# Chapter 33

# Semiclassical quantization

(G. Vattay, G. Tanner and P. Cvitanović)

We DERIVE HERE the Gutzwiller trace formula and the semiclassical zeta function, the central results of the semiclassical quantization of classically chaotic systems. In chapter 34 we will rederive these formulas for the case of scattering in open systems. Quintessential wave mechanics effects such as creeping, diffraction and tunneling will be taken up in chapter 37.

## 33.1 Trace formula

Our next task is to evaluate the Green's function trace (30.17) in the semiclassical approximation. The trace

$$\operatorname{tr} G_{sc}(E) = \int d^D q\, G_{sc}(q,q,E) = \operatorname{tr} G_0(E) + \sum_j \int d^D q\, G_j(q,q,E)$$

receives contributions from "long" classical trajectories labeled by $j$ which start and end in $q$ after finite time, and the "zero length" trajectories whose lengths approach zero as $q' \to q$.

First, we work out the contributions coming from the finite time *returning* classical orbits, i.e., trajectories that originate and end at a given configuration point $q$. As we are identifying $q$ with $q'$, taking of a trace involves (still another!) stationary phase condition in the $q' \to q$ limit,

$$\left.\frac{\partial S_j(q,q',E)}{\partial q_i}\right|_{q'=q} + \left.\frac{\partial S_j(q,q',E)}{\partial q'_i}\right|_{q'=q} = 0\,,$$


**Figure 33.1:** A returning trajectory in the configuration space. The orbit is periodic in the full phase space only if the initial and the final momenta of a returning trajectory coincide as well.

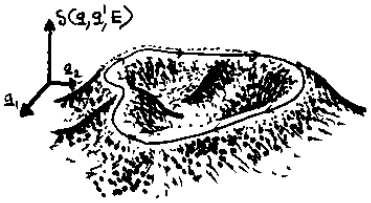


**Figure 33.2:** A romanticized sketch of $S_p(E) = S(q,q,E) = \oint p(q,E)dq$ landscape orbit. Unstable periodic orbits traverse isolated ridges and saddles of the mountainous landscape of the action $S(q_\parallel, q_\perp, E)$. Along a periodic orbit $S_p(E)$ is constant; in the transverse directions it generically changes quadratically.

meaning that the initial and final momenta (32.40) of contributing trajectories should coincide

$$p_i(q,q,E) - p'_i(q,q,E) = 0\,, \qquad q \in j\text{th periodic orbit}\,, \tag{33.1}$$

so the trace receives contributions only from those long classical trajectories which are *periodic* in the full phase space.

For a periodic orbit the natural coordinate system is the intrinsic one, with $q_\parallel$ axis pointing in the $\dot{q}$ direction along the orbit, and $q_\perp$, the rest of the coordinates transverse to $\dot{q}$. The $j$th periodic orbit contribution to the trace of the semiclassical Green's function in the intrinsic coordinates is

$$\mathrm{tr}\, G_j(E) = \frac{1}{i\hbar(2\pi\hbar)^{(d-1)/2}} \oint_j \frac{dq_\parallel}{\dot{q}} \int_j d^{d-1}q_\perp |\det D_\perp^j|^{1/2} e^{\frac{i}{\hbar}S_j - \frac{i\pi}{2}m_j},$$

where the integration in $q_\parallel$ goes from 0 to $L_j$, the geometric length of small tube around the orbit in the configuration space. As always, in the stationary phase approximation we worry only about the fast variations in the phase $S_j(q_\parallel, q_\perp, E)$, and assume that the density varies smoothly and is well approximated by its value $D_\perp^j(q_\parallel, 0, E)$ on the classical trajectory, $q_\perp = 0$ . The topological index $m_j(q_\parallel, q_\perp, E)$ is an integer which does not depend on the initial point $q_\parallel$ and not change in the infinitesimal neighborhood of an isolated periodic orbit, so we set $m_j(E) = m_j(q_\parallel, q_\perp, E)$.

The transverse integration is again carried out by the stationary phase method, with the phase stationary on the periodic orbit, $q_\perp = 0$. The result of the transverse integration can depend only on the parallel coordinate

$$\mathrm{tr}\, G_j(E) = \frac{1}{i\hbar} \oint \frac{dq_\parallel}{\dot{q}} \left| \frac{\det D_{\perp j}(q_\parallel, 0, E)}{\det D'_{\perp j}(q_\parallel, 0, E)} \right|^{1/2} e^{\frac{i}{\hbar}S_j - \frac{i\pi}{2}m_j},$$

where the new determinant in the denominator, $\det D'_{\perp j} =$

$$\det\left(\frac{\partial^2 S(q,q',E)}{\partial q_{\perp i}\partial q_{\perp j}}+\frac{\partial^2 S(q,q',E)}{\partial q'_{\perp i}\partial q_{\perp j}}+\frac{\partial^2 S(q,q',E)}{\partial q_{\perp i}\partial q'_{\perp j}}+\frac{\partial^2 S(q,q',E)}{\partial q'_{\perp i}\partial q'_{\perp j}}\right),$$

is the determinant of the second derivative matrix coming from the stationary phase integral in transverse directions. Mercifully, this integral also removes most of the $2\pi\hbar$ prefactors in (??).

The ratio $\det D_{\perp j}/\det D'_{\perp j}$ is here to enforce the periodic boundary condition for the semiclassical Green's function evaluated on a periodic orbit. It can be given a meaning in terms of the monodromy matrix of the periodic orbit by following observations

$$\begin{aligned}\det D_\perp &= \left\|\frac{\partial p'_\perp}{\partial q_\perp}\right\| = \left\|\frac{\partial(q'_\perp,p'_\perp)}{\partial(q_\perp,q'_\perp)}\right\| \\ \det D'_\perp &= \left\|\frac{\partial p_\perp}{\partial q_\perp}-\frac{\partial p'_\perp}{\partial q_\perp}+\frac{\partial p_\perp}{\partial q'_\perp}-\frac{\partial p'_\perp}{\partial q'_\perp}\right\| = \left\|\frac{\partial(p_\perp-p'_\perp,q_\perp-q'_\perp),}{\partial(q_\perp,q'_\perp)}\right\| .\end{aligned}$$

Defining the $2(D-1)$-dimensional transverse vector $x_\perp = (q_\perp, p_\perp)$ in the full phase space we can express the ratio

$$\begin{aligned}\frac{\det D'_\perp}{\det D_\perp} &= \left\|\frac{\partial(p_\perp-p'_\perp,q_\perp-q'_\perp)}{\partial(q'_\perp,p'_\perp)}\right\| = \left\|\frac{\partial(x_\perp-x'_\perp)}{\partial x'_\perp}\right\| \\ &= \det\,(M-\mathbf{1})\ , \end{aligned} \tag{33.2}$$

in terms of the monodromy matrix $M$ for a surface of section transverse to the orbit within the constant energy $E = H(q,p)$ shell.

The classical periodic orbit action $S_j(E) = \oint p(q_\parallel,E)dq_\parallel$ is an integral around a loop defined by the periodic orbit, and does not depend on the starting point $q_\parallel$ along the orbit, see figure 33.2. The eigenvalues of the monodromy matrix are also independent of where $M_j$ is evaluated along the orbit, so $\det(1-M_j)$ can also be taken out of the the $q_\parallel$ integral

$$\mathrm{tr}\,G_j(E) = \frac{1}{i\hbar}\sum_j \frac{1}{|\det(1-M_j)|^{1/2}} e^{r(\frac{i}{\hbar}S_j-\frac{i\pi}{2}m_j)}\oint\frac{dq_\parallel}{\dot q_\parallel}\ .$$

Here we have assumed that $M_j$ has no marginal eigenvalues. The determinant of the monodromy matrix, the action $S_p(E) = \oint p(q_\parallel,E)dq_\parallel$ and the topological index are all classical invariants of the periodic orbit. The integral in the parallel direction we now do exactly.

First, we take into account the fact that any repeat of a periodic orbit is also a periodic orbit. The action and the topological index are additive along the

trajectory, so for $r$th repeat they simply get multiplied by $r$. The monodromy matrix of the $r$th repeat of a prime cycle $p$ is (by the chain rule for derivatives) $M_p^r$, where $M_p$ is the prime cycle monodromy matrix. Let us denote the time period of the prime cycle $p$, the single, shortest traversal of a periodic orbit by $T_p$. The remaining integral can be carried out by change of variables $dt = dq_{\|}/\dot{q}(t)$

$$\int_0^{L_p} \frac{dq_{\|}}{\dot{q}(t)} = \int_0^{T_p} dt = T_p \,.$$

Note that the spatial integral corresponds to a *single* traversal. If you do not see why this is so, rethink the derivation of the classical trace formula (16.23) - that derivation takes only three pages of text. Regrettably, in the quantum case we do not know of an honest derivation that takes less than 30 pages. The final result, the *Gutzwiller trace formula*

$$\mathrm{tr}\, G_{sc}(E) = \mathrm{tr}\, G_0(E) + \frac{1}{i\hbar} \sum_p T_p \sum_{r=1}^{\infty} \frac{1}{|\det\left(1 - M_p^r\right)|^{1/2}} e^{r\left(\frac{i}{\hbar} S_p - \frac{i\pi}{2} m_p\right)}\,, \qquad (33.3)$$

an expression for the trace of the semiclassical Green's function in terms of periodic orbits, is beautiful in its simplicity and elegance.

The topological index $m_p(E)$ counts the number of changes of sign of the matrix of second derivatives evaluated along the prime periodic orbit $p$. By now we have gone through so many stationary phase approximations that you have surely lost track of what the total $m_p(E)$ actually is. The rule is this: The topological index of a closed curve in a $2D$ phase space is the sum of the number of times the partial derivatives $\frac{\partial p_i}{\partial q_i}$ for each dual pair $(q_i, p_i)$, $i = 1, 2, \ldots, D$ (no sum on $i$) change their signs as one goes once around the curve.

### 33.1.1 Average density of states

We still have to evaluate $\mathrm{tr}\, G_0(E)$, the contribution coming from the infinitesimal trajectories. The real part of $\mathrm{tr}\, G_0(E)$ is infinite in the $q' \to q$ limit, so it makes no sense to write it down explicitly here. However, the imaginary part is finite, and plays an important role in the density of states formula, which we derive next.

The semiclassical contribution to the density of states (30.17) is given by the imaginary part of the Gutzwiller trace formula (33.3) multiplied with $-1/\pi$. The contribution coming from the zero length trajectories is the imaginary part of (32.48) for $q' \to q$ integrated over the configuration space

$$d_0(E) = -\frac{1}{\pi} \int d^D q\, \mathrm{Im}\, \mathrm{G}_0(\mathrm{q}, \mathrm{q}, \mathrm{E}),$$

The resulting formula has a pretty interpretation; it estimates the number of quantum states that can be accommodated up to the energy $E$ by counting the

available quantum cells in the phase space. This number is given by the *Weyl rule* , as the ratio of the phase space volume bounded by energy $E$ divided by $h^D$, the volume of a quantum cell,

$$N_{sc}(E) = \frac{1}{h^D} \int d^D p d^D q \, \Theta(E - H(q,p)) \,. \tag{33.4}$$

where $\Theta(x)$ is the Heaviside function (30.22). $N_{sc}(E)$ is an estimate of the spectral staircase (30.21), so its derivative yields the average density of states

$$d_0(E) = \frac{d}{dE} N_{sc}(E) = \frac{1}{h^D} \int d^D p d^D q \, \delta(E - H(q,p)) \,, \tag{33.5}$$

precisely the semiclassical result (33.6). For Hamiltonians of type $p^2/2m + V(q)$, the energy shell volume in (33.5) is a sphere of radius $\sqrt{2m(E - V(q))}$. The surface of a $d$-dimensional sphere of radius $r$ is $\pi^{d/2} r^{d-1}/\Gamma(d/2)$, so the average density of states is given by [exercise 33.3]

$$d_0(E) = \frac{2m}{\hbar^D 2^d \pi^{D2} \Gamma(D/2)} \int_{V(q)<E} d^D q \, [2m(E - V(q))]^{D/2-1} \,, \tag{33.6}$$

and

$$N_{sc}(E) = \frac{1}{h^D} \frac{\pi^{D/2}}{\Gamma(1 + D/2)} \int_{V(q)<E} d^D q \, [2m(E - V(q))]^{D/2} \,. \tag{33.7}$$

Physically this means that at a fixed energy the phase space can support $N_{sc}(E)$ distinct eigenfunctions; anything finer than the quantum cell $h^D$ cannot be resolved, so the quantum phase space is effectively finite dimensional. The average density of states is of a particularly simple form in one spatial dimension [exercise 33.4]

$$d_0(E) = \frac{T(E)}{2\pi\hbar} \,, \tag{33.8}$$

where $T(E)$ is the period of the periodic orbit of fixed energy $E$. In two spatial dimensions the average density of states is

$$d_0(E) = \frac{m\mathcal{A}(E)}{2\pi\hbar^2} \,, \tag{33.9}$$

where $\mathcal{A}(E)$ is the classically allowed area of configuration space for which $V(q) < E$. [exercise 33.5]

The semiclassical density of states is a sum of the average density of states and the oscillation of the density of states around the average, $d_{sc}(E) = d_0(E) + d_{osc}(E)$, where

$$d_{osc}(E) = \frac{1}{\pi\hbar} \sum_p T_p \sum_{r=1}^{\infty} \frac{\cos(rS_p(E)/\hbar - r m_p \pi/2)}{|\det(1 - M_p^r)|^{1/2}} \tag{33.10}$$

follows from the trace formula (33.3).

### 33.1.2 Regularization of the trace

The real part of the $q' \to q$ zero length Green's function (32.48) is ultraviolet divergent in dimensions $d > 1$, and so is its formal trace (30.17). The short distance behavior of the real part of the Green's function can be extracted from the real part of (32.48) by using the Bessel function expansion for small $z$

$$Y_\nu(z) \approx \begin{cases} -\frac{1}{\pi}\Gamma(\nu)\left(\frac{z}{2}\right)^{-\nu} & \text{for } \nu \neq 0 \\ \frac{2}{\pi}(\ln(z/2)+\gamma) & \text{for } \nu = 0 \end{cases} ,$$

where $\gamma = 0.577...$ is the Euler constant. The real part of the Green's function for short distance is dominated by the singular part

$$G_{sing}(|q-q'|,E) = \begin{cases} -\frac{m}{2\hbar^2\pi^{\frac{d}{2}}}\Gamma((d-2)/2)\frac{1}{|q-q'|^{d-2}} & \text{for } d \neq 2 \\ \frac{m}{2\pi\hbar^2}(\ln(2m(E-V)|q-q'|/2\hbar)+\gamma) & \text{for } d = 2 \end{cases} .$$

The *regularized* Green's function

$$G_{reg}(q,q',E) = G(q,q',E) - G_{sing}(|q-q'|,E)$$

is obtained by subtracting the $q' \to q$ ultraviolet divergence. For the regularized Green's function the Gutzwiller trace formula is

$$\mathrm{tr}\, G_{reg}(E) = -i\pi d_0(E) + \frac{1}{i\hbar}\sum_p T_p \sum_{r=1}^{\infty} \frac{e^{r(\frac{i}{\hbar}S_p(E) - \frac{i\pi}{2}m_p(E))}}{|\det(1-M_p^r)|^{1/2}} . \tag{33.11}$$

Now you stand where Gutzwiller stood in 1990. You hold the trace formula in your hands. You have no clue how good is the $\hbar \to 0$ approximation, how to take care of the sum over an infinity of periodic orbits, and whether the formula converges at all.

## 33.2 Semiclassical spectral determinant

The problem with trace formulas is that they diverge where we need them, at the individual energy eigenvalues. What to do? Much of the quantum chaos literature responds to the challenge of wrestling the trace formulas by replacing the delta functions in the density of states (30.18) by Gaussians. But there is no need to do this - we can compute the eigenenergies without any further ado by remembering that the smart way to determine the eigenvalues of linear operators is by determining zeros of their spectral determinants.

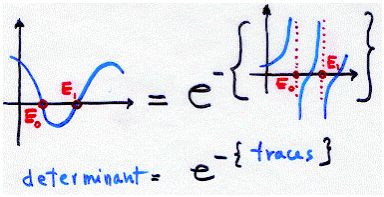


**Figure 33.3:** A sketch of how spectral determinants convert poles into zeros: The trace shows $1/(E-E_n)$ type singularities at the eigenenergies while the spectral determinant goes smoothly through zeroes.

A sensible way to compute energy levels is to construct the spectral determinant whose zeroes yield the eigenenergies, $\det(\hat{H}-E)_{sc}=0$. A first guess might be that the spectral determinant is the Hadamard product of form

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

but this product is not well defined, since for fixed $E$ we multiply larger and larger numbers $(E-E_n)$. This problem is dealt with by *regularization*, discussed below in appendix 33.1.2. Here we offer an impressionistic sketch of regularization.

The logarithmic derivative of $\det(\hat{H}-E)$ is the (formal) trace of the Green's function

$$-\frac{d}{dE}\ln\det(\hat{H}-E)=\sum_n \frac{1}{E-E_n}=\mathrm{tr}\,G(E).$$

This quantity, not surprisingly, is divergent again. The relation, however, opens a way to derive a convergent version of $\det(\hat{H}-E)_{sc}$, by replacing the trace with the regularized trace

$$-\frac{d}{dE}\ln\det(\hat{H}-E)_{sc}=\mathrm{tr}\,G_{reg}(E).$$

The regularized trace still has $1/(E-E_n)$ poles at the semiclassical eigenenergies, poles which can be generated only if $\det(\hat{H}-E)_{sc}$ has a zero at $E=E_n$, see figure 33.3. By integrating and exponentiating we obtain

$$\det(\hat{H}-E)_{sc}=\exp\left(-\int^E dE'\,\mathrm{tr}\,G_{reg}(E')\right)$$

Now we can use (33.11) and integrate the terms coming from periodic orbits, using the relation (32.17) between the action and the period of a periodic orbit, $dS_p(E)=T_p(E)dE$, and the relation (30.21) between the density of states and the spectral staircase, $dN_{sc}(E)=d_0(E)dE$. We obtain the *semiclassical zeta function*

$$\det(\hat{H}-E)_{sc}=e^{i\pi N_{sc}(E)}\exp\left(-\sum_p\sum_{r=1}^{\infty}\frac{1}{r}\frac{e^{ir(S_p/\hbar-m_p\pi/2)}}{|\det(1-M_p^r)|^{1/2}}\right). \qquad (33.12)$$

[chapter 18]

We already know from the study of classical evolution operator spectra of chapter 17 that this can be evaluated by means of cycle expansions. The beauty of this formula is that everything on the right side – the cycle action $S_p$, the topological index $m_p$ and monodromy matrix $M_p$ determinant – is intrinsic, coordinate-choice independent property of the cycle $p$.

## 33.3 One-dof systems

It has been a long trek, a stationary phase upon stationary phase. Let us check whether the result makes sense even in the simplest case, for quantum mechanics in one spatial dimension.

In one dimension the average density of states follows from the 1-dof form of the oscillating density (33.10) and of the average density (33.8)

$$d(E) = \frac{T_p(E)}{2\pi\hbar} + \sum_r \frac{T_p(E)}{\pi\hbar} \cos(rS_p(E)/\hbar - rm_p(E)\pi/2). \tag{33.13}$$

The classical particle oscillates in a single potential well with period $T_p(E)$. There is no monodromy matrix to evaluate, as in one dimension there is only the parallel coordinate, and no transverse directions. The $r$ repetition sum in (33.13) can be rewritten by using the Fourier series expansion of a delta spike train

$$\sum_{n=-\infty}^{\infty} \delta(x-n) = \sum_{k=-\infty}^{\infty} e^{i2\pi kx} = 1 + \sum_{k=1}^{\infty} 2\cos(2\pi kx).$$

We obtain

$$d(E) = \frac{T_p(E)}{2\pi\hbar} \sum_n \delta(S_p(E)/2\pi\hbar - m_p(E)/4 - n). \tag{33.14}$$

This expression can be simplified by using the relation (32.17) between $T_p$ and $S_p$, and the identity (14.7) $\delta(x-x^*) = |f'(x)|\delta(f(x))$, where $x^*$ is the only zero of the function $f(x^*) = 0$ in the interval under consideration. We obtain

$$d(E) = \sum_n \delta(E - E_n),$$

where the energies $E_n$ are the zeroes of the arguments of delta functions in (33.14)

$$S_p(E_n)/2\pi\hbar = n - m_p(E)/4\,,$$

where $m_p(E) = m_p = 2$ for smooth potential at both turning points, and $m_p(E) = m_p = 4$ for two billiard (infinite potential) walls. These are precisely the *Bohr-Sommerfeld quantized energies* $E_n$, defined by the condition

$$\oint p(q, E_n)dq = h\left(n - \frac{m_p}{4}\right). \tag{33.15}$$

In this way the trace formula recovers the well known 1-dof quantization rule. In one dimension, the average of states can be expressed from the quantization condition. At $E = E_n$ the exact number of states is $n$, while the average number of states is $n - 1/2$ since the staircase function $N(E)$ has a unit jump in this point

$$N_{sc}(E) = n - 1/2 = S_p(E)/2\pi\hbar - m_p(E)/4 - 1/2. \tag{33.16}$$

The 1-dof spectral determinant follows from (33.12) by dropping the monodromy matrix part and using (33.16)

$$\det(\hat{H} - E)_{sc} = \exp\left(-\frac{i}{2\hbar}S_p + \frac{i\pi}{2}m_p\right)\exp\left(-\sum_r \frac{1}{r}e^{\frac{i}{\hbar}rS_p - \frac{i\pi}{2}rm_p}\right). \tag{33.17}$$

Summation yields a logarithm by $\sum_r t^r/r = -\ln(1-t)$ and we get

$$\begin{aligned}\det(\hat{H} - E)_{sc} &= e^{-\frac{i}{2\hbar}S_p + \frac{im_p}{4} + \frac{i\pi}{2}}(1 - e^{\frac{i}{\hbar}S_p - i\frac{m_p}{2}}) \\ &= 2\sin\left(S_p(E)/\hbar - m_p(E)/4\right).\end{aligned}$$

So in one dimension, where there is only one periodic orbit for a given energy E, nothing is gained by going from the trace formula to the spectral determinant. The spectral determinant is a real function for real energies, and its zeros are again the Bohr-Sommerfeld quantized eigenenergies (33.15).

## 33.4 Two-dof systems

For flows in two configuration dimensions the monodromy matrix $M_p$ has two eigenvalues $\Lambda_p$ and $1/\Lambda_p$, as explained in sect. 7.2. Isolated periodic orbits can be elliptic or hyperbolic. Here we discuss only the hyperbolic case, when the eigenvalues are real and their absolute value is not equal to one. The determinant appearing in the trace formulas can be written in terms of the expanding eigenvalue as

$$|\det(1 - M_p^r)|^{1/2} = |\Lambda_p^r|^{1/2}\left(1 - 1/\Lambda_p^r\right),$$

and its inverse can be expanded as a geometric series

$$\frac{1}{|\det(1 - M_p^r)|^{1/2}} = \sum_{k=0}^{\infty} \frac{1}{|\Lambda_p^r|^{1/2}\Lambda_p^{kr}}.$$

With the 2-dof expression for the average density of states (33.9) the spectral determinant becomes

$$\begin{aligned}\det(\hat{H}-E)_{sc} &= e^{i\frac{m\mathcal{A}E}{2\hbar^2}}\exp\left(-\sum_p\sum_{r=1}^{\infty}\sum_{k=0}^{\infty}\frac{e^{ir(S_p/\hbar-m_p\pi/2)}}{r|\Lambda_p^r|^{1/2}\Lambda_p^{kr}}\right)\\ &= e^{i\frac{m\mathcal{A}E}{2\hbar^2}}\prod_p\prod_{k=0}^{\infty}\left(1-\frac{e^{\frac{i}{\hbar}S_p-\frac{i\pi}{2}m_p}}{|\Lambda_p|^{1/2}\Lambda_p^k}\right). \qquad (33.18)\end{aligned}$$

## Résumé

Spectral determinants and dynamical zeta functions arise both in classical and quantum mechanics because in both the dynamical evolution can be described by the action of linear evolution operators on infinite-dimensional vector spaces. In quantum mechanics the periodic orbit theory arose from studies of semi-conductors, and the unstable periodic orbits have been measured in experiments on the very paradigm of Bohr's atom, the hydrogen atom, this time in strong external fields.

In practice, most "quantum chaos" calculations take the stationary phase approximation to quantum mechanics (the Gutzwiller trace formula, possibly improved by including tunneling periodic trajectories, diffraction corrections, etc.) as the point of departure. Once the stationary phase approximation is made, what follows is *classical* in the sense that all quantities used in periodic orbit calculations - actions, stabilities, geometrical phases - are classical quantities. The problem is then to understand and control the convergence of classical periodic orbit formulas.

While various periodic orbit formulas are formally equivalent, practice shows that some are preferable to others. Three classes of periodic orbit formulas are frequently used:

*Trace formulas.* The trace of the semiclassical Green's function

$$\mathrm{tr}\, G_{sc}(E) = \int dq\, G_{sc}(q,q,E)$$

is given by a sum over the periodic orbits (33.11). While easiest to derive, in calculations the trace formulas are inconvenient for anything other than the leading eigenvalue estimates, as they tend to be divergent in the region of physical interest. In classical dynamics trace formulas hide under a variety of appellations such as the $f-\alpha$ or multifractal formalism; in quantum mechanics they are known as the Gutzwiller trace formulas.

Zeros of *Ruelle or dynamical zeta functions*

$$1/\zeta(s) = \prod_p (1-t_p), \quad t_p = \frac{1}{|\Lambda_p|^{1/2}} e^{\frac{i}{\hbar}S_p - i\pi m_p/2}$$

yield, in combination with cycle expansions, the semiclassical estimates of *quantum* resonances. For hyperbolic systems the dynamical zeta functions have good convergence and are a useful tool for determination of classical and quantum mechanical averages.

*Spectral determinants, Selberg-type zeta functions, Fredholm determinants, functional determinants* are the natural objects for spectral calculations, with convergence better than for dynamical zeta functions, but with less transparent cycle expansions. The 2-dof semiclassical spectral determinant (33.18)

$$\det(\hat{H}-E)_{sc} = e^{i\pi N_{sc}(E)} \prod_p \prod_{k=0}^{\infty} \left(1 - \frac{e^{iS_p/\hbar - i\pi m_p/2}}{|\Lambda_p|^{1/2}\Lambda_p^k}\right)$$

is a typical example. Most periodic orbit calculations are based on cycle expansions of such determinants.

As we have assumed repeatedly during the derivation of the trace formula that the periodic orbits are isolated, and do not form families (as is the case for integrable systems or in KAM tori of systems with mixed phase space), the formulas discussed so far are valid only for hyperbolic and elliptic periodic orbits.

For deterministic dynamical flows and number theory, spectral determinants and zeta functions are exact. The quantum-mechanical ones, derived by the Gutzwiller approach, are at best only the stationary phase approximations to the exact quantum spectral determinants, and for quantum mechanics an important conceptual problem arises already at the level of derivation of the semiclassical formulas; how accurate are they, and can the periodic orbit theory be systematically improved?

## Commentary

**Remark 33.1** Gutzwiller quantization of classically chaotic systems. The derivation given here and in sects. 32.3 and 33.1 follows closely the excellent exposition [2] by Martin Gutzwiller, the inventor of the trace formula. The derivation presented here is self contained, but refs. [3, 1] might also be of help to the student.

**Remark 33.2** Zeta functions. For "zeta function" nomenclature, see remark 17.4 on page 296.

## Exercises

33.1. **Monodromy matrix from second variations of the action.** Show that

$$D_{\perp j}/D'_{\perp j} = (\mathbf{1} - M) \tag{33.19}$$

33.2. **Jacobi gymnastics.** Prove that the ratio of determinants in (S.48) can be expressed as

$$\frac{\det D'_{\perp j}(q_{\|}, 0, E)}{\det D_{\perp j}(q_{\|}, 0, E)} = \det \begin{pmatrix} I - M_{qq} & -M_{qp} \\ -M_{pq} & I - M_{pp} \end{pmatrix} = \det (1 - M_j)\,, \tag{33.20}$$

where $M_j$ is the monodromy matrix of the periodic orbit.

33.3. **Volume of $d$-dimensional sphere.** Show that the volume of a $d$-dimensional sphere of radius $r$ equals $\pi^{d/2} r^d / \Gamma(1 + d/2)$. Show that $\Gamma(1 + d/2) = \Gamma(d/2) d/2$.

33.4. **Average density of states in 1 dimension.** Show that in one dimension the average density of states is given by (33.8)

$$\bar{d}(E) = \frac{T(E)}{2\pi\hbar},$$

where $T(E)$ is the time period of the 1-dimensional motion and show that

$$\bar{N}(E) = \frac{S(E)}{2\pi\hbar}\,, \tag{33.21}$$

where $S(E) = \oint p(q, E)\, dq$ is the action of the orbit.

33.5. **Average density of states in 2 dimensions.** Show that in 2 dimensions the average density of states is given by (33.9)

$$\bar{d}(E) = \frac{m\mathcal{A}(E)}{2\pi\hbar^2}\,,$$

where $\mathcal{A}(E)$ is the classically allowed area of configuration space for which $U(q) < E$.

## References


[33.1] R.G. Littlejohn, *J. Stat. Phys.* **68**, 7 (1992).

[33.2] L.D. Landau and E.M. Lifshitz, *Mechanics* (Pergamon, London, 1959).

[33.3] R.G. Littlejohn, "Semiclassical structure of trace formulas," in G. Casati and B. Chirikov, eds., *Quantum Chaos*, (Cambridge University Press, Cambridge 1994).

[33.4] M.C. Gutzwiller, *J. Math. Phys.* **8**, 1979 (1967); **10**, 1004 (1969); **11**, 1791 (1970); **12**, 343 (1971).

[33.5] M.C. Gutzwiller, *J. Math. Phys.* **12**, 343 (1971)

[33.6] M.C. Gutzwiller, *J. Phys. Chem.* **92**, 3154 (1984).

[33.7] A. Voros, *J. Phys.* **A 21**, 685 (1988).

[33.8] A. Voros, *Aspects of semiclassical theory in the presence of classical chaos*, *Prog. Theor. Phys. Suppl.* **116**, 17 (1994).

[33.9] P. Cvitanović and P.E. Rosenqvist, in G.F. Dell'Antonio, S. Fantoni and V.R. Manfredi, eds., *From Classical to Quantum Chaos*, *Soc. Italiana di Fisica Conf. Proceed.* **41**, pp. 57-64 (Ed. Compositori, Bologna 1993).

[33.10] A. Wirzba, "Validity of the semiclassical periodic orbit approximation in the 2-and 3-disk problems," *CHAOS* **2**, 77 (1992).