# Chapter 3

# Smoothing quantum oscillations

This chapter is devoted to the inclusion of finite temperature and impurity scattering in semiclassical approximations. The common microscopic approach is outlined, and another, more mathematically oriented ansatz is presented. The comparison of the two procedures allows an extension of the smoothing formalism to higher-order contributions in  $\hbar$ . This section provides some of the technical details which will be important when considering  $\hbar$  corrections in the subsequent chapters.

## Contents

3.2	The	relation	between smoothing and amplitude damping
3.3	$\mathbf{Smo}$	othing h	beyond the leading order in $\hbar$
:	3.3.1	Includin	g oscillating amplitudes
		3.3.1.1	Oscillating real amplitudes
		3.3.1.2	Special case: Tangent bifurcations
		3.3.1.3	Oscillating complex amplitudes
		3.3.1.4	Special case: Grazing
;	3.3.2	The fold	ing approach
3.4	$\mathbf{Smo}$	othing f	or other reasons

The quantum mechanical level density of pure systems is given by a sum of  $\delta$ -functions centered at the eigenenergies. Experiments on mesoscopic systems, however, are performed at finite temperatures. Furthermore, the samples are not ideally clean, but incorporate impurities (contaminations, lattice defects, etc.). These effects broaden the levels to a finite width, thus *smoothing* the level density. If the line width is smaller than the mean level spacing, the individual quantum states can still be observed. This situation will be referred to as *full quantization*. For larger smoothing widths, i. e. line widths larger that the mean level spacing, the individual levels cannot be resolved. This is called the *coarse-grained* level density in the following.

Only for very peculiar systems, like the harmonic oscillator, are the levels regularly distributed in energy. The generic situation for finite fermion systems are groups of levels, separated by gaps larger than the mean level spacing. These groups are called *shells* according to the canonical example of the electronic s-, p-, d-, ... shells in atoms. This *shell structure* survives even for strong broadening of the lines. It is therefore often the only experimentally observable reminiscence of the quantum nature of a sample. Those shell effects are a typical feature of finite fermion systems. Prominent examples include the abundance spectra of alkali clusters [50, 26] or the stability of nuclei [117].

This chapter deals with techniques that include the effects which lead to finite line widths in the semiclassical trace formula. The common ansatz starts with including the microscopic effects on a quantum mechanical level and re-derives the semiclassical approximation along the same line as calculating the original trace formula. The resulting expression differs from the simple trace formula Eq. (2.14) by additional terms that damp the amplitudes of the periodic orbit contributions.

In Sec. 3.2, an alternative ansatz is derived. The essential idea is to establish a formal relation between line shapes and amplitude damping schemes. Provided the knowledge of the correct line shape, this method can also be used for the calculation of the corresponding amplitude damping factors.

In leading order of  $\hbar$ , these two approaches lead of course to equivalent results. The second technique, however, can be generalized to higher-order contributions. The idea exploited in Sec. 3.3 is to replace the microscopic ansatz by the second approach if higher orders in  $\hbar$  are to be included. This will be of great importance for the examination of higher-order contributions in  $\hbar$  to the trace sum in the subsequent chapters.

A couple of nice side results from the inclusion of finite line widths in the trace formula are discussed in Sec. 3.4.

## 3.1 The microscopic approach to smoothing

The general scheme how to include finite temperatures, impurity scattering, and related effects on a microscopic level necessitates the re-derivation of the trace formula. After incorporating the effect in the quantum mechanical calculation, e.g. by including weak disorder or finite temperature by the appropriate ensemble averages, the Green's functions are replaced by their semiclassical approximations. Subsequent stationary phase approximations lead to trace formulae similar to Eq. (2.14). This approach opens up the possibility of a semiclassical calculation of line shapes and line widths. Note, however, that despite recent progress [60] the quantum mechanical calculation of line shapes and

line widths is still a mostly unsettled problem.<sup>1</sup> Since the semiclassical approximation starts from the quantum formalism, this is equally true for for semiclassics. This work is not intended to contribute to questions related to line shapes and relative amplitudes, so that temperature and scattering will only be included along the simple lines outlined below.

For the very low temperatures used in the measurement of mesoscopic semiconductor devices, phonons (and their interaction with charge carriers) can be neglected. The only relevant temperature-related effect concerning the level density stems from the Fermi distribution. For this situation, the inclusion of finite temperature on the oscillating part of the level density is simply given by

$$\delta g(\mu, T) = \int_0^\infty dE \,\,\delta g(E, T = 0) \,f'(E - \mu) \,, \tag{3.1}$$

with the Fermi distribution function

$$f(E - \mu) = \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} .$$
(3.2)

The derivative of the Fermi distribution is strongly peaked around the Fermi energy  $\mu$ , so that Eq. (3.1) mainly introduces an energy average over a typical width of  $k_BT$ . Performing this integration leads to an additional temperature-dependent factor R in the trace formula

$$R(T_{\rm po}) = \frac{T_{\rm po}/\tau_T}{\sinh(T_{\rm po}/\tau_T)} .$$
(3.3)

Here  $T_{\rm po}$  is the period of the orbit and  $\tau_T = \hbar k_B T / \pi$  defines the thermal cutoff time  $\tau_T$ . For a detailed derivation, see for example Refs. [96, 105, 100, 17].

The inclusion of impurities in semiclassical formulae is, even on an elementary level, much more elaborate than including finite temperature. In the semiclassical picture, scattering enters via three distinct effects:

- 1. The amplitudes of the periodic orbits are reduced due to the finite probability of scattering out of the trajectory. This effect is relevant even for small impurity concentrations.
- 2. New orbits which include scattering events (i. e. closed 'hopping' orbits from scattering center to scattering center) occur. These orbits are for example responsible for universal conductance fluctuations (UCF) and weak localization. This effect is only relevant for sufficiently high concentrations of scatterers.
- 3. Scattering may introduce interference between otherwise coherent orbits (like in degenerate orbit families).

In ballistic systems, the first of these effects dominates. Since scattering will only be considered with respect to transport properties in later sections, the discussion about the inclusion of the effects is postponed until then. Here only the main result of this analysis

 $<sup>^{1}</sup>$ This applies especially to transport properties. So for example not even the amplitude of the Shubnikovde-Haas oscillations of the free 2DEG is understood theoretically [125].

should be stated, namely that for ballistic systems the procedure is very similar to the inclusion of finite temperatures. The effect of the scatterers can be approximated by a damping factor F depending exponentially on the orbit length

$$F(L_{\rm po}) = e^{-L_{\rm po}/(2\ell)} .$$
(3.4)

Here  $\ell$  is the elastic mean-free path of the system and  $L_{\rm po}$  denotes the orbit length. For billiards, where  $L_{\rm po} = v_F T_{\rm po}$ , this damping can also be expressed in terms of the scattering time  $\tau_s$  by

$$F(T_{\rm po}) = e^{-T_{\rm po}/(2\tau_s)} , \qquad (3.5)$$

where the scattering time is related to the mobility  $\mu$  by  $\tau_s = m^* \mu/e$ .

These two results establish a first connection between smoothing and amplitude damping, a relation that will be examined more deeply in the following section. Please note that the semiclassical inclusion of finite temperature and mean-free path is – just as the trace formula itself – only correct up to leading order in  $\hbar$ . Therefore this approach is not appropriate for the inclusion of higher-order  $\hbar$  terms. For those contributions, a modified smoothing scheme needs to be developed.

# 3.2 The relation between smoothing and amplitude damping

Finite temperature and scattering lead to finite widths of the individual energy levels. The effect is equivalent to a convolution of the  $\delta$ -functions constituting the level density with the line shape induced by temperature and impurity effects. This section discusses from a more mathematical point of view how this convolution integral can be implemented in the trace formula. The main result is Eq. (3.18), which states a one-to-one relation between line shapes and amplitude damping functions.

The general form of a trace formula is given by

$$\delta g = \sum_{\Gamma} A_{\Gamma}(E) e^{i \frac{S_{\Gamma}(E)}{\hbar} - i\sigma_{\Gamma} \frac{\pi}{2}}, \qquad (3.6)$$

where  $\Gamma$  is a one-dimensional classification of the classical periodic orbits. If there is a generalized energy e(E), and functions  $G(\Gamma, E)$  and  $\tilde{\sigma}(G)$ , which fulfill

$$\frac{S_{\Gamma}(E)}{\hbar} - \sigma_{\Gamma} \frac{\pi}{2} = eG - \tilde{\sigma}(G) , \qquad (3.7)$$

the trace formula can be rewritten as

$$\delta g = \sum_{G} A_2(e, G) e^{ieG} .$$
 (3.8)

For the last step it was assumed that every orbit is uniquely determined by its value of G. By rescaling,  $G \in \mathbb{N}$  can always be obtained; the rescaling factors should be included in  $A_2(e, G)$ . The most simple situation is that  $A_2$  factorizes in terms depending only on the generalized energy e and the classification variable G:

$$A_2(e,G) = A_G(G) A_e(e) . (3.9)$$

Approximating Eq. (3.8) by an integral

$$\delta g \approx A_e(e) \int A_G(G) e^{ieG} dG .$$
(3.10)

gives (apart from normalization constants) the oscillating part of the level density  $\delta g$  as the Fourier transform of  $A_G(G)$ :

$$\delta g(e) \approx \sqrt{2\pi} A_e(e) \mathcal{F}[A_G(G)].$$
(3.11)

The Fourier transform is denoted by

$$\mathcal{F}[A_G(G)] := \frac{1}{\sqrt{2\pi}} \int A_G(G) e^{ieG} \, dG \,. \tag{3.12}$$

Using the well-known folding theorem, an arbitrary window function F(G) leads to

$$\int F(G) A_2(e, G) e^{ieG} dG \approx \delta g(e) * f(e) .$$
(3.13)

Here  $f(e) = \mathcal{F}[F(G)]$  denotes the Fourier transform of F(G) and "\*" stands for the convolution integral. Therefore

$$\delta g^F := \sum_{\Gamma} F(G) A_{\Gamma}(E) e^{i \frac{S_{\Gamma}(E)}{\hbar} - i\sigma_{\Gamma} \frac{\pi}{2}} \approx \delta g(e) * f(e) , \qquad (3.14)$$

where  $\delta g^F$  denotes the trace formula with damped amplitudes. This relation shows that folding the semiclassical level density with a *smoothing function* f(e) is equivalent to a multiplication of the amplitudes with a *window function* F(G). Unfortunately the restrictions of Eqs. (3.7) and (3.9) are quite severe and often prevent the application of Eq. (3.14). With two additional approximations these restrictions can be relaxed.

In the generic situation Eq. (3.9) is violated and only the common dependence of the amplitudes on e can be separated out:

$$A_2(e,G) = A_G(e,G) A_e(e) . (3.15)$$

In this case Eq. (3.14) is still a good approximation if the variation of  $A_G(e, G)$  in e is sufficiently slow. Denoting the characteristic width of f(e) with  $\gamma$ , this means that  $A_G(e, G)$  has to be nearly constant over a region  $\gamma$  in e.

If, on the other hand, there are no functions e(E) and  $G(E, \Gamma)$  that fulfill Eq. (3.7), a local expansion of the action S in powers of e can be used:

$$\frac{S}{\hbar} = \frac{S(e_0)}{\hbar} + G(e_0) (e - e_0) + \mathcal{O}(e - e_0)^2 .$$
(3.16)

If this approximation is valid in a region in e that is wider than the typical width  $\gamma$  of the smoothing function, Eq. (3.14) still holds. In the general case G is therefore given by the first derivative of the classical action with respect to e:

$$G(E) = \frac{1}{\hbar} \frac{\mathrm{d}S}{\mathrm{d}e} \bigg|_{E} \,. \tag{3.17}$$

With e = E,  $\hbar G$  is the period T of the orbit, so that  $\hbar G$  is referred to as the quasiperiod. For systems with constant absolute velocity along the orbit (this holds especially for billiards), the choice e = k leads to

$$\frac{\mathrm{d}S}{\mathrm{d}e} = \frac{\mathrm{d}S}{\mathrm{d}E}\frac{\mathrm{d}E}{\mathrm{d}k} = T \cdot \frac{k\hbar^2}{m} = \hbar L \; ,$$

where L is the geometrical orbit length.

Putting all approximations together, it was shown that damping the amplitudes in the trace formula with a window function F(G) results in an approximation for the level density folded with the Fourier transform of F(G):

$$\delta g^F \approx f(e) * \delta g . \tag{3.18}$$

This is the main result of this section. Eq. (3.18) holds if the conditions

$$S \approx S(e_0) + G(e_0) \ (e - e_0) \tag{3.19}$$

and

$$A_2(e,G) \approx \text{const}$$
 (3.20)

are fulfilled in a region wider than the typical width  $\gamma$  of the smoothing function. These conditions depend mainly on the behavior of the actions and amplitudes of the orbits. In order to match them, a well-adapted choice of the generalized energy is essential. Note that for narrow smoothing functions (small  $\gamma$ ), the conditions are less restrictive. Therefore, using Eq. (3.18) is often justified for a full quantization, whereas for the calculation of the gross-shell structure the conditions Eqs. (3.19) and (3.20) put tight limits on the use of the amplitude damping ansatz – which might seem counter-intuitive at first sight. Since every orbit is uniquely determined by its value of G, and G should be sufficiently smooth in practical applications, the amplitude damping scheme may not depend explicitly on the repetition number of the orbit. For most of the the applications of Eq. (3.18) in the present work this limitation will be irrelevant. Note, however, that for the damping scheme commonly used for the free 2DEG (compare to chapter 6), Eq. (3.18) does not apply.

A simple example might be helpful to illustrate the result. Pure billiard systems are those where the the action along the orbits scales with the wave number:  $S = \hbar k \cdot L$ , and L, the geometric orbit length, is independent of the energy. Setting

$$e(E) = k = \sqrt{\frac{2mE}{\hbar^2}}$$
 and  $G(\Gamma) = L$ , (3.21)

Eq. (3.19) is fulfilled trivially. If Eq. (3.20) is also matched, then the use of a window function F depending on the orbit length L is equivalent to a folding of the level density

in k. Evaluating the trace formula with a Gaussian depending on the orbit length L as window function yields the level density folded with a Gaussian in k. This is the technique commonly practiced for the computation of trace formulas for billiard systems. Eq. (3.18) is somewhat more general, since it is not restricted to billiard systems nor to special window functions.

The use of Eq. (3.18) is very convenient. Its range of validity can easily be checked using Eqs. (3.19) and (3.20). Furthermore, there is no general limitation of its applicability to the leading order in  $\hbar$ . In the following section Eq. (3.18) will be modified so that it can deal with two  $\hbar$  corrections which occur in the disk billiard.

# 3.3 Smoothing beyond the leading order in $\hbar$

The microscopic ansatz for the inclusion of scattering and finite temperature in the trace formula is, as already pointed out, limited to the contributions of leading order in  $\hbar$ . It is therefore questionable to use this smoothing scheme for higher-order  $\hbar$  terms like bifurcations or grazing, since thereby the influence of the corrections on the smoothing is neglected. The examination of the impact of higher-order  $\hbar$  corrections thus demands a generalized smoothing scheme which is applicable to the relevant  $\hbar$  corrections. But just as the inclusion of  $\hbar$  corrections necessitates an adaption to the smoothing scheme, so does the exclusion thereof. This comes about as omitting  $\hbar$  corrections does not only lead to missing terms in the trace sum, but also renders the inclusion of the smoothing inaccurate. A way to distinguish these two effects is desired.

A complete inclusion of second leading order  $\hbar$  effects in the microscopic calculation of Sect. 3.1 requires the derivation of the trace formula itself to second order. This task is, as already pointed out, both numerically and analytically so involved that it renders the semiclassical approach useless for practical applications. This work therefore follows a different approach, namely to replace the microscopic approach by the formulas stating the equivalence between smoothing and amplitude damping. The latter formulae shall be found much easier to generalize.

Along this path, the following section derives explicit amplitude damping formulas applicable to two kinds of higher-order  $\hbar$  corrections, namely bifurcations and grazing. The ansatz is, however, not restricted to these specific cases but can be used to derive analogous formulae for a large class of corrections.

After that, Sec. 3.3.2 will introduce the *folding approach*, a simple numerical scheme cutting down the influence of higher-order  $\hbar$  contributions on the smoothing procedure. This method does not rely on the knowledge of the correction terms, so that it makes the separation of the two contributions of  $\hbar$  corrections to the trace formula discussed above possible.

#### 3.3.1 Including oscillating amplitudes

The general procedure to implement smoothing in trace formulae has been derived in Sec. 3.2. The main result is restated here in a notation convenient for a generalization:

For an energy variable e(E) and a trace formula

$$\delta g = \mathcal{I}m\left[\sum_{\Gamma} A_{\Gamma}(e) e^{ix_{\Gamma}(e)}\right] = \sum_{\Gamma} A_{\Gamma}(e) \sin[x_{\Gamma}(e)], \qquad (3.22)$$

the smoothing, i. e. the convolution with the line shape function f(e), can be approximated by damping the semiclassical amplitudes with a window function  $F(T_{\Gamma})$ :

$$\delta g^F = \sum_{\Gamma} A_{\Gamma}(e) F(T_{\Gamma}) \sin[x_{\Gamma}(e)] \approx f(e) * \delta g .$$
(3.23)

This approximation is only valid for slowly varying real amplitudes. The implementation of two kinds of  $\hbar$  corrections to the trace formula for the disk billiard, namely tangent bifurcations and grazing, will lead to oscillating amplitudes. This motivates a generalization of Eq. (3.23) to oscillating real and complex amplitudes.

#### 3.3.1.1 Oscillating real amplitudes

Any real amplitude  $A_{\Gamma}(e)$  can be written as

$$A_{\Gamma}(e) = M_{\Gamma}(e) \cdot \cos[\Theta_{\Gamma}(e)], \qquad (3.24)$$

where  $\Theta(e)$  is monotonous in e and M(e) is real and does not change sign. Inserting this in Eq. (3.22) and using

$$\sin(x)\cos(\Theta) = \frac{1}{2}[\sin(x-\Theta) + \sin(x+\Theta)], \qquad (3.25)$$

the two terms can individually be treated according to Eq. (3.23). This leads to the following smoothing scheme generally applicable to oscillating real amplitudes:

$$\delta g^{F} = \sum_{\Gamma} M_{\Gamma} \left[ \bar{F} \cos(\Theta_{\Gamma}) \sin(x_{\Gamma}) + \Delta F \sin(\Theta_{\Gamma}) \cos(x_{\Gamma}) \right] \\ = \sum_{\Gamma} A_{\Gamma} \bar{F} \sin(x_{\Gamma}) + \sum_{\Gamma} \Delta F M_{\Gamma} \sin(\Theta_{\Gamma}) \cos(x_{\Gamma}) , \qquad (3.26)$$

where

$$\bar{F} = \frac{F^+ + F^-}{2} ; \quad \Delta F = \frac{F^+ - F^-}{2} ; F^+ = F(x' + \Theta') ; \quad F^- = F(x' - \Theta') .$$
(3.27)

The dashes denote the derivatives with respect to e. For slowly oscillating amplitudes  $(\Theta' \ll x')$  the second term in Eq. (3.26) is negligible, whereas the first term reproduces the previous result for non-oscillating amplitudes Eq. (3.14). The second term gives a correction depending mainly on  $\Theta'$ , i.e. the frequency of the amplitude oscillation. As expected, this correction is large for rapidly oscillating amplitudes.

#### **3.3.1.2** Special case: Tangent bifurcations

The uniform approximation of the tangent bifurcation according to Eqs. (B.8) and (B.7) leads to the Airy function as semiclassical amplitude. For this special case

$$\delta g = \sum_{\Gamma} Ai(y_{\Gamma}) \sin(x_{\Gamma})$$
(3.28)

one gets, using Eq. (3.26),

$$\delta g^F = \sum_{\Gamma} \left[ \bar{F} Ai(y_{\Gamma}) \sin(x_{\Gamma}) + \Delta F Bi(y_{\Gamma}) \cos(x_{\Gamma}) \right] .$$
(3.29)

The frequency  $\Theta'$  can be expressed as

$$\Theta'(e) = \frac{Ai(e)Bi'(e) - Ai'(e)Bi(e)}{Ai(e)^2 + Bi(e)^2} \cdot y'.$$
(3.30)

These formulas are used in Sec. 4.3.3 on the treatment of the tangent bifurcations in the disk billiard. There, the corrections to the smoothing scheme (i.e. mainly the second term of Eq. (3.29)) will be seen to be comparable to the corrections stemming from the uniform treatment of the bifurcations. This shows that the correct implementation of the smoothing is vital for an examination of higher-order  $\hbar$  contributions to the trace formula.

#### 3.3.1.3 Oscillating complex amplitudes

For oscillating complex amplitudes, Eq. (3.26) can be applied to the real and the imaginary part of  $A_{\Gamma}$  separately, so that no special treatment has to be introduced. For the special case that the amplitude can be written as

$$A_{\Gamma}(e) = M_{\Gamma}(e) \cdot \exp\{i\Theta_{\Gamma}(e)\}, \qquad (3.31)$$

the implementation of smoothing is simply given by

$$\delta g^F = \sum_{\Gamma} M_{\Gamma} F^+ \sin(x_{\Gamma} + \Theta_{\Gamma}) . \qquad (3.32)$$

Note that now both the oscillating term and the damping via the window function F only depend on  $x_{\Gamma} + \Theta_{\Gamma}$ . This is similar to the original formula for slowly varying amplitudes Eq. (3.23).

#### 3.3.1.4 Special case: Grazing

Eq. (3.32) can be used for the Fresnel integrals occurring in grazing corrections (see, e. g., Sec. 4.3.4). Setting

$$\tilde{I}(y) = \left(C(y) - \frac{1}{2}\right) + i\left(S(y) - \frac{1}{2}\right) , \qquad (3.33)$$

I can be written according to Eq. (3.31). Using Eq. (3.32), some straight-forward calculations show that the smoothing of a trace formula

$$\delta g = \mathcal{I}m\left[\sum_{\Gamma} \left[\mathcal{C}(y_{\Gamma}) + i\alpha \mathcal{S}(y_{\Gamma})\right] e^{ix_{\Gamma}}\right]$$
(3.34)

can be implemented by

$$\delta g^{F} = \sum_{\Gamma} \left( F^{+} \left[ C(y) \sin(x) + \alpha S(y) \cos(x) \right] + \frac{F(x') - F^{+}}{\sqrt{2}} \sin\left(x + \alpha \frac{\pi}{4}\right) \right), \quad (3.35)$$

where  $\alpha = \pm 1$  and  $\Theta = \pi/2 \cdot y^2$ . Note that now, in contrast to Eq. (3.32), a correction term with an amplitude depending mainly on  $\Theta'$  shows up.

## 3.3.2 The folding approach

The smoothing procedure presented above can only be applied if the  $\hbar$  corrections can be calculated explicitly. But, as already pointed out, also the neglected (and thus unknown) corrections affect the validity of the amplitude damping ansatz for the implementation of smoothing. This is especially clear for bifurcations: Neglecting bifurcations leads to diverging Gutzwiller amplitudes. In the vicinity of the bifurcation condition Eq. (3.20) of Sec. 3.2 is thus violated. The convolution of the trace sum with the line shape is therefore no longer equivalent to the common amplitude damping. Since at bifurcations the contribution to the trace sum is lower in powers of  $\hbar$ , the microscopic approach also fails, as the leading-order assumption is not fulfilled.

The simplest technique to separate the direct influence of higher-order  $\hbar$ -terms on the trace formula from the effects they have on the implementation of smoothing is to perform the smoothing exactly by a numerical convolution with the appropriate line shape. With the plausible assumption that higher-order  $\hbar$  contributions do not influence the line shape, this can be taken according to Sec. 3.2 as the Fourier transform of the amplitude damping function. This numerical procedure to implement smoothing in the trace formula will be referred to as folding approach.

Both the example of the disk billiard in chapter 4 and the magnetoconductance of the channel with antidots in chapter 7 will show that for systems where many orbits contribute, the dominating effect of bifurcations is not given by the additional terms they introduce in the trace formula, but stems from their influence on the implementation of smoothing. Neglecting the  $\hbar$ -corrections of the bifurcations in trace formulae, but correctly implementing the smoothing, will prove to be a good approximation in these cases.

# 3.4 Smoothing for other reasons

Even for systems where no experimental smoothing is relevant,<sup>2</sup> the implementation of a smoothing scheme as presented above might be useful.

A first motivation is given by the mathematical properties of semiclassical trace formulae. In the form used in this work, they exhibit non-trivial convergence properties. From a

<sup>&</sup>lt;sup>2</sup>See for example the disk billiard in chapter 4, which is only compared to the pure quantum result.

mathematical point of view they cannot be summed up straight-forwardly. This is already clear from the fact that the quantum mechanical single particle level densities are sums of  $\delta$ -functions. These are not functions in a mathematical sense, but *distributions*, which need special treatment. For various attempts establishing proper resummation schemes of trace formulae see Refs. [111, 101].

If one considers, on the other hand, the smoothed level density, the mathematical problems vanish to a great extent. Calculating the trace formula without smoothing as the limit of vanishing smoothing width allows to ignore the convergence properties of the trace sums within the context of this work.

Another application of smoothing is to cope with the technical limits of a numerical evaluation of the trace formula. Eq. (2.14) consists of a sum over all classical periodic orbits of a system, usually infinitely many. In a numerical approach, this sum has to be truncated. The impact of this truncation can be controlled according to Sec. 3.2 by identifying the cut-off with the window function F(G). Eq. (3.18) thus allows a precise estimate of the error introduced by the truncation in a numerical evaluation.

It is however often more effective to use the relation between smoothing and amplitude damping in the other direction: Given the tolerated numerical effort, the question is how to choose the orbits which are included in the numerical evaluation. This problem is equivalent to the standard problem of Fourier spectroscopy, namely how to get the best spectrum from a finite range of measured intensities. There, special window functions in analogy to Sec. 3.2 are used. There is a large variety of reasonable window-functions at hand. For a detailed discussion see Ref. [43]. There is no optimal window function for all applications, as there is a fundamental trade-off between the width of the peaks and the intensity of spurious sidebands. For the evaluation of the trace formula it is usually convenient to use window functions which already include the (unavoidable) truncation. Choosing a F(G)which is nonzero only in a finite range automatically controls the truncation error. In this work, a triangular window function is used.

The last reason for the implementation of a smoothing scheme like Eq. (3.18) is closely related to the problem of the numerical evaluation of trace formulae mentioned above. For any given window function (which may be only due to the truncation scheme implemented), the expected line width and line shape can be calculated. This method provides the basis for a very precise numerical calculation of the semiclassical single-particle energies. For details see Sec. 4.6 of Ref. [1]. In Ref. [2] this ansatz was used to prove the identity of the EBK and the Gutzwiller result for the disk billiard numerically.