

## Appendix A45

# Semiclassical quantization, with corrections

In fact I'm Vattay Gábor, just these Indo-Europeans mix up the right order.

(G. Vattay)

**T**HE GUTZWILLER TRACE FORMULA is only a good approximation to the quantum mechanics when  $\hbar$  is small. Can we improve the trace formula by adding quantum corrections to the semiclassical terms? A similar question can be posed when the classical deterministic dynamics is disturbed by some way Gaussian white noise with strength  $D$ . The deterministic dynamics then can be considered as the weak noise limit  $D \rightarrow 0$ . The effect of the noise can be taken into account by adding noise corrections to the classical trace formula. A formal analogy exists between the noise and the quantum problem. This analogy allows us to treat the noise and quantum corrections together.



### A45.1 Periodic orbits as integrable systems

From now on, we use the language of quantum mechanics, since it is more convenient to visualize the results there. Where it is necessary we will discuss the difference between noise and quantum cases.

First, we introduce periodic orbits from an unusual point of view, which can convince you, that chaotic and integrable systems are in fact not as different from each other, than we might think. If we start orbits in the neighborhood of a periodic orbit and look at the picture on the Poincaré section we can see a regular picture. For stable periodic orbits the points form small ellipses around the center and for unstable orbits they form hyperbolas (see figure [A45.1](#)).

**Figure A45.1:** Poincaré section close to a stable and an unstable periodic orbit.

The motion close to a periodic orbit is regular in both cases. This is due to the fact, that we can linearize the Hamiltonian close to an orbit, and linear systems are always integrable. The linearized Hamilton's equations close to the periodic orbit  $(q_p(t) + q, p_p(t) + p)$  are of the form

$$\begin{aligned}\dot{q} &= +\partial_{pq}^2 H(q_p(t), p_p(t)) q + \partial_{pp}^2 H(q_p(t), p_p(t)) p \\ \dot{p} &= -\partial_{qq}^2 H(q_p(t), p_p(t)) q - \partial_{qp}^2 H(q_p(t), p_p(t)) p,\end{aligned}$$

where the new coordinates  $q$  and  $p$  are relative to a periodic orbit. This linearized equation can be regarded as a  $D$  dof oscillator with time periodic frequencies (where 'dof' stands for the Hamiltonian 'degree of freedom'). These equations are representing the equation of motion in a redundant way since more than one combination of  $q$ ,  $p$  and  $t$  determines the same point of the phase space. This can be cured by an extra restriction on the variables, a constraint the variables should fulfill. This constraint can be derived from the time independence or stationarity of the full Hamiltonian

$$\partial_t H(q_p(t) + q, p_p(t) + p) = 0. \quad (\text{A45.1})$$

Using the linearized form of this constraint we can eliminate one of the linearized equations. It is very useful, although technically difficult, to do one more transformation and to introduce a coordinate, which is parallel with the Hamiltonian flow ( $x_{\parallel}$ ) and others which are orthogonal. In the orthogonal directions we again get linear equations. These equations with  $x_{\parallel}$  dependent rescaling can be transformed into normal coordinates, so that we get tiny oscillators in the new coordinates with constant frequencies. This result has first been derived by Poincaré for equilibrium points and later it was extended for periodic orbits by V.I. Arnol'd and co-workers. In the new coordinates, the Hamiltonian reads as

$$H_0(x_{\parallel}, p_{\parallel}, x_n, p_n) = \frac{1}{2} p_{\parallel}^2 + U(x_{\parallel}) + \sum_{n=1}^{D-1} \frac{1}{2} (p_n^2 \pm \omega_n^2 x_n^2), \quad (\text{A45.2})$$

which is the general form of the Hamiltonian in the neighborhood of a periodic orbit. The  $\pm$  sign denotes, that for stable modes the oscillator potential is positive while for an unstable mode it is negative. For the unstable modes,  $\omega$  is the Lyapunov exponent of the orbit

$$\omega_n = \ln \Lambda_{p,n} / T_p, \quad (\text{A45.3})$$

where  $\Lambda_{p,n}$  is the expanding eigenvalue of the Jacobi matrix. For the stable directions the eigenvalues of the Jacobi matrix are connected with  $\omega$  as

$$\Lambda_{p,n} = e^{-i\omega_n T_p}. \quad (\text{A45.4})$$

The Hamiltonian close to the periodic orbit is integrable and can be quantized by the Bohr-Sommerfeld rules. The result of the Bohr-Sommerfeld quantization for

the oscillators gives the energy spectra

$$\begin{aligned} E_n &= \hbar\omega_n \left( j_n + \frac{1}{2} \right) && \text{for stable modes} \\ E_n &= -i\hbar\omega_n \left( j_n + \frac{1}{2} \right) && \text{for unstable modes,} \end{aligned} \quad (\text{A45.5})$$

where  $j_n = 0, 1, \dots$ . It is convenient to introduce the index  $s_n = 1$  for stable and  $s_n = -i$  for unstable directions. The parallel mode can be quantized implicitly through the classical action function of the mode:

$$\frac{1}{2\pi} \oint p_{\parallel} dx_{\parallel} = \frac{1}{2\pi} S_{\parallel}(E_m) = \hbar \left( m + \frac{m_p \pi}{2} \right), \quad (\text{A45.6})$$

where  $m_p$  is the topological index of the motion in the parallel direction. The latter condition can be rewritten by a very useful trick into the equivalent form (39.18)

$$1 - e^{iS_{\parallel}(E_m)/\hbar - im_p \pi/2} = 0. \quad (\text{A45.7})$$

The eigenenergies of a semiclassically quantized periodic orbit are all the possible energies

$$E = E_m + \sum_{n=1}^{D-1} E_n. \quad (\text{A45.8})$$

This relation allows us to change in (A45.7)  $E_m$  with the full energy minus the oscillator energies  $E_m = E - \sum_n E_n$ . All the possible eigenenergies of the periodic orbit then are the zeroes of the expression

$$\Delta_p(E) = \prod_{j_1, \dots, j_{D-1}} \left( 1 - e^{iS_{\parallel}(E - \sum_n \hbar s_n \omega_n (j_n + 1/2))/\hbar - im_p \pi/2} \right). \quad (\text{A45.9})$$

If we Taylor expand the action around  $E$  to first order

$$S_{\parallel}(E + \epsilon) \approx S_{\parallel}(E) + T(E)\epsilon, \quad (\text{A45.10})$$

where  $T(E)$  is the period of the orbit, and use the relations of  $\omega$  and the eigenvalues of the Jacobi matrix, we get the expression of the Selberg product

$$\Delta_p(E) = \prod_{j_1, \dots, j_{D-1}} \left( 1 - \frac{e^{iS_p(E)/\hbar - im_p \pi/2}}{\prod_n \Lambda_{p,n}^{(1/2 + j_n)}} \right). \quad (\text{A45.11})$$

If we use the right convention for the square root we get exactly the  $D$  dof expression of the Selberg product formula we derived from the Gutzwiller trace formula in (39.19). Just here we derived it in a different way! The function  $\Delta_p(E)$  is the semiclassical zeta function for one prime orbit.

Now, if we have many prime orbits and we would like to construct a function which is zero, whenever the energy coincides with the Bohr-Sommerfeld quantized energy of one of the periodic orbits, we have to take the product of these determinants:

$$\Delta(E) = \prod_p \Delta_p(E). \quad (\text{A45.12})$$

The miracle of the semiclassical zeta function is, that if we take infinitely many periodic orbits, the infinite product will have zeroes not at these energies, but close to the eigenenergies of the whole system!

So we have learned that both stable and unstable orbits are integrable systems, and can be individually quantized semiclassically by the old Bohr-Sommerfeld rules. We have thus almost completed the program of Sommerfeld to quantize general systems with the method of Bohr. *A remark: In addition to the Bohr-Sommerfeld rules, we used the unjustified approximation (A45.10). Sommerfeld would never do this! At that point we loose some important precision compared to the Bohr-Sommerfeld rules and we get somewhat worse results than a semiclassical formula is able to do. We will come back to this point in sect. A45.4, when we discuss the quantum corrections.* To complete the program of full scale Bohr-Sommerfeld quantization of chaotic systems we have to go beyond the linear approximation around the periodic orbit.

The Hamiltonian close to a periodic orbit in the parallel and normal coordinates can be written as the ‘harmonic’ plus ‘anaharmonic’ perturbation

$$H(x_{||}, p_{||}, x_n, p_n) = H_0(x_{||}, p_{||}, x_n, p_n) + H_A(x_{||}, x_n, p_n), \quad (\text{A45.13})$$

where the anaharmonic part can be written as a sum of homogeneous polynomials of  $x_n$  and  $p_n$  with  $x_{||}$  dependent coefficients,

remark A45.1

$$\begin{aligned} H_A(x_{||}, x_n, p_n) &= \sum_{k=3} H^k(x_{||}, x_n, p_n) \\ H^k(x_{||}, x_n, p_n) &= \sum_{\sum \ell_n + m_n = k} H_{\ell_n, m_n}^k(x_{||}) x_n^{\ell_n} p_n^{m_n}. \end{aligned} \quad (\text{A45.14})$$

This classical Hamiltonian is hopeless from Sommerfeld’s point of view, since it is non integrable. However, Birkhoff in 1927 introduced the concept of normal form, which gives successive integrable approximations to a non-integrable problem. <sup>3</sup>

## A45.2 The Birkhoff normal form

Birkhoff studied the canonical perturbation theory close to an equilibrium point of a Hamiltonian. Equilibrium point is where the potential has a minimum  $\nabla U = 0$  and small perturbations lead to oscillatory motion. We can linearize the problem and by introducing normal coordinates  $x_n$  and conjugate momenta  $p_n$  the quadratic part of the Hamiltonian will be a set of oscillators

$$H_0(x_n, p_n) = \sum_{n=1}^D \frac{1}{2} (p_n^2 + \omega_n^2 x_n^2). \quad (\text{A45.15})$$

<sup>3</sup> It is a pity that in 1926 Schrödinger introduced wave mechanics, thus blocking the development of Sommerfeld’s concept.

The full Hamiltonian can be rewritten with the new coordinates

$$H(x_n, p_n) = H_0(x_n, p_n) + H_A(x_n, p_n), \quad (\text{A45.16})$$

where  $H_A$  is the anaharmonic part of the potential in the new coordinates. The anaharmonic part can be written as a series of homogeneous polynomials

$$\begin{aligned} H_A(x_n, p_n) &= \sum_{j=3}^{\infty} H^j(x_n, p_n) \\ H^j(x_n, p_n) &= \sum_{|\ell|+|m|=j} h_{\ell m}^j x^\ell p^m, \end{aligned}$$

where  $h_{\ell m}^j$  are real constants and we used the multi-indices  $\ell := (\ell_1, \dots, \ell_D)$  with definitions

$$|\ell| = \sum \ell_n, \quad x^\ell := x_1^{\ell_1} x_2^{\ell_2} \dots x_D^{\ell_D}.$$

Birkhoff showed, that that by successive canonical transformations one can introduce new momenta and coordinates such, that in the new coordinates the anaharmonic part of the Hamiltonian up to any given  $n$  polynomial will depend only on the variable combination

$$\tau_n = \frac{1}{2}(p_n^2 + \omega_n^2 x_n^2), \quad (\text{A45.17})$$

where  $x_n$  and  $p_n$  are the new coordinates and momenta, but  $\omega_n$  is the original frequency. This is called the Birkhoff normal form of degree  $N$ :

$$H(x_n, p_n) = \sum_{j=2}^N H^j(\tau_1, \dots, \tau_D), \quad (\text{A45.18})$$

where  $H^j$  are homogeneous degree  $j$  polynomials of  $\tau$ 's. This is an integrable Hamiltonian, the non-integrability is pushed into the remainder, which consists of polynomials of degree higher than  $N$ . We run into trouble only when the oscillator frequencies are commensurate, i.e., when it is possible to find a set of integers  $m_n$  such that the linear combination

$$\sum_{n=1}^D \omega_n m_n,$$

vanishes. This extra problem has been solved by Gustavson in 1966 and we call the object Birkhoff-Gustavson normal form. The procedure of the successive canonical transformations can be computerized and can be carried out up to high orders ( $\sim 20$ ).

Of course, we pay a price for forcing the system to be integrable up to degree  $N$ . For a non-integrable system the high order terms behave quite wildly and the series is not convergent. Therefore we have to use this tool carefully. Now, we learned how to approximate a non-integrable system with a sequence of integrable systems and we can go back and carry out the Bohr-Sommerfeld quantization.

### A45.3 Bohr-Sommerfeld quantization of periodic orbits

There is some difference between equilibrium points and periodic orbits. The Hamiltonian (A45.2) is not a sum of oscillators. One can transform the parallel part, describing circulation along the orbit, into an oscillator Hamiltonian, but this would make the problem extremely difficult. Therefore, we carry out the canonical transformations dictated by the Birkhoff procedure only in the orthogonal directions. The  $x_{\parallel}$  coordinate plays the role of a parameter. After the transformation up to order  $N$  the Hamiltonian (A45.14) is

$$H(x_{\parallel}, p_{\parallel}, \tau_1, \dots, \tau_{D-1}) = H_0(x_{\parallel}, p_{\parallel}, \tau_1, \dots, \tau_{D-1}) + \sum_{j=2}^N U^j(x_{\parallel}, \tau_1, \dots, \tau_{D-1}), \quad (\text{A45.19})$$

where  $U^j$  is a  $j$ th order homogeneous polynomial of  $\tau$ 's with  $x_{\parallel}$  dependent coefficients. The orthogonal part can be Bohr-Sommerfeld quantized by quantizing the individual oscillators, replacing  $\tau$ 's as we did in (A45.5). This leads to a 1-dimensional effective potential indexed by  $j_1, \dots, j_{D-1}$

$$H(x_{\parallel}, p_{\parallel}, j_1, \dots, j_{D-1}) = \frac{1}{2} p_{\parallel}^2 + U(x_{\parallel}) + \sum_{n=1}^{D-1} \hbar s_n \omega_n (j_n + 1/2) + \sum_{k=2}^N U^k(x_{\parallel}, \hbar s_1 \omega_1 (j_1 + 1/2), \hbar s_2 \omega_2 (j_2 + 1/2), \dots, \hbar s_{D-1} \omega_{D-1} (j_{D-1} + 1/2)), \quad (\text{A45.20})$$

where  $j_n$  can be any non-negative integer. The term with index  $k$  is proportional with  $\hbar^k$  due to the homogeneity of the polynomials.

The parallel mode now can be Bohr-Sommerfeld quantized for any given set of  $j$ 's

$$\begin{aligned} S_p(E, j_1, \dots, j_{D-1}) &= \oint dx_{\parallel} p_{\parallel} \\ &= \oint dx_{\parallel} \sqrt{E - \sum_{n=1}^{D-1} \hbar s_n \omega_n (j_n + 1/2) - U(x_{\parallel}, j_1, \dots, j_{D-1})} \\ &= 2\pi\hbar(m + m_p/2), \end{aligned}$$

where  $U$  contains all the  $x_{\parallel}$  dependent terms of the Hamiltonian. The spectral determinant becomes

$$\Delta_p(E) = \prod_{j_1, \dots, j_{D-1}} (1 - e^{iS_p(E, j_1, \dots, j_{D-1})/\hbar - m_p\pi/2}).$$

This expression completes the Sommerfeld method and tells us how to quantize chaotic or general Hamiltonian systems. Unfortunately, Schrödinger's wave mechanics postponed this nice formula until our book.

The formula has been derived with the help of the semiclassical Bohr-Sommerfeld quantization rule and the classical normal form theory. Indeed, if we expand  $S_p$  in the exponent in the powers of  $\hbar$

$$S_p = \sum_{k=0}^N \hbar^k S_k,$$

we get more than just a constant and a linear term. This formula already gives us corrections to the semiclassical zeta function in all powers of  $\hbar$ . There is a very attractive feature of this semiclassical expansion.  $\hbar$  in  $S_p$  shows up only in the combination  $\hbar s_n \omega_n (j_n + 1/2)$ . A term proportional with  $\hbar^k$  can only be a homogeneous expression of the oscillator energies  $s_n \omega_n (j_n + 1/2)$ . For example in two dimensions there is only one possibility of the functional form of the order  $k$  term

$$S_k = c_k(E) \cdot \omega_n^k (j + 1/2)^k,$$

where  $c_k(E)$  is the only function to be determined.

The corrections derived so far are *doubly* semiclassical, since they give semiclassical corrections to the semiclassical approximation. What can quantum mechanics add to this? As we have stressed in the previous section, the exact quantum mechanics is not invariant under canonical transformations. In other context, this phenomenon is called the operator ordering problem. Since the operators  $\hat{x}$  and  $\hat{p}$  do not commute, we run into problems, when we would like to write down operators for classical quantities like  $x^2 p^2$ . On the classical level the four possible orderings  $xpxp$ ,  $ppxx$ ,  $pxpx$  and  $xxpp$  are equivalent, but they are different in the quantum case. The expression for the energy (A45.20) is not exact. We have to go back to the level of the Schrödinger equation in order to obtain the exact expression.

## A45.4 Quantum calculation of $\hbar$ corrections

The Gutzwiller trace formula has originally been derived from the saddle point approximation of the Feynman path integral form of the propagator. The exact trace is a path-sum for all closed paths of the system

$$\text{tr} G(x, x', t) = \int dx G(x, x, t) = \int \mathcal{D}x e^{iS(x,t)/\hbar}, \quad (\text{A45.21})$$

where  $\int \mathcal{D}x$  denotes the discretization and summation for all paths of time length  $t$  in the limit of the infinite refinement and  $S(x, t)$  is the classical action calculated along the path. The trace in the saddle point calculation is a sum for classical periodic orbits and zero length orbits, since these are the extrema of the action  $\delta S(x, t) = 0$  for closed paths:

$$\text{tr} G(x, x', t) = g_0(t) + \sum_{p \in PO} \int \mathcal{D}\xi_p e^{iS(\xi_p + x_p(t), t)/\hbar}, \quad (\text{A45.22})$$

where  $g_0(t)$  is the zero length orbit contribution. We introduced the new coordinate  $\xi_p$  with respect to the periodic orbit  $x_p(t)$ ,  $x = \xi_p + x_p(t)$ . Now, each path sum  $\int \mathcal{D}\xi_p$  is computed in the vicinity of periodic orbits. Since the saddle points are taken in the configuration space, only spatially distinct periodic orbits, the so called prime periodic orbits, appear in the summation. So far nothing new has been invented. If we continue the standard textbook calculation scheme, we have to Taylor expand the action in  $\xi_p$  and keep the quadratic term in the exponent while treating the higher order terms as corrections. Then we can compute the path integrals with the help of Gaussian integrals. The key point here is that we do not compute the path sum directly. We use the correspondence between path integrals and partial differential equations. This idea comes from Maslov, and a good summary is given in ref. [2]. We search for that Schrödinger equation, which leads to the path sum

$$\int \mathcal{D}\xi_p e^{iS(\xi_p+x_p(t),t)/\hbar}, \quad (\text{A45.23})$$

where the action around the periodic orbit is in a multi-dimensional Taylor expanded form:

$$S(x, t) = \sum_{\mathbf{n}} s_{\mathbf{n}}(t)(x - x_p(t))^{\mathbf{n}}/\mathbf{n}! \quad (\text{A45.24})$$

The symbol  $\mathbf{n} = (n_1, n_2, \dots, n_D)$  denotes the multi index for  $D$  dofs,  $\mathbf{n}! = \prod_{i=1}^D n_i!$  the multi factorial and  $(x - x_p(t))^{\mathbf{n}} = \prod_{i=1}^D (x_i - x_{p,i}(t))^{n_i}$ , respectively. The expansion coefficients of the action can be determined from the Hamilton-Jacobi equation

$$\partial_t S + \frac{1}{2}(\nabla S)^2 + U = 0, \quad (\text{A45.25})$$

in which the potential is expanded in a multidimensional Taylor series around the orbit

$$U(x) = \sum_{\mathbf{n}} u_{\mathbf{n}}(t)(x - x_p(t))^{\mathbf{n}}/\mathbf{n}!. \quad (\text{A45.26})$$

The Schrödinger equation

$$i\hbar\partial_t\psi = \hat{H}\psi = -\frac{\hbar^2}{2}\Delta\psi + U\psi, \quad (\text{A45.27})$$

with this potential also can be expanded around the periodic orbit. Using the WKB ansatz

$$\psi = \varphi e^{iS/\hbar}, \quad (\text{A45.28})$$

we can construct a Schrödinger equation corresponding to a given order of the Taylor expansion of the classical action. The Schrödinger equation induces the Hamilton-Jacobi equation (A45.25) for the phase and the transport equation of Maslov and Fjedoruk [15] for the amplitude:

$$\partial_t\varphi + \nabla\varphi\nabla S + \frac{1}{2}\varphi\Delta S - \frac{i\hbar}{2}\Delta\varphi = 0. \quad (\text{A45.29})$$



This partial differential equation, solved in the neighborhood of a periodic orbit with the expanded action (A45.24), belongs to the local path-sum (A45.23).

If we know the Green's function  $G_p(\xi, \xi', t)$  corresponding to the local equation (A45.29), then the local path sum can be converted back into a trace:

$$\int \mathcal{D}\xi_p e^{i/\hbar \sum_n S_n(x_p(t), t) \xi_p^n / n!} = \text{tr } G_p(\xi, \xi', t). \quad (\text{A45.30})$$

The saddle point expansion of the trace in terms of local traces then becomes

$$\text{tr } G(x, x', t) = \text{tr } G_W(x, x', t) + \sum_p \text{tr } G_p(\xi, \xi', t), \quad (\text{A45.31})$$

where  $G_W(x, x', t)$  denotes formally the Green's function expanded around zero length orbits, known as the Weyl term [3–5]. Each Green's function can be Fourier-Laplace transformed independently and by definition we get in the energy domain

$$\text{tr } G(x, x', E) = g_0(E) + \sum_p \text{tr } G_p(\xi, \xi', E). \quad (\text{A45.32})$$

Note that we do not need here to take further saddle points in time, since we are dealing with exact time and energy domain Green's functions.

The spectral determinant is a function which has zeroes at the eigenenergies  $E_n$  of the Hamilton operator  $\hat{H}$ . Formally it is

$$\Delta(E) = \det(E - \hat{H}) = \prod_n (E - E_n).$$

The logarithmic derivative of the spectral determinant is the trace of the energy domain Green's function:

$$\text{tr } G(x, x', E) = \sum_n \frac{1}{E - E_n} = \frac{d}{dE} \log \Delta(E). \quad (\text{A45.33})$$

We can define the spectral determinant  $\Delta_p(E)$  also for the local operators, writing

$$\text{tr } G_p(\xi, \xi', E) = \frac{d}{dE} \log \Delta_p(E). \quad (\text{A45.34})$$

Using (A45.32) we can express the full spectral determinant as a product for the sub-determinants

$$\Delta(E) = e^{W(E)} \prod_p \Delta_p(E),$$

where  $W(E) = \int^E g_0(E') dE'$  is the term coming from the Weyl expansion.

The construction of the local spectral determinants can be done easily. We have to consider the stationary eigenvalue problem of the local Schrödinger problem and keep in mind, that we are in a coordinate system moving together with the periodic orbit. If the classical energy of the periodic orbit coincides with an

eigenenergy  $E$  of the local Schrödinger equation around the periodic orbit, then the corresponding stationary eigenfunction fulfills

$$\psi_p(\xi, t + T_p) = \int d\xi' G_p(\xi, \xi', t + T_p) \psi_p(\xi', t) = e^{-iET_p/\hbar} \psi_p(\xi, t), \quad (\text{A45.35})$$

where  $T_p$  is the period of the prime orbit  $p$ . If the classical energy of the periodic orbit is not an eigenenergy of the local Schrödinger equation, the non-stationary eigenfunctions fulfill

$$\psi_p^\ell(\xi, t + T_p) = \int d\xi' G_p(\xi, \xi', t + T_p) \psi_p(\xi', t) = e^{-iET_p/\hbar} \lambda_p^\ell(E) \psi_p^\ell(t), \quad (\text{A45.36})$$

where  $\ell = (\ell_1, \ell_2, \dots)$  is a multi-index of the possible quantum numbers of the local Schrödinger equation. If the eigenvalues  $\lambda_p^\ell(E)$  are known the local functional determinant can be written as

$$\Delta_p(E) = \prod_{\ell} (1 - \lambda_p^\ell(E)), \quad (\text{A45.37})$$

since  $\Delta_p(E)$  is zero at the eigenenergies of the local Schrödinger problem. We can insert the ansatz (A45.28) and reformulate (A45.36) as

$$e^{\frac{i}{\hbar}S(t+T_p)} \varphi_p^\ell(t + T_p) = e^{-iET_p/\hbar} \lambda_p^\ell(E) e^{\frac{i}{\hbar}S(t)} \varphi_p^\ell(t). \quad (\text{A45.38})$$

The phase change is given by the action integral for one period  $S(t + T_p) - S(t) = \int_0^{T_p} L(t) dt$ . Using this and the identity for the action  $S_p(E)$  of the periodic orbit

$$S_p(E) = \oint p dq = \int_0^{T_p} L(t) dt + ET_p, \quad (\text{A45.39})$$

we get

$$e^{\frac{i}{\hbar}S_p(E)} \varphi_p^\ell(t + T_p) = \lambda_p^\ell(E) \varphi_p^\ell(t). \quad (\text{A45.40})$$

Introducing the eigenequation for the amplitude

$$\varphi_p^\ell(t + T_p) = R_{\ell,p}(E) \varphi_p^\ell(t), \quad (\text{A45.41})$$

the local spectral determinant can be expressed as a product for the quantum numbers of the local problem,

$$\Delta_p(E) = \prod_{\ell} (1 - R_{\ell,p}(E) e^{\frac{i}{\hbar}S_p(E)}).$$

Since  $\hbar$  is a small parameter we can develop a perturbation series for the amplitudes

$$\varphi_p^\ell(t) = \sum_{m=0}^{\infty} \left( \frac{i\hbar}{2} \right)^m \varphi_p^{\ell(m)}(t)$$

which can be inserted into the equation (A45.29) and we get an iterative scheme starting with the semiclassical solution  $\varphi^{\ell(0)}$ :

$$\begin{aligned} \partial_t \varphi^{\ell(0)} + \nabla \varphi^{\ell(0)} \nabla S + \frac{1}{2} \varphi^{\ell(0)} \Delta S &= 0, \\ \partial_t \varphi^{\ell(m+1)} + \nabla \varphi^{\ell(m+1)} \nabla S + \frac{1}{2} \varphi^{\ell(m+1)} \Delta S &= \Delta \varphi^{\ell(m)}. \end{aligned} \quad (\text{A45.42})$$

The eigenvalue can also be expanded in powers of  $i\hbar/2$ :

$$R_{\ell,p}(E) = \exp \left\{ \sum_{m=0}^{\infty} \left( \frac{i\hbar}{2} \right)^m C_{\ell,p}^{(m)} \right\} = e^{C_{\ell,p}^{(0)}} \left\{ 1 + \frac{i\hbar}{2} C_{\ell,p}^{(1)} + \left( \frac{i\hbar}{2} \right)^2 \left( \frac{1}{2} (C_{\ell,p}^{(1)})^2 + C_{\ell,p}^{(2)} \right) + \dots \right\}. \quad (\text{A45.43})$$

The eigenvalue equation (A45.41) in  $\hbar$  expanded form reads as

$$\begin{aligned} \varphi_p^{\ell(0)}(t+T_p) &= e^{C_{\ell,p}^{(0)}} \varphi_p^{\ell(0)}(t) \\ \varphi_p^{\ell(1)}(t+T_p) &= e^{C_{\ell,p}^{(0)}} \left[ \varphi_p^{\ell(1)}(t) + C_{\ell,p}^{(1)} \varphi_p^{\ell(0)}(t) \right] \\ \varphi_p^{\ell(2)}(t+T_p) &= e^{C_{\ell,p}^{(0)}} \left[ \varphi_p^{\ell(2)}(t) + C_{\ell,p}^{(1)} \varphi_p^{\ell(1)}(t) + (C_{\ell,p}^{(2)} + \frac{1}{2} (C_{\ell,p}^{(1)})^2) \varphi_p^{\ell(0)}(t) \right], \end{aligned}$$

and so on. These equations are the conditions selecting the eigenvectors and eigenvalues and they hold for all  $t$ .

It is convenient to expand the functions  $\varphi_p^{\ell(m)}(x, t)$  in Taylor series around the periodic orbit and to solve the equations (A45.43) in this basis [9], since only a couple of coefficients should be computed to derive the first corrections. One can derive in general the zero order term  $C_{\ell}^{(0)} = i\pi\nu_p + \sum_{i=1}^{D-1} (\ell_i + \frac{1}{2}) u_{p,i}$ , where  $u_{p,i} = \log \Lambda_{p,i}$  are the logarithms of the eigenvalues of the monodromy matrix  $M_p$  and  $\nu_p$  is the topological index of the periodic orbit. The first correction is given by the integral

$$C_{\ell,p}^{(1)} = \int_0^{T_p} dt \frac{\Delta \varphi_p^{\ell(0)}(t)}{\varphi_p^{\ell(0)}(t)}.$$

When the theory is applied for billiard systems, the wave function should fulfill the Dirichlet boundary condition on hard walls, e.g. it should vanish on the wall. The wave function determined from (A45.29) behaves discontinuously when the trajectory  $x_p(t)$  hits the wall. For the simplicity we consider a 2 dof billiard system here. The wave function on the wall before the bounce ( $t_{-0}$ ) is given by

$$\psi_{in}(x, y(x), t) = \varphi(x, y(x), t_{-0}) e^{iS(x, y(x), t_{-0})/\hbar}, \quad (\text{A45.44})$$

where  $y(x) = Y_2 x^2/2! + Y_3 x^3/3! + Y_4 x^4/4! + \dots$  is the parametrization of the wall around the point of reflection (see Fig 1.). The wave function on the wall after the bounce ( $t_{+0}$ ) is

$$\psi_{out}(x, y(x), t) = \varphi(x, y(x), t_{+0}) e^{iS(x, y(x), t_{+0})/\hbar}. \quad (\text{A45.45})$$

The sum of these wave functions should vanish on the hard wall. This implies that the incoming and the outgoing amplitudes and the phases are related as

$$S(x, y(x), t_{-0}) = S(x, y(x), t_{+0}), \quad (\text{A45.46})$$

and

$$\varphi(x, y(x), t_{-0}) = -\varphi(x, y(x), t_{+0}). \quad (\text{A45.47})$$

The minus sign can be interpreted as the topological phase coming from the hard wall.

Now we can reexpress the spectral determinant with the local eigenvalues:

$$\Delta(E) = e^{W(E)} \prod_p \prod_{\ell} (1 - R_{\ell,p}(E) e^{\frac{i}{\hbar} S_p(E)}). \quad (\text{A45.48})$$

This expression is the quantum generalization of the semiclassical Selberg-product formula [19]. A similar decomposition has been found for quantum baker maps in refs. [18, 20]. The functions

$$\zeta_{\ell}^{-1}(E) = \prod_p (1 - R_{\ell,p}(E) e^{\frac{i}{\hbar} S_p(E)}) \quad (\text{A45.49})$$

are the generalizations of the Ruelle type [17] zeta functions. The trace formula can be recovered from (A45.33):

$$\text{tr } G(E) = g_0(E) + \frac{1}{i\hbar} \sum_{p,\ell} \left( T_p(E) - i\hbar \frac{d \log R_{\ell,p}(E)}{dE} \right) \frac{R_{\ell,p}(E) e^{\frac{i}{\hbar} S_p(E)}}{1 - R_{\ell,p}(E) e^{\frac{i}{\hbar} S_p(E)}}. \quad (\text{A45.50})$$


We can rewrite the denominator as a sum of a geometric series and we get

$$\text{tr } G(E) = g_0(E) + \frac{1}{i\hbar} \sum_{p,r,\ell} \left( T_p(E) - i\hbar \frac{d \log R_{\ell,p}(E)}{dE} \right) (R_{\ell,p}(E))^r e^{\frac{i}{\hbar} r S_p(E)}. \quad (\text{A45.51})$$

The new index  $r$  can be interpreted as the repetition number of the prime orbit  $p$ . This expression is the generalization of the semiclassical trace formula for the exact quantum mechanics. We would like to stress here, that the perturbation calculus introduced above is just one way to compute the eigenvalues of the local Schrödinger problems. Non-perturbative methods can be used to calculate the local eigenvalues for stable, unstable and marginal orbits. Therefore, our trace formula is not limited to integrable or hyperbolic systems, it can describe the most general case of systems with mixed phase space.

The semiclassical trace formula can be recovered by dropping the sub-leading term  $-i\hbar d \log R_{\ell,p}(E)/dE$  and using the semiclassical eigenvalue  $R_{\ell,p}^{(0)}(E) = e^{C_p^{(0)}} = e^{-iv_p\pi} e^{-\sum_i (\ell_i + 1/2) u_{p,i}}$ . Summation for the indexes  $\ell_i$  yields the celebrated semiclassical amplitude

$$\sum_{\ell} (R_{\ell,p}^{(0)}(E))^r = \frac{e^{-irv_p\pi}}{|\det(\mathbf{1} - M_p^r)|^{1/2}}. \quad (\text{A45.52})$$

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## Commentary

**Remark A45.1.** Birkhoff normal form. Normal forms of equilibria stability manifolds for 1D Hamiltonian (are-preserving) systems were introduced by Birkhoff [6]. Their convergence is discussed by Moser [16]. In 1927 Birkhoff [7] extended the concept of normal form to give successive integrable approximations to a non-integrable problem.

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## A45.5 Examples

**Example A45.1. The first correction  $C_{p,\ell}^{(1)}$  to 2 dof billiards.** To have an impression about the improvement caused by the quantum corrections we have developed a numerical code which calculates the first correction  $C_{p,\ell}^{(1)}$  for general 2 dof billiard systems. The first correction depends only on some basic data of the periodic orbit such as the lengths of the free flights between bounces, the angles of incidence and the first three Taylor expansion coefficients  $Y_2, Y_3, Y_4$  of the wall in the point of incidence. To check that our new local method gives the same result as the direct calculation of the Feynman integral, we computed the first  $\hbar$  correction  $C_{p,0}^{(1)}$  for the periodic orbits of the 3-disk scattering system [11–13] where the quantum corrections have been found to agree up to the fifth decimal digit, while our method generates these numbers with any desired precision. Unfortunately, the  $\ell \neq 0$  coefficients cannot be compared to ref. [1], since the  $\ell$  dependence was not realized there due to the lack of general formulas (A45.48) and (A45.49). However, the  $\ell$  dependence can be checked on the 2 disk scattering system [21, 22]. On the standard example [1, 8, 10–13, 21, 22], when  $R$ , the distance of the centers, is 6 times the disk radius  $a$ , we obtain

$$C_{\ell}^{(1)} = \frac{1}{\sqrt{2E}}(-0.625 \ell^3 - 0.3125 \ell^2 + 1.4375 \ell + 0.625).$$

For  $\ell = 0$  and 1 this has been confirmed by A. Wirzba, who was able to compute  $C_0^{(1)}$  from his exact quantum calculation. Our method makes it possible to utilize the Cvitanović–Eckhardt [8] symmetry reduction and to repeat the fundamental domain cycle expansion calculation of ref. [8] with the first quantum correction. We computed the correction to the leading 226 prime periodic orbits with 10 or less bounces in the fundamental domain. Table A45.1 shows the numerical values of the exact quantum calculation [21, 22], the semiclassical cycle expansion [9] and our corrected calculation. The error of the corrected calculation vs. the error of the semiclassical calculation decreases with the

**Figure A45.2:** A typical bounce off a billiard wall. The wall can be characterized by the local expansion  $y(x) = Y_2x^2/2! + Y_3x^3/3! + Y_4x^4/4! + \dots$

**Table A45.1:** Real part of the resonances ( $\text{Re } k$ ) of the 3-disk scattering system at disk separation 6:1. Semiclassical and first corrected cycle expansion versus exact quantum calculation and the error of the semiclassical  $\delta_{SC}$  divided by the error of the first correction  $\delta_{Corr}$ . The magnitude of the error in the imaginary part of the resonances remains unchanged.

Quantum	Semiclassical	First correction	$\delta_{SC}/\delta_{Corr}$
0.697995	0.758313	0.585150	0.53
2.239601	2.274278	2.222930	2.08
3.762686	3.787876	3.756594	4.13
5.275666	5.296067	5.272627	6.71
6.776066	6.793636	6.774061	8.76
...	...	...	...
30.24130	30.24555	30.24125	92.3
31.72739	31.73148	31.72734	83.8
32.30110	32.30391	32.30095	20.0
33.21053	33.21446	33.21048	79.4
33.85222	33.85493	33.85211	25.2
34.69157	34.69534	34.69152	77.0

wavenumber. Besides the improved results, a convergence up to six decimal digits is observed, in contrast to just three decimal digits obtained in the full domain calculation [1, 10].

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