tau = T/T_H$, where T_H is the Heisenberg time, and all non-universal features are restricted to small τ-regimes, near $\tau = 0$ and $\tau = 1$.

The semiclassical theory for the form factor was developed by Berry [31] and extended by Bogomolny and Keating [32]. By using a sum rule for the periodic orbits [79] the form factor can be described correctly in the ranges $\tau \ll 1$ and $\tau \approx 1$. Up to now these are the only regimes which are fully accessible to a semiclassical analysis. For $\tau \gg 1$ a different reasoning is applied. It can be shown that the exact form factor approximates the value 1 for large values of τ if the spectrum doesn't have systematic degeneracies. Based on the assumption that the semiclassical form factor shows the same behaviour, this leads to a semiclassical sum rule for the periodic orbits, equivalent to $K_{sc}(\tau) \approx 1$ for $\tau \gg 1$.

In the article [P8] we show that the semiclassical form factor does not necessarily obey this semiclassical sum rule, in fact it can drastically deviate from it. We consider in [P8] systems for which the Maslov index for all periodic orbits is equal to zero. Examples are defocusing billiard systems with Neumann boundary conditions or the geodesic motion on certain Riemann surfaces with constant negative curvature. For these systems the correspondence between the form factor and its semiclassical approximation depends very sensitively on the form of the averaging procedure that is chosen for evaluating $K(\tau)$. A natural choice would be a Gaussian averaging, however, as is shown in [P8], this leads to an exponentially increasing semiclassical form factor for sufficiently large τ.

The exponential increase of $K_{\rm sc}(\tau)$ is shown in [P8] by numerical as well as analytical calculations, where the analytical results are obtained by approximating the sum over periodic orbits by an integral. This is only possible if all Maslov indices vanish. A better understanding of this unexpected behaviour of $K_{\rm sc}(\tau)$ is obtained by considering a system for which Gutzwiller's trace formula for the spectral density is exact and corresponds to the Selberg trace formula, the example in [P8] is an asymmetric hyperbolic octagon. For this system the exponential increase can be proven rigorously. The only semiclassical approximation that is made for $K_{\rm sc}(\tau)$ for this system consists in linearizing the energy dependence of the action when taking the Fourier transform of the two-level correlation function. It can be shown that this leads to an exact replacement of the form factor for the energy spectrum by the form factor for the momentum spectrum. The hyperbolic octagon has, however, an imaginary momentum eigenvalue that correspond to the zero-mode energy $E = 0$, and this is the origin of the exponential increase. The imaginary momentum eigenvalue is also the reason why Berry's semiclassical sum rule is not valid for the momentum spectrum.

There are several remedies to the exponentially increasing semiclassical form factor. One can subtract the mean exponential behaviour of the periodic orbit sum, one can use

a different averaging that cuts off the zero-mode contribution, e. g. a window averaging, or one can push the start of the exponential increase to larger values of τ by going higher up in the spectrum. We note that the exponential $K_{\rm sc}(\tau)$ does not interfere with the action correlations in section 3.1 as discussed in detail in [80].

4 Semiclassical methods in diffractive and mixed systems

4.1 Uniform approximation for diffractive contributions in trace formulas

By varying the boundary of a billiard system one can generate a large variety of dynamical systems. Besides integrable, mixed and chaotic dynamics, billiard systems can exhibit also dynamical behaviour that is not found in smooth Hamiltonian systems. An example is the class of pseudo-integrable billiards. These systems have as many independent constants of motion as degrees of freedom, and the motion in the $2n$-dimensional phase space is restricted to an n-dimensional surface. Due to singularities in the boundary, however, this surface does not have the topology of a torus as in the case of an integrable system, but it is of higher genus (see the discussion in [81] and references therein). For pseudo-integrable systems semiclassical approximations cannot be purely expressed in terms of the periodic orbits. For some of these systems it is not even known if periodic orbits exist. Instead there are additional semiclassical contributions which are related to the diffraction of quantum wave functions on the singularities of the boundary.

Pseudointegrable systems are only one example of billiard systems in which diffractive effects influence the spectral properties. More general, if part of the billiard boundary is concave or if it has corners with angles different from π/n then there are additional contributions in semiclassical trace formulas which are not related to periodic orbits. They can be expressed in terms of creeping orbits that creep along a part of the convex boundary, or diffractive orbits that run into a corner from where they can depart in arbitrary directions.

A theory for the treatment of these additional contributions was already developed in the fifties for electromagnetic waves by Keller (see e. g. [82]). Keller's geometrical theory of diffraction (GTD) can be considered as an extension of geometrical optics that includes the treatment of diffractive effects by additional non-classical trajectories. These additional contributions appear also in the context of semiclassical trace formulas, and they were derived within the framework of Keller's theory in [43, 44, 45].

Let us consider now a billiard system with corners. One might ask whether a trace formula which includes the contributions of diffractive orbits, derived from GTD, is sufficient for describing, for example, spectral properties of pseudo-integrable systems. This is in general not the case, since Keller's theory has only a limited range of validity. It diverges at optical boundaries which, in the language of geometrical optics, separate illuminated and shadowed regions. The regions where Keller's theory is not valid shrink with increasing energy, but this is counterbalanced by the fact that longer orbits, that become relevant for a larger energy, approach optical boundaries on average closer than shorter orbits. There is a very similar effect in mixed systems for orbits near bifurcations (see section 4.2). In mixed systems short orbits near bifurcations can be considered isolated if the energy is sufficiently high, but there are always longer orbits for which this cannot be done, independently how large the energy is.

The reason for the divergence of Keller's theory is that diffractive orbits contribute with a lower power in $\hbar$ on optical boundaries. Consequently, Keller's theory breaks down where the contributions of diffractive orbits are most important. In order to remedy this

situation, a uniform approximation for the semiclassical contributions of diffractive orbits is derived in [P9]. This uniform approximation interpolates between the two asymptotic regimes, the optical boundary and the regime where Keller's theory is valid. The derivation is based on the boundary integral method and an exact integral representation for the Green function of an infinite wedge with an arbitrary angle. The final result is valid for orbits which run once into a corner. This gives the most important diffractive contribution. The method can, in principle, also be applied to orbits with arbitrary points in corners, but the corresponding expressions become increasingly more complex and involve multiple Fresnel integrals.

Numerical applications in [P9] show that the uniform approximation is in excellent agreement with quantum results, whereas the simple geometrical theory of diffraction is in many cases inadequate. For example, the uniform approximation has also to be applied if a corner angle is close to a value π/n where n is an integer. Results of [P9] reveal a further similarity between diffractive orbits and bifurcating periodic orbits. If a corner angle is varied and goes through a value π/n then a new periodic orbit is born out of a diffractive orbit. This kind of bifurcation is correctly described by the uniform approximation.

4.2 Uniform approximations and bifurcations of periodic orbits

The form of semiclassical approximations depends on the structure of the underlying classical motion. In integrable systems the energy surface is filled by layers of tori on which the classical motion is confined. In the semiclassical limit wave functions concentrate on single tori that are selected by the EBK-quantization conditions. In chaotic systems on the other hand a typical trajectory fills the whole energy surface in phase space ergodically, and no manifolds are left invariant under the classical flow except the whole energy surface, and the set of periodic orbits. This is reflected by the quantum ergodicity [83, 84, 85, 86], i. e. the property that almost all wave functions are distributed uniformly over the energy surface in phase space in the limit of large energies. In a general system the structures in phase space are much more complicated. Regular and irregular regions coexist in phase space and are intermingled in a complex form. We discuss this structure briefly for two-dimensional conservative systems.

As an integrable system is disturbed all rational tori, i. e. tori which consist of periodic orbits, break-up immediately into an equal number of stable and unstable periodic orbits. This is a consequence of the Poincaré-Birkhoff theorem (see e. g. [87]). Around the stable orbits there are small islands of regular motion whereas the unstable orbits are contained in a small layer of chaotic motion that surrounds the islands. On a Poincaré surface of section this structure appears as a chain of islands with a layer of stochastic motion around them. According to the KAM-theorem many of the irrational tori of the unperturbed integrable system will survive a small perturbation and are only slightly deformed. These KAM-tori separate neighbouring chains of islands. The original torus-structure of the integrable system is thus replaced by alternating layers of KAM-tori and island-chains that are surrounded by a layer of chaotic trajectories exploring a tiny portion of the phase space. The whole structure is self-similar, since the islands consist again of alternating invariant tori and secondary island chains and this pattern repeats itself up to arbitrary small scales.

As the perturbation is increased, more and more of the KAM-tori will be destroyed and the stochastic regions that were separated by them will merge. When the last invariant

torus that remains of the integrable system is destroyed all chaotic layers of the primary structure will have merged into a global chaotic sea in which the remaining invariant tori of the islands are embedded. A fully chaotic system is obtained only if all invariant tori are destroyed, also those of the secondary and higher-order structures.

The difficulty for semiclassical theories in mixed systems is that they have to take these complicated classical patterns into account. At a fixed value of the energy, quantum mechanics does not resolve all the details of the phase space structures since it smoothes over regions of the order of $\hbar^2$. However, as E is increased (or $\hbar$ diminished) more and more structures will be resolved. The difficulty in performing the semiclassical limit $E \to \infty$ or $\hbar \to 0$ is due to the fact that classical structures exist up to arbitrary small scales. No matter how large E is there are always new details that become semiclassically relevant. Up to now, no general semiclassical theory has been developed that can handle these difficulties. Semiclassical methods that are applied in mixed systems are typically restricted to some energy regime, and if the energy is changed then also the method has to be adjusted to the new relevant structures in phase space.

An example are EBK-like quantization rules that can be applied also to weakly disturbed integrable systems (see e. g. [88]). They interpolate smoothly over the island-chain structures if the energy is not too high. As the energy is increased they become inaccurate. However, when the energy is high enough so that wave functions can concentrate on one of the islands, then EBK-quantization rules can be applied again, but now for the quantization of the islands. This is because the islands have a very similar structure as the perturbed integrable system [89]. It is an interesting mechanism how the EBK-quantization conditions for the primary KAM-structure is replaced by the EBK-conditions for the primary islands for a particular island chain [90]. The application of the torus quantization requires the knowledge of the two action variables for two irreducible circuits around an torus. These can be determined for the invariant tori of the islands, and for the periodic orbits, but not for the regions in between. In order to apply the EBK-quantization rules one therefore has to interpolate the action variables over the regions between the invariant tori. Although this method often works well, it does not have a firm theoretical basis.

The alternative approach to the semiclassical approximation follows the line of Gutzwiller's periodic orbit theory. Periodic orbits give in general the leading order oscillatory contribution to the level density since they correspond to stationary points in representations of the level density by oscillatory integrals. This applies also to mixed systems. The difference with respect to chaotic systems is that in mixed systems periodic orbits can also be stable, and stable orbits are never isolated from other periodic orbits in their neighbourhood. A semiclassical contribution of stable periodic orbits was derived by Gutzwiller by a linearization of the motion around them [2]. This approximation neglects the presence of other neighbouring periodic orbits and yields

$$d_\gamma(E) = \frac{1}{\pi\hbar} \sum_{m=1}^{\infty} \frac{T_\gamma(E)}{2\sin\left(\frac{m\alpha_\gamma}{2}\right)} \cos\left(\frac{S_\gamma(E)}{\hbar} - \frac{\pi}{2}\nu_\gamma\right) \ . \tag{6}$$

Here the sum runs over all repetitions m of the orbit γ. $S_\gamma(E)$, $T_\gamma(E)$, and ν_γ are the action, period and the number of turning points of the orbit, respectively. The quantity α_γ is the stability angle that specifies the angle by which neighbouring trajectories wind around the stable orbit in phase space during one traversal. They are related to the two

eigenvalues of the stability matrix by $\lambda_{1,2} = \exp(\pm i\alpha_\gamma)$.

The form (6) yields direct quantization conditions for a set of energy levels. They are obtained by expanding the fraction with the sine function in the denominator into a geometric series and applying the Poisson summation formula. This yields a sum over delta-functions whose positions are determined by the condition [91]

$$S_\gamma(E) - \alpha_\gamma \hbar \left(m + \frac{1}{2}\right) = 2\pi\hbar \left(n + \frac{\nu}{4}\right) . \tag{7}$$

The same quantization condition was obtained by Voros by applying EBK-quantization to the torus structure that is obtained by a linearization of the motion around a stable orbit [92]. Rigorous results are given by Ralston [93]. The energy levels determined by (7) correspond to quasimodes that are approximate solutions of the Schrödinger equation.

The quantization conditions (7) in general cannot be good approximations to quantum levels if the corresponding wave functions are not concentrated sufficiently close to the stable orbit, since the actual island structure around a stable orbit differs distinctly from the torus structure that is obtained from the linearization. Thus there are restrictions to the values of m and n for which (7) is good. The formula (6) on the other hand sums over semiclassical energies $E_{n,m}$ for all values $m, n \geq 0$ and thus has to be modified.

That equation (6) must be wrong in general can also be seen directly. The sine in the denominator is zero if its argument is a multiple of π. If α_γ is a rational multiple of 2π then there is always a positive integer m such that the sine is zero and the formula (6) diverges. The reason for this divergence is, as mentioned before, the fact that a stable periodic orbit is never isolated from neighbouring periodic orbits. The divergence of the m-th term in the sum in (6) implies that the stability matrix of the m-th repetition of the stable orbit has eigenvalues $\lambda_{1,2} = 1$ which in turn means that there is another periodic orbit in an infinitesimal neighbourhood. This occurs either if a periodic orbit is part of a family of orbits or if it coalesces with another periodic orbit in a bifurcation. Since generically there are no families in mixed systems, it signifies that the orbit undergoes a bifurcation.

Bifurcations are a typical phenomenon in mixed systems and occur very often. Every arbitrarily small but finite change of α_γ, as caused for example by a small parameter change of the system, immediately causes an infinite number of different bifurcations since α_γ will go through an infinite number of rational multiples of 2π. Most of these bifurcations occur for large values of m, i. e. for orbits with long periods. Bifurcations are the reason for the strong increase of the number of periodic orbits when an integrable system is transformed into a chaotic system (from a power law dependence on the period to an exponential dependence).

In order to treat bifurcations semiclassically one has to apply approximations that take neighbouring orbits into account. In the derivation of semiclassical trace formulas this is equivalent to the semiclassical evaluation of oscillatory integrals with almost coalescing stationary points. Such integrals cannot be evaluated by stationary phase approximations which diverge if different stationary points coalesce. One has to apply uniform approximations that are valid at bifurcations as well as in regions where orbits are well separated and stationary phase approximations can be applied. Uniform approximations are typically necessary when there is a transition between two different asymptotic regimes. In the case of bifurcations coalescing periodic orbits contribute semiclassically with a different power in $\hbar$ than isolated periodic orbits. The difference in the power is given by

the singularity index of the bifurcation. The derivation of uniform approximations for all typical bifurcations in two-dimensional systems is the topic of the articles [P10-P12].

Bifurcations occur in several different forms. The appearance or disappearance of periodic orbits in smooth systems is always connected to bifurcations. But bifurcations can also occur in the form that orbits become identical and then part again. A classification of all different bifurcations that typically occur in two-dimensional systems without symmetries was given by Meyer and Bruno [94, 95, 96]. These bifurcations are realized if one parameter in a system is changed, they are called bifurcations of codimension one. One finds that the form of the bifurcation depends only on the lowest repetition number m of a stable orbit for which the stability matrix has eigenvalues $\lambda_{1,2} = 1$. The corresponding bifurcations are period-m-tupling bifurcations since they involve other periodic orbits which have a primitive period that is m times larger than that of the considered stable orbit.

There is only a finite number of different characteristic forms of the bifurcations. For $m = 1$ one has a saddle-node or tangent bifurcation in which two periodic orbits appear (or disappear). The case $m = 2$ is a pitchfork bifurcation in which a central orbit changes its stability from stable to unstable or vice versa, and a new orbit appears (or disappears). For $m = 3$ two orbits coalesce in a touch-and-go bifurcation and part again. For $m = 4$ there are two forms of the bifurcation. One case looks like a touch-and-go bifurcation, but it involves three orbits in contrast to the case $m = 3$. One orbit disappears at the bifurcation and a new one appears. The second case is an island-chain bifurcation in which two new orbits are born, one stable and one unstable. The remaining cases $m \geq 5$ all have the form of island-chain bifurcations.

In the following we briefly discuss how the uniform approximations are obtained in [P10-P12]. Semiclassical contributions for bifurcating periodic orbits follow from a semiclassical evaluation of the trace of the Green function which leads to integrals of the form

$$d_\xi(E) = \int \mathrm{d}q \int \mathrm{d}p \; a(q,p) \exp\left\{\frac{i}{\hbar} f(q,p)\right\} \tag{8}$$

where the stationary points of the function $f(q,p)$ correspond to the positions of the periodic orbits in a Poincaré section of surface. In the vicinity of a bifurcation the integral (8) can be evaluated by expressing $f(q,p)$ in terms of the normal form of the bifurcation that describes the positions of the neighbouring periodic orbits, and considering $a(q,p)$ constant [48]. This expresses $d_\xi(E)$ in terms of catastrophe diffraction integrals. It yields a transitional approximation that is only valid in the vicinity of a bifurcation. It does not give the correct contributions of isolated periodic orbits far away from the bifurcation.

In [P10] a method was developed for obtaining a complete uniform approximation. It involves the extension of the normal form by including higher-order correction terms. The extended normal form is inserted into (8) and the exponent is simplified by appropriate coordinate transformations. Furthermore the amplitude factor $a(q,p)$ is also expanded up to an order consistent with the expansion of the exponent. By this way a uniform approximation is obtained that has the correct Gutzwiller limit far away from the bifurcation. An application of this formula was given in the article [P13].

In [P11] uniform approximations were derived for the cases $m = 1$, $m = 2$ and $m = 3$ by applying the method of [P10]. The results were tested on the example of a kicked top and compared to the exact quantum result, the transitional approximation and the

Gutzwiller approximation, respectively. There was hardly any difference between the uniform approximation and the quantum calculation, whereas the transitional approximation showed clear deviations in some distance from the bifurcation, and the Gutzwiller approximation diverged at the bifurcation.

The article [P12] treats the remaining case $m = 4$ which is more complicated because it involves three periodic orbits that have to be treated on the same footing. It is the only case in which the uniform approximation cannot be expressed in terms of known functions. We used a different method for the derivation in [P12]. It consist in a mapping of the function $f(q, p)$ onto the normal form by an implicitly defined coordinate transformation. The amplitude factor $a(q, p)$ is then approximated by an interpolating function that has the correct values at the positions of the stationary points. The resulting uniform approximation was again tested on the kicked top with similar results as for $m = 1$, $m = 2$ and $m = 3$.

The articles [P10-P12] give a complete treatment of uniform approximations for all generic bifurcations that occur in two-dimensional systems. In systems with discrete symmetries further types of bifurcations can occur, which however often have the normal forms of generic bifurcations but with a different interpretation. For example pitchfork bifurcations occur in which not one orbit with twice the period is born, but two symmetric orbits with the same period as the central stable orbit. Bifurcations of this kind can be treated by slight modifications of the generic formulas.

Although the treatment of the generic bifurcations in [P10-P12] is for many applications sufficient, it does not allow a complete semiclassical treatment of mixed systems. As longer and longer orbits are involved, bifurcations occur more and more rapidly, and there is a point were different subsequent bifurcations of a periodic orbit cannot be treated separated. This requires an extension of the normal forms such that it describes also the treatment of subsequent bifurcations. A series of bifurcations can often also be considered as a bifurcation of a higher codimension since the different bifurcations can typically be brought to a coalescence if one varies several parameters of a system. Bifurcations of codimension two are treated in [49, 50, 51].

4.3 Semiclassical transition from an elliptical to an oval billiard

In integrable systems semiclassical approximations are generally considered to be rather simple. The generalization of the WKB-approximation to higher dimensions leads to the EBK-quantization rules, and by applying the Poisson summation formula one obtains the Berry-Tabor trace formula in terms of a sum over all tori of periodic orbits. Yet also in integrable systems complications can occur. There can be separatrices that separate different dynamical regimes, there can be isolated periodic orbits, stable as well as unstable, that are not part of a periodic torus, and there can be bifurcations of periodic orbits that lead to the appearance of new tori of periodic orbits as a parameter of the system is changed. All these features can be observed in an apparently simple system like a billiard in form of an ellipse.

One motivation for studying the elliptical billiard and small deformations of it in [P13] was the interest in the relation between bifurcations in integrable and mixed systems. Generic bifurcations in mixed systems involve only a finite number of periodic orbits, whereas in integrable systems whole tori appear (or disappear). But bifurcations in the integrable case can be considered as a limit of bifurcations in mixed systems. If a torus is

close to undergoing a bifurcation, and the integrable system is perturbed, then the torus breaks up into a finite number of periodic orbits, and the distribution of the periodic orbits in phase space is then identical to that of the orbits near a generic bifurcation. For this reason, the uniform approximations of the last section 4.2 describe also the break-up of tori near bifurcations as an integrable system is perturbed. [P13] contains thus an application and a first numerical test of the results of [P10]. (Only the results for bifurcations with high repetition numbers were needed in [P13].)

The first part of [P13] gives a short overview of classical and quantum properties of the elliptical billiard. It discusses further the EBK-quantization rules that require a uniformization in the elliptical billiard. There is a separatrix in the ellipse that separates the classical motion between the two foci from the motion around the two foci. This separatrix leads to a discontinuity in the EBK-quantization conditions since the Maslov index is different for both regions. The discontinuity is removed by an interpolating uniform approximation for the Maslov index [97].

Starting from the uniformized EBK-quantization rules a trace formula is derived in [P13] for the ellipse which includes a uniform treatment of the bifurcations. Numerical tests of this formula with quantum calculations show a good agreement, and the small semiclassical error was taken as a reference for the semiclassical calculations in a nearly-integrable system that was examined in the second part of [P13].

This second part investigates how the semiclassical approximations change if the ellipse is slightly deformed into a non-integrable oval. One has to distinguish two cases. For tori not involved in a bifurcation one can apply general uniform approximations for the break-up of generic tori [98, 99, 100, 101]. The break-up of tori which are close to a bifurcation on the other hand is described by the uniform formulas for generic bifurcations as discussed above. By using these formulas numerical examinations in [P13] show that the semiclassical error in the near-integrable oval billiard is of the same size as the semiclassical error in the elliptical billiard. This confirms that the uniform approximations are indeed the appropriate substitute for torus or isolated orbit contributions in trace formulas.

5 Semiclassical methods in nuclear physics

Many properties of multi-fermion systems like atoms, nuclei or metallic clusters can be explained by assuming that the particles move independently in a common potential. In this approximation the correlations between the positions of the particles are neglected and the particle interaction is incorporated into a mean field that determines the common potential. This mean field depends itself on the density of the particles and has to be determined in a self-consistent way, as is done by the Hartree-Fock method or the density functional method. In this way the N-particle problem is reduced to N one-particle problems.

Mean-field approximations can be used, for example, to explain and determine "magic numbers" that denote the number of particles in a system for which it is most stable. These magic numbers are a consequence of the fact that the energy levels of the single-particle spectrum for the collective potential are not uniformly distributed, but show a strong clustering that is due to high symmetries of the systems. The appearance of magic numbers is thus a typical shell effect that can be observed in large fluctuations of the coarse grained level density. It is in applications like these that semiclassical methods are most powerful. It often suffices to sum only over a few periodic orbits in order to determine fluctuations in the spectrum of a system that are responsible for the main shell structure. (For the determination of magic numbers this applies to metallic clusters. In nuclei additional spin-orbit forces are essential for an understanding of closed shells.)

In the same context semiclassical methods have been successful in explaining ground state deformations of atomic nuclei [34] and small metallic clusters [35], and the occurrence of "supershells" in the metallic clusters that show up as long-range oscillations in the coarse grained level density superposing the fluctuations corresponding to the shell structure [4, 36]. In the articles [P14,P15] we present a further application of semiclassical periodic orbit approximations in nuclear physics. It allows a simple interpretation of the origin of the asymmetric fission of heavy atomic nuclei.

The fission of many actinide nuclei results in an asymmetric mass distribution of the fission fragments. This mass asymmetry cannot be explained by the classical liquid drop model that favors symmetric fission. In order to explain the asymmetry one has to include shell corrections, i. e. deviations from the mean distribution of the single particle energies due to the discreteness of the spectra, as is done by Strutinsky's shell correction method [102]. According to Strutinsky the total binding energy of a nucleus consisting of N neutrons and Z protons has the form

$$E_{\rm tot}(N,Z;def) = E_{\rm LDM}(N,Z;def) + \delta E_n(N;def) + \delta E_p(Z;def) \qquad (9)$$

where $E_{\rm LDM}$ is the liquid drop model (LDM) energy, and $\delta E_n(N;def)$ and $\delta E_p(Z;def)$ are the shell-correction energies of the neutrons and protons, respectively. All quantities depend on the shape of the nucleus which is described by several deformation parameters summarized by 'def'.

The shell corrections in (9) where calculated in the seventies from realistic nuclear shell-model potentials of Wood-Saxon form [103]. For a typical actinide nucleus they lead to three characteristic deviations from the liquid drop model: the ground state is deformed and not spherical, the potential energy has a second local minimum for larger deformations, the so-called fission isomer, and, starting from the fission isomer, left-right asymmetric deformations are energetically more favourable than symmetric deformations.

(All these deformations still have an axial symmetry.) The shell-correction method thus yields an asymmetric mass distribution and it has been very successful in reproducing experimental nuclear binding energies and fission barriers, however, it does not lead to an intuitive understanding of the physical origin of the asymmetry.

In [P14,P15] we give a simple and transparent semiclassical interpretation of the asymmetric fission. We use a simple model for the nuclear mean field by replacing it by a three-dimensional cavity, and we neglect spin-orbit interactions. Furthermore, we consider only the neutron contributions δE_n in (9) since they contain the main shell effects. The boundary of the cavity is parameterized by three parameters c, h and α, where c determines the longitudinal elongation of the cavity, h regulates the formation of a neck that leads to the scission of the nucleus into two fragments, and α controls the left-right asymmetry. The parameters are chosen such that an increase of c with $h = \alpha = 0$ follows the adiabatic path through the parameter space in the liquid drop model.

In this model we calculate the shell correction δE for the neutrons. It is obtained from the level density for the neutrons by summing over all energies up to the Fermi energy and subtracting the mean level density. This leads to a trace formula of the form:

$$\delta E = \sum_{\gamma} A_\gamma(E_F) \left(\frac{\hbar}{T_\gamma(E_F)}\right)^2 \cos\left(\frac{S_\gamma(E_F)}{\hbar} - \frac{\pi}{2}\sigma_\gamma\right) , \tag{10}$$

where E_F denotes here the Fermi energy. Eq. (10) sums over the contributions of one-parameter families of periodic orbits in the axially symmetric billiard system, and the quantity σ_γ takes half-integer values. The formula differs from the oscillatory part of the level density by a factor $(\hbar/T_\gamma)^2$.

In order to evaluate (10) the shortest orbits of the system were determined as a function of the parameters. Since the starting point for the development of left-right asymmetric shapes is the fission isomer, it is sufficient to restrict the consideration to large deformations of the cavity. For these the shortest orbits all lie in planes perpendicular to the symmetry axis of the billiard. In one such plane the orbits are those of a circular billiard.

If one changes the parameters then one finds that the number of these equatorial planes are not constant. During the neck formation two new planes of periodic orbits arise in a bifurcation, and this requires a modification of the contributions in the trace formula (10). As in section 4.2 one has to derive a uniform approximation for their contribution. The particular bifurcation is not generic. It is a bifurcation of codimension two corresponding to the cusp bifurcation of catastrophe theory. Its uniform approximation is expressed in terms of Pearcey's integral and its derivatives [P14]. A test of this uniform approximation is carried out in [P15] by comparing it to quantum calculations for the three-dimensional cavity.

With this modification the shell-correction energy is evaluated. By plotting it as a function of the parameters one finds that this simple semiclassical calculation produces correctly the gross parameter dependence of δE, as obtained previously from quantum calculations for a realistic Wood-Saxon potential, including spin-orbit interaction and pairing correlations. In particular the semiclassical calculations predict correctly the onset of the asymmetry at the fission isomer. Furthermore, the adiabatic path that the system follows in the parameter space starting from the fission isomer in the semiclassical approximations follows the line on which the actions of the most important periodic orbits are constant. This provides a simple intuitive interpretation of the asymmetric fission, it relates it semiclassically to the constancy of the shortest periodic orbits.

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Appendices