Chapter 2

Semiclassical approximations

Semiclassics are usually defined as approximations of the quantum mechanical equations to leading order in $\hbar$. This definition is accurate, short, and self-contained — but by no means self-explaining. This chapter first provides the necessary context by giving a short overview of the history of semiclassical approximations before presenting the modern form used in the subsequent chapters.

Contents

The classification of semiclassical approximations in theories for integrable, purely chaotic and mixed systems follows roughly the historical development of the discipline. This chapter introduces the central ideas of semiclassical approximations for the different situations following more or less this chronological order. It does not attempt, however, to review the whole variety of different approaches developed so far, but will concentrate on key ideas and methods relevant for the present work.

2.1 Integrable systems

The first attempts that – from a modern point of view – would be called semiclassical date back prior to the development of wave mechanics. The empirical Bohr-Sommerfeld quantization rule

$$S = \oint \boldsymbol{p}\, d\boldsymbol{q} = 2\pi\hbar \cdot n \quad (n \in \mathbb{N}) \tag{2.1}$$

successfully explained the spectrum of hydrogen and ionized helium. Despite huge efforts, however, it completely failed for neutral helium. When in 1926 the wave mechanical approach successfully explained this long-considered problem, it superseded the Bohr-Sommerfeld scheme, and the role closed orbits play for quantization was ignored for nearly half a century.

Soon after, an expansion of the new wave mechanical quantum theory in powers of $\hbar$ was given by Wentzel, Kramers and Brillouin [85, 51, 20]. It is usually called *WKB-approximation*. The two key ideas are

1. Separate the wave function in a real amplitude and a (unit) phase factor according to

$$\Psi(\boldsymbol{r},t) \;=\; A(\boldsymbol{r},t)e^{iR(\boldsymbol{r},t)/\hbar}\;. \tag{2.2}$$

The quantum momentum of the particle

$$\langle\ \Psi\ |\ -i\hbar\nabla\ |\ \Psi\ \rangle\ = \nabla R A^2 - i\hbar A\nabla A \tag{2.3}$$

is well defined and finite in the *semiclassical limit* $\hbar \to 0$. Inserting this ansatz in the Schrödinger equation yields two equations for A and R, equivalent to the time evolution of the real and the complex part of the wave function. For a Hamiltonian $H = \boldsymbol{p}^2/2m + V(\boldsymbol{r})$ this results in

$$\frac{\partial R}{\partial t} + \frac{(\nabla R)^2}{2m} + V(\boldsymbol{r}) - \frac{\hbar^2}{2m}\frac{\nabla A}{A} \;=\; 0\;, \tag{2.4}$$

and

$$\frac{\partial A}{\partial t} + \frac{\nabla R \nabla A}{m} + \frac{A\nabla R}{2m} \;=\; 0\;. \tag{2.5}$$

These equations are the starting point of Madelung's *hydrodynamic picture* of quantum mechanics [56]. The naming was motivated by the fact that with $\rho := A^2$ and $\boldsymbol{v} := \nabla R/m$ Eq. (2.5) takes the form of a continuity equation $\dot{\rho} + \nabla(\rho\boldsymbol{v}) = 0$.

2. The semiclassical approximation corresponds to the limit $\hbar \to 0$, which is well defined for Eqs. (2.4) and (2.5). In this limit the last term in Eq. 2.4, the so-called *quantum potential*, vanishes[1]. This equation then takes the form of a classical Hamilton-Jacobi equation $\dot{R} + H(\boldsymbol{r}, \nabla R) = 0$. Using this analogy it can be shown that R is in fact given by Hamilton's principal function along a classical path.

For one-dimensional (or separable) systems the Hamilton-Jacobi equation can be solved in general. The condition of the simple-valuedness of the wave function leads to quantization conditions. These can be written down explicitly,[2] taking exactly the form of the Bohr-Sommerfeld rule Eq. (2.1).

The classical turning points, however, introduce additional subtleties.[3] This was first realized by Kramers [51], who derived additional phase factors $\mu\pi/2$ using his *connection formulas*. These factors correspond to phase shifts at reflections. In Sec. 4.3.2 this point will be considered in some more detail. The quantization condition is modified by the additional phases according to

$$S = \oint \boldsymbol{p}\, d\boldsymbol{q} = 2\pi\hbar \left(n + \frac{\mu}{4}\right) \quad (n \in \mathbb{N}) \,. \tag{2.6}$$

The additional phases from the classical turning points shift the energy spectrum. As such, they are responsible for the quantum mechanical zero point energy.

The WKB approach can be generalized to *integrable systems*, i. e. systems with as many constants of motion as degrees of freedom. In these systems the phase-space motion is confined to a torus.[4] The closed paths along which the quantization in analogy to Eq. (2.6) has to be performed are the topological invariant closed paths on this torus. In this form, it is usually named *EBK* after Einstein, Brillouin and Keller [45]. Whereas for (effectively) one-dimensional systems the classical turning points lead to additional phases, in higher dimensions their role is taken by focusing points of trajectories in configuration space, the so-called *caustics*. These correspond to foldings in phase space, where the orientation of the configuration-space surface changes. The additional phases, which are nowadays called *Maslov indices*[5], only depend on the topology of the classical path.

The Maslov indices are one ingredient necessary for a successful semiclassical quantization of the neutral helium which was missed by Heisenberg and coworkers in their attempts prior to 1926. The second problem they did not take into account is that Helium, a three-body problem, is not integrable, but chaotic. The role of classical orbits for the quantization of chaotic problems remained unclear for another decade.

2.2 Chaotic systems

The methods presented above result in an energy quantization rule which depends on individual, characteristic orbits of the system. The general hope was that the close con-

[1] The alternative interpretation of quantum mechanics presented by Bohm [109] preserves the quantum potential. It solves the Hamilton-Jacobi equation including this amplitude-dependent term. A recent work shows that this ansatz might be helpful in the interpretation of the quantum measurement process [102].

[2] For explicit examples, see, e. g., section 2.4 of Ref. [100].

[3] The formal reason is that at classical turning points the quantum potential is not negligible.

[4] This holds for bounded systems, to be precise.

[5] The definition of the Maslov index is not consistent in the literature. In this work, the term is laxly used for all additional phases in multiples of $\pi/2$.

nection between single orbits of the system and individual quantum states established for integrable systems would also hold in the non-integrable case. This belief turned out to be wrong, and obscured for a long time the way to a semiclassical treatment of chaotic systems. In a series of papers [36, 37, 38, 39, 40] starting in 1967, Gutzwiller established the long-searched bridge between classical chaotic dynamics and quantum properties of the system. This work constitutes the foundation of modern semiclassical theories. The central result, the famous *trace formula* for the level density of a completely chaotic system, has by now been re-derived using various alternative approaches. Whereas the original work of Gutzwiller started out with the Feynman path integral, Bogomolny uses a description of the Schrödinger equation in terms of a semiclassical transfer operator acting on the Poincaré map [16], and Smilansky employs a scattering approach [106]. Citanović and coworkers [101] calculate the quantum mechanical propagator K using the fact that K itself solves the Schrödinger equation. The corresponding wave function is approximated by a very nice generalization of the multidimensional WKB scheme to non-integrable systems. Readers interested in details on these derivations are referred to the original literature or to the recent reviews Refs. [100, 105]. Here, only the main ideas leading to the Gutzwiller trace formula will be sketched.

2.2.1 The semiclassical Propagator

The quantum mechanical propagator K is the operator that propagates a wave function Ψ through time :

$$\Psi(\boldsymbol{r}, t) = K(\boldsymbol{r}, \boldsymbol{r'}; t)\, \Psi(\boldsymbol{r'}, 0)\ . \tag{2.7}$$

A semiclassical approximation can be derived starting out with the Feynman path integral expression of the propagator

$$K(\boldsymbol{r}, \boldsymbol{r'}; t) = \int \mathcal{D}\boldsymbol{r}\ \exp\left(\frac{i}{\hbar} R(\boldsymbol{r}, \boldsymbol{r'}; t)\right)\ , \tag{2.8}$$

where R is Hamilton's principal function. $\int \mathcal{D}\boldsymbol{r}$ denotes an infinite-dimensional integration. It extends over all paths from $\boldsymbol{r'}$ to $\boldsymbol{r}$ in time t. The integrand is rapidly oscillating, so that most of the contributions to K cancel. This type of integrals can be well approximated using the *stationary phase approximation*, one of the central techniques in semiclassics. In one dimension, it is given by

$$\begin{aligned} \int_{\gamma_1}^{\gamma_2} e^{\frac{i}{\hbar}R(\gamma)}\ d\gamma &= \int_{\gamma_1}^{\gamma_2} e^{\frac{i}{\hbar}(R_0 + R_2(\gamma-\gamma_0)^2 + R_3(\gamma-\gamma_0)^3 + \ldots)}\ d\gamma \\ &\approx \int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(R_0 + R_2(\gamma-\gamma_0)^2)}\ d\gamma\ =\ e^{\frac{i}{\hbar}R_0}\sqrt{\frac{\pi}{|R_2|}}\, e^{i\ \mathrm{sign}(R_2)\pi/4}\ . \end{aligned} \tag{2.9}$$

If more stationary points exists, their contributions have to be summed up. The generalization to more dimensions is straight forward. The stationary points of the exponent of Eq. (2.8) correspond to the classical paths. Therefore the stationary phase approximation of K consists of the replacement of the integral over *all* paths from $\boldsymbol{r'}$ to $\boldsymbol{r}$ by the appropriately weighted *classical* ones.

The resulting approximation of the propagator was – apart from the indices ν, which again stem from caustic points[6] – already proposed by Van Vleck [86] back in 1928:

$$K_{\mathrm{sc}}(\boldsymbol{r},\boldsymbol{r'};t) = \left(\frac{1}{2\pi i\hbar}\right)^{D/2} \sum_{\Gamma(\boldsymbol{r},\boldsymbol{r'};t)} \sqrt{\det\left|\frac{\partial^2 R}{\partial \boldsymbol{r}\partial \boldsymbol{r'}}\right|} \quad \exp\left(\frac{i}{\hbar}R(\boldsymbol{r},\boldsymbol{r'};t) - i\nu\frac{\pi}{2}\right) \ . \tag{2.10}$$

Here $\Gamma(\boldsymbol{r},\boldsymbol{r'};t)$ denotes the sum over all classical paths connecting $\boldsymbol{r}$ and $\boldsymbol{r'}$ in time t, and D is the system dimension. Eq. (2.10) is one of the key formulas to modern semiclassical theories.

2.2.2 The semiclassical Green's function

More convenient than the propagator is the Green's function, its (half-sided) Fourier transform with respect to time

$$G(\boldsymbol{r},\boldsymbol{r'};E) = -\frac{i}{\hbar}\lim_{\varepsilon\to 0}\int_0^\infty K(\boldsymbol{r},\boldsymbol{r'};t)\ \exp\left(\frac{i}{\hbar}(E-i\varepsilon)t\right)\ dt\,. \tag{2.11}$$

Gutzwiller treated the case where all classical orbits are *isolated* in phase space, i. e. have no neighbor with the same energy and action at infinitesimal distance. If additionally the actions S of the classical trajectories are much larger than $\hbar$, the integrations perpendicular to the classical paths can be performed in stationary phase approximation. This leads to the semiclassical approximation of the Green's function according to

$$G_{\mathrm{sc}}(\boldsymbol{r},\boldsymbol{r'};E) = \frac{2\pi}{(2\pi i\hbar)^{\frac{D+1}{2}}} \sum_{\Gamma(\boldsymbol{r},\boldsymbol{r'};E)} \sqrt{\det\begin{vmatrix} S_{\boldsymbol{r'}\boldsymbol{r}} & S_{\boldsymbol{r'}E} \\ S_{E\boldsymbol{r}} & S_{EE}\end{vmatrix}}\ \exp\left(\frac{i}{\hbar}S(\boldsymbol{r},\boldsymbol{r'};E) - i\mu\frac{\pi}{2}\right)\ , \tag{2.12}$$

where S_{kl} denotes the partial derivatives $\partial^2 S/(\partial k\,\partial l)$. The summation extends over all classical paths Γ with fixed energy E connecting $\boldsymbol{r'}$ and $\boldsymbol{r}$.

The general strategy for semiclassical approximations is to find an exact expression of the desired quantity in terms of Green's functions. Replacing the Green's functions by their semiclassical approximations yields a semiclassical formula for the desired observable. This procedure will be used in the following section to derive a semiclassical formula for the level density. In chapter 5 the same approach will lead to a semiclassical expression for the conductivity.

2.2.3 The semiclassical level density

The level density can be expressed in terms of Green's function as

$$g(E) = -\frac{1}{\pi}\lim_{\varepsilon\to 0}\mathcal{I}m\left[\mathrm{Tr}(G(\boldsymbol{r},\boldsymbol{r},E+i\varepsilon))\right]\ . \tag{2.13}$$

The classical paths from $\boldsymbol{r}$ to $\boldsymbol{r}$, i. e. the closed paths, fall into two groups: The orbits with zero length, and finite length orbits returning to $\boldsymbol{r}$. The contribution of the zero length orbits has to be evaluated separately, since they violate the condition $S \gg \hbar$,

[6] These *Morse indices* slightly differ from the Maslov indices μ.

which is required for the validity of the stationary phase approximation. These orbits lead to the average density of states $\tilde{g}(E)$, which alternatively can be calculated using the familiar Thomas-Fermi relation. From now on, only the contributions of finite-length orbits will be considered. These are responsible for the oscillatory deviations $\delta g(E)$ from the smooth part $\tilde{g}(E)$. Performing another stationary phase approximation to evaluate the trace integral yields the famous Gutzwiller *trace formula*

$$\delta g(E) \approx \frac{1}{\pi\hbar} \sum_{\mathrm{po}} \underbrace{\frac{T_{\mathrm{PPO}}}{\sqrt{|\det(\widetilde{M} - \mathbb{1})|}}}_{:= A_{\mathrm{po}}} \cos\left(\frac{S}{\hbar} - \mu\frac{\pi}{2}\right) \ . \tag{2.14}$$

The summation extends over all classical *periodic* orbits po of the system. T_{PPO} is the period of the *primitive* orbit, i. e. the part of the orbit until it first closes in phase space. The *stability matrix* $\widetilde{M}$ is given by the non-trivial part of the *Monodromy matrix* M. It is related to the stability of an orbit. This quantity is explained in detail in appendix A.1.2. The factors in front of the cos-term are usually collectively called *semiclassical amplitude* A_{po} of an orbit. Formula Eq. (2.14) is often given in an analog form which separates the sum over the different orbits from the sum over their repetitions. In this thesis the sum over the repetitions should always be included in the sum over all orbits.

Please note that the trace formula for the semiclassical quantization of chaotic systems has a completely different structure than the quantization conditions for the integrable case. Whereas for the latter individual paths in the system are related to single quantum states, in chaotic systems each periodic orbit contributes to all energy levels.

The Gutzwiller trace formula provided the basis for a successful semiclassical treatment of neutral helium, which was finally accomplished in 1991 [28]. 65 years after the same problem had set an end to the empirical quantization rules, this was a great success for the growing semiclassical community. In the following years searching for traces of classical orbits in quantum spectra as well as superposing classical trajectories to approximate shell structures or even individual quantum levels have been recognized as powerful theoretical tools.

For the purpose of this work, two generalizations of the trace formula are needed, namely the extension to continuous symmetries and to systems with mixed phase space. These will be presented in the following sections.

2.3 Continuous symmetries

For systems with continuous symmetries the Fourier integral Eq. (2.11) can not be evaluated as sketched above. A suitable adaption of the procedure has been proposed by Strutinsky and Magner [76] and, in a more general form, by Creagh and Littlejohn [23]. The main idea of the latter generalization is a separation into a symmetry-free system which is treated in analogy to the Gutzwiller case, and the symmetry degrees of freedom, over which the integrations are performed exactly. The structure of the trace formula Eq. (2.14) remains essentially unchanged by this procedure, but the definition of the amplitudes is different, reflecting the different structure of the underlying classical dynamics:

$$\delta g(E) \quad \approx \quad -\frac{1}{\pi}\mathcal{I}m\left[\frac{1}{i\hbar}\frac{1}{(2\pi i\hbar)^{k/2}}\sum_{po}\int_{po} dt\, d\boldsymbol{\mu}(\boldsymbol{g})\, |K_{po}|^{-1/2} e^{i\frac{S_{po}}{\hbar} - i\sigma_{po}\frac{\pi}{2}}\right] =$$

$$=: \quad -\left(\frac{1}{\pi\hbar}\right)^{\frac{k+2}{2}} \mathcal{I}m \left[\sum_{po} A_{po} e^{i\frac{S_{po}}{\hbar} - i\sigma_{po}\frac{\pi}{2}}\right] . \tag{2.15}$$

The dimensionality of the symmetry is denoted by k. The integral over t replaces the period of the primitive orbit T_{PPO} in the Gutzwiller case. $\int_{po} d\boldsymbol{\mu}(\boldsymbol{g})$ is the integration over the symmetry, where $\boldsymbol{\mu}(\boldsymbol{g})$ denotes the measure of the symmetry group. The stability term of the Gutzwiller formula is replaced by $|K|^{1/2}$, where

$$K = Q \det(W) \det(\widetilde{M} - I) . \tag{2.16}$$

Here $\widetilde{M}$ is the stability matrix of the symmetry-reduced system. Q depends only on the type of symmetry. For Abelian symmetries $Q = 1$, and for three-dimensional rotational symmetry $Q = J^{-2}$, where J denotes the total angular momentum. Trajectories which are periodic in the symmetry-reduced system do not necessarily close in complete phase space. This leads to the additional factor $\det(W)$, where

$$W_{ij} = \frac{\partial \Theta_i}{\partial J_j} . \tag{2.17}$$

The Θ_i are the operators of the symmetry and the J_i are the corresponding conserved quantities. The topological index σ is given by $\sigma = \mu - \delta$, where δ is the number of negative eigenvalues of W. The Maslov index μ is the same as in the original Gutzwiller formula.

This approach can deal with continuous symmetries of arbitrary dimensionality. Each symmetry dimension corresponds to one constant of motion J_i. Eq. (2.15) applies even to integrable systems, where the number of J_i equals the degrees of freedom. The trace formula of Creagh and Littlejohn therefore provides a unified description of integrable and chaotic systems. Although it can also be applied to systems with mixed phase space, it cannot deal with the transition from regular motion to chaos. This problem will be dealt with in the following section.

The power in $\hbar$ of the contributions of the classical periodic orbits depends on the dimension of the symmetry. This implies that the amplitude of the oscillating part of the level density is larger for highly symmetric systems. In systems where different orbits have different dimensions of symmetry, their power in $\hbar$ is different. The leading-order contribution in $\hbar$ stems from the orbits with the highest continuous symmetry, whereas the other orbits give rise to $\hbar$ corrections. In chapter 4 this point will be discussed in more detail for the example of the disk billiard.

2.4 Mixed phase space

The semiclassical methods described above apply either to the integrable or to the completely chaotic situation. Many realistic physical systems, however, show a mixed phase-space structure. This introduces additional complications for semiclassic approximations, which are not completely settled by now. Only the ansatz of Bogomolny [16] does not explicitly assume regular or chaotic motion, so that it can deal with mixed phase space as well – but unfortunately only on a numerical level. The standard Gutzwiller approach cannot cope with the transition from regular to chaotic behavior. The extensions which

have been worked out to overcome this limitation will be introduced in this section. They build the basis for the considerations in the following chapters.

As pointed out above, the phase-space motion of an integrable system is confined to a torus. The periodic orbits of those systems are given by the repetitions of the elementary loops of the Bohr-Sommerfeld quantization. There are only a few such orbits up to a given maximum period T_m. Their number increases as a power law with T_m. In completely chaotic[7] systems, however, the number of periodic orbits increases exponentially with the period according to $N \propto 1/(hT_m)\exp(hT_m)$, where h is the topological entropy.

This implies that a system on its way from regular to chaotic motion creates new classical periodic orbits. These creation points are called *orbit bifurcations*. The underlying mechanism is visualized in Fig. 2.1. There, the situation prior to the integration of Eq. (2.13) is illustrated. The solid line gives the action in dependence of $\boldsymbol{r}$, and the arrows indicate the stationary points, i. e. the classical *periodic* paths. Varying an external parameter of

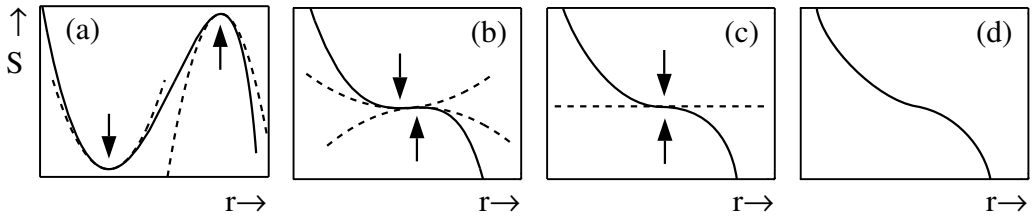

Figure 2.1: *The classical action $S(\boldsymbol{r}, \boldsymbol{r}; E)$ of a one-dimensional system in dependence of an external parameter. The parabolas give the local quadratic approximations at the stationary points.*

the system changes the functional dependence of S on $\boldsymbol{r}$. The two extrema, i. e., the two periodic orbits in (a) approach (b), fall together (c) and finally disappear (d). From right to left, these pictures illustrate the birth of two periodic orbits. This is the simplest type of bifurcation, called tangent bifurcation.

In Gutzwiller's derivation, the integration of Eq. (2.13) is performed in stationary phase approximation. According to Eq. (2.9), this means to replace the integral over $\boldsymbol{r}$ by the integrals over the parabolas approximating $S(\boldsymbol{r}, \boldsymbol{r}; E)$ at the stationary points. These second-order approximations are given by the dotted lines in Fig. 2.1. Obviously the stationary phase approximation gets inaccurate for orbits in close vicinity. At the point where the orbits coincide the fit parabolas have zero curvature. Since the amplitude of the orbits is in this approximation proportional the inverse curvature of these parabolas, the Gutzwiller approximation diverges at bifurcation points.

To overcome this problem, a local expansion to higher order in the action has been proposed by de Almeida and Hannay [8] or Kus *et al.* [53]. Such a local approximation, however, does not reproduce the Gutzwiller limit of well separated orbits. Retaining both the correct asymptotic and local behavior is possible using *uniform approximations*, which interpolate smoothly between the limiting cases. These have been developed most systematically by Schomerus and Sieber [72, 70, 73]. Bifurcations can be classified according to their normal form, and the authors give explicit formulas for all generic bifurcations in terms of the amplitudes, actions and Maslov indices of the orbits engaged. Non-generic cases, e. g. systems with discrete symmetries, are not directly covered by these formulas and need special care. The expressions for the two types of bifurcations relevant for this

[7] This holds for ergodic systems, to be precise.

thesis are given in appendix B. Eqs. (B.7) and (B.8) apply to the tangent bifurcation, and Eq. (B.15) to the period doubling bifurcation.

The Gutzwiller approximation only contains information about the classical phase-space structure. At first sight, the uniform approximations of Schomerus and Sieber are expressed in dependence of the same terms. They include, however, also contributions of *ghost orbits*, i. e., analytic continuations of orbits beyond the regime where they classically exist. This exceeds the purely classical phase space properties. In systems where the periodic orbits are known analytically, this additional information is readily available. If the equations of motion are solved numerically, however, this information can hardly be accessed. This problem will be examined in more detail in chapter 7.

As can be deduced from the analytical local form of the bifurcation, the contributions of the orbits engaged in a bifurcation are increased by a factor $\hbar^{-\delta}$ [70]. δ is positive; its value depends on the type of the bifurcation. The negative exponent shows that the bifurcations are of leading order in $\hbar$. Thus, these points dominate in the semiclassical limit $\hbar/S \to 0$ (with S being the action of a typical periodic orbit in the system). This gives a more formal explanation for the divergence of the standard Gutzwiller-like approximation at these points. The problems related with bifurcations will be examined in detail for the level density of the disk billiard in chapter 4 and for the magnetoconductance of a channel with antidots in chapter 7.

Systems with mixed phase space may exhibit even more complicated structures in the classical dynamics than the bifurcations discussed above. Just as bifurcations occur when in dependence of an external parameter two (or more) orbits approach and finally coincide, also two bifurcations can approach and fall together. This is called a bifurcation of codimension 2.[8] Treating those requires normal forms of even higher order in the action. The bifurcations of codimension 2 have recently been classified by Schomerus [69, 71]. He also presented formulas for their uniform approximation. For bifurcations of higher codimension, however, a general treatment is still lacking. The analytic complexity of the corresponding uniform formulae would anyway make them useless for practical applications. For the context of this work, the consideration of the 'ordinary' bifurcations of codimension 1 will be sufficient.

With the extension to systems with continuous symmetries of Sec. 2.3 and including the bifurcations by uniform approximations, integrable and chaotic systems as well as systems with mixed phase space can be described semiclassically. This generalized trace formula constitutes the main tool for the present work.

Prior to the application of this semiclassical trace formula to the disk billiard, some technical details have to be worked out. This will be done in chapter 3, where the convergence properties of the orbit sum are examined in the necessary detail. Readers mainly interested in physics are invited to page 27 immediately.

[8] This is not the exact definition of a bifurcation of codimension 2, since some "bifurcations of bifurcations" can still be described in a one-dimensional parameter space. This distinction, however, is irrelevant in the context of this work.