Spectral determinant

It can be more efficient to consider spectral determinants. They are entire functions of the energy E whose zeros are given by the quantum energy levels, and they are real valued for real E

$$\Delta(E) = \prod_{n=1}^{\infty} A(E, E_n)\,(E - E_n).$$

The amplitudes depend on the regularisation. For example, for a two-dimensional billiard system the mean density of states $\bar{d}(E) \approx mA/(2\pi\hbar^2)$ is constant. This implies that the trace of the Green function

$$\mathrm{Tr}\, G(E) = \sum_n \frac{1}{E - E_n}$$

is divergent. It can be regularised by considering instead

$$\mathrm{Tr}\, G^{\mathrm{reg}}(E) = \mathrm{Tr}(G(E) - G(0)) = \sum_n \frac{1}{E - E_n} + \frac{1}{E_n} = \sum_n \frac{E}{(E - E_n)E_n},$$

which is finite. The regularised determinant is then obtained from

$$\Delta(E) = \exp\left(\int_0^E \mathrm{d}E'\ \mathrm{Tr}\, G^{\mathrm{reg}}(E')\right) = \exp\left(\sum_n \log(1 - E/E_n) + E/E_n\right)$$

Spectral determinant

We obtain

$$\Delta(E) = \prod_{n=1}^{\infty} \left(1 - \frac{E}{E_n}\right) \mathrm{e}^{E/E_n} \qquad \Longrightarrow \qquad A(E, E_n) = -\frac{1}{E_n} \mathrm{e}^{E/E_n}.$$

This is an example of a Weierstrass regularisation.

After inserting the semiclassical approximation for the trace of the Green function, one can derive the following expression

$$\Delta(E) \approx B(E)\, \mathrm{e}^{i\pi \bar{N}(E)}\, \zeta(E),$$

where $B(E)$ is real-valued for real E. The function $\zeta(E)$ is obtained from the periodic orbit

$$\zeta(E) = \sum_{n=0}^{\infty} C_n\, \mathrm{e}^{i\mathcal{S}_n/\hbar}$$

The sum is over composite orbits (or pseudo-orbits) which are combinations of periodic orbits

$$\mathcal{S}_n = \sum_{p \in \mathcal{P}_n} m_p\, S_p.$$

n labels all possible finite linear combinations of actions of periodic orbits with positive coefficients. There is a zero-length term with $\mathcal{S}_0 = 0$ and $C_0 = 1$.

Spectral determinant

Motivated by the Riemann-Siegel formula for the Riemann zeta function, Berry and Keating derived a semiclassical resummation of the spectral determinant

$$\Delta(E) \approx 2\,\mathrm{Re}[\Delta(E)]^{\mathrm{sc,tr}}$$

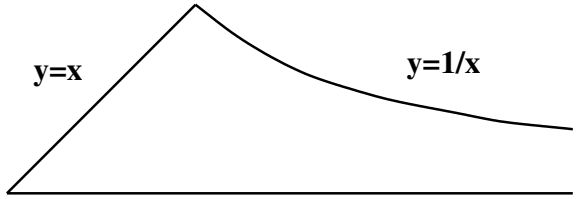
where

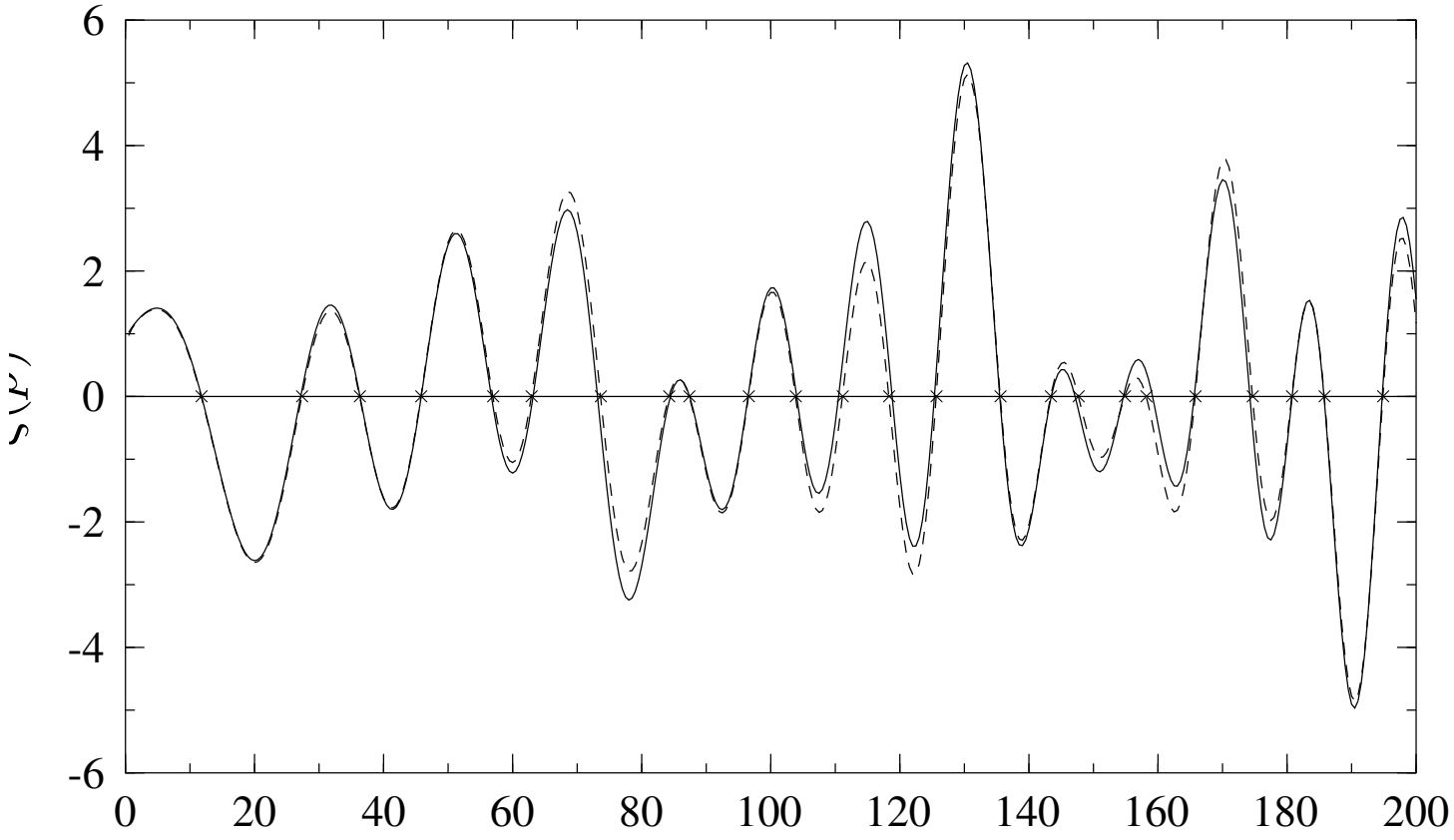
$$[\Delta(E)]^{\mathrm{sc,tr}} = B(E) \sum_{n=0}^{\infty} C_n \mathrm{e}^{-\mathrm{i}\pi\bar{N}(E)+\mathrm{i}\mathcal{S}_n/\hbar}\ \theta^{\mathrm{tr}}(T_{\mathrm{H}}/2 - \mathcal{T}_n)$$

and $\mathcal{T}_n = \mathrm{d}\mathcal{S}_n/\mathrm{d}E$. The function θ^{tr} smoothly truncates the sum

Heuristic explanation: The spectral determinant is real valued for real E. The Fourier transform of a real function $f(E)$ satisfies $\mathcal{F}(T) = \mathcal{F}(-T)^*$. Since the energy dependence of the oscillatory terms is $\sim [-\pi\bar{d} + \mathcal{T}_n/\hbar]E$ we obtain a relation between the contributions of orbits with periods beyond $T_{\mathrm{H}}/2 = \pi\bar{d}\hbar$ and those of orbits with period smaller than $T_{\mathrm{H}}/2$.

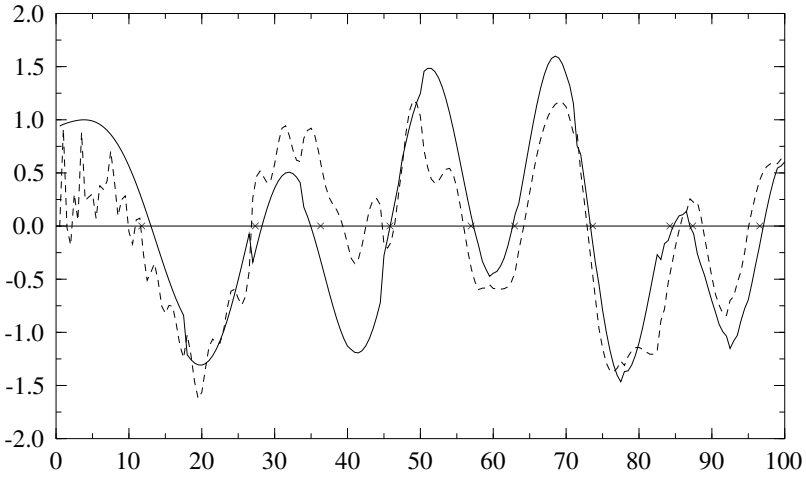
Numerical results for the hyperbola billiard

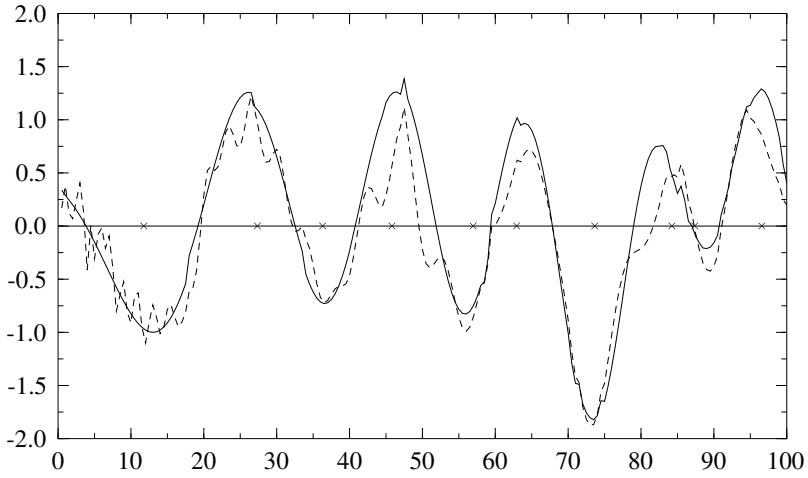




Numerical results for the hyperbola billiard

The contributions of orbits below and above the cut-off, respectively. Left: real parts (with same sign). Right: imaginary parts (with opposite signs).





Exercise 6

Obtain the trace formula for the density of states and the spectral determinant for a particle in a box.

Wave functions

Approximation for wave functions

Bogomolny considered the local density of states

$$d(\boldsymbol{q}, E) = \sum_n |\psi_n(\boldsymbol{q})|^2 \, \delta(E - E_n) = -\frac{1}{\pi} \lim_{\varepsilon \to 0} \operatorname{Im} G(\boldsymbol{q}, \boldsymbol{q}, E + i\varepsilon)$$

This leads to the approximation

$$\left\langle |\psi_n(\boldsymbol{q})|^2 \right\rangle_E = \frac{\left\langle -\frac{1}{\pi} \operatorname{Im} G(\boldsymbol{q}, \boldsymbol{q}, E) \right\rangle_E}{\langle d(E) \rangle_E}$$

where $\langle \ldots \rangle_E$ denotes averaging over an energy window ΔE. For $\Delta E \approx 1/\bar{d}(E)$ one need orbits with time $T_\xi < T_{\mathrm{H}}$.

This approach is similar to using the trace formula for finding semiclassical energies. Is there an analogue to the approach with the spectral determinants? There are several approaches to this topic, most use quantised Poincare sections (Fishman et al., . . .). In the following I will discuss an approach that uses low rank perturbations.

Perturbation by a point scatterer

We consider the perturbation of a system by a point scatterer. We start with one-dimensional systems for which a delta-function potential is well-defined. Consider a quantum Hamiltonian of the form $H = H_0 + \lambda A$ where $A = |q\rangle\langle q|$. Then the time-independent Schrödinger equation has the form

$$0 = (H_0 - E)\,|\psi\rangle + \lambda |q\rangle\,\langle q|\psi\rangle$$

Multiplying from the left with $\langle q|\,G_0$ where $G_0 = (E - H_0)^{-1}$ is the resolvent leads to

$$0 = (1 - \lambda \langle q|G_0|q\rangle)\,\langle q|\psi\rangle$$

The solutions are given by unperturbed energies E_m if the corresponding eigenstate vanishes at q, and by the zeros of the bracket on the right-hand side.

The resolvent $G(E) = (E - H)^{-1}$ of the perturbed Hamiltonian is obtained from the general relation $G = G_0 + G_0 \lambda A G$

$$G = \frac{1}{1 - G_0 \lambda |q\rangle\langle q|}\, G_0$$

The eigenvalues of the Hamiltonian H are given by the poles of the resolvent G. Hence the new spectral determinant has the form

$$\Delta_1(E,\lambda,q) = \Delta_0(E)\ \det(1-\lambda G_0|q\rangle\langle q|)$$

Applying $\det M = \mathrm{e}^{\mathrm{Tr}\log M}$ and $\mathrm{Tr}\, G_0|q\rangle\langle q| = \langle q|G_0|q\rangle$ yields

$$\Delta_1(E,\lambda,q) = \Delta_0(E)\,[1-\lambda G_0(q,q,E)]$$

where $G_0(q,q',E) = \langle q|G_0|q'\rangle$ is the Green function of the unperturbed system. Note that the poles of the Green function cancel the zeros of $\Delta_0(E)$ if they are non-degenerate and the corresponding wave function does not vanish at q.

An alternative representation of the Green function can be obtained by using

$$\frac{1}{1-G_0\lambda|q\rangle\langle q|} = 1 + \frac{\lambda G_0|q\rangle\langle q|}{1-\lambda\langle q|G_0|q\rangle},$$

from which follows that

$$G = G_0 + G_0|q\rangle\frac{\lambda}{1-\lambda\langle q|G_0|q\rangle}\langle q|G_0$$

If the fraction is expanded into a geometric series one obtains an expression that can be interpreted as a sum over diffractive orbits, see later discussion.

A point-like scatterer in two and three dimensions

A delta-function potential is not well-defined in two or three dimensions. This is reflected by the fact that $\langle \boldsymbol{q}|G_0|\boldsymbol{q}\rangle$ is infinite in these cases. The standard method to define a point-like perturbation is to apply the theory a self-adjoint extension to a Hamiltonian from whose domain one point has been removed. The resulting expressions for $\Delta(E)$ and $G(E)$ are very similar to the one-dimensional case. The difference is that the Green function $G_0(\boldsymbol{q},\boldsymbol{q},E) = \langle \boldsymbol{q}|G_0|\boldsymbol{q}\rangle$ is regularised.

$$\Delta_1(E,\lambda,\boldsymbol{q}) = \Delta_0(E)\left[1-\lambda G_0^{\mathrm{reg}}(\boldsymbol{q},\boldsymbol{q},E)\right]$$

and

$$G = G_0 + G_0|q\rangle \frac{\lambda}{1-\lambda\langle q|G_0^{\mathrm{reg}}|q\rangle}\langle q|G_0$$

The regularization of the Green function is not unique. Different regularizations can differ by an arbitrary *real* constant. However, all different regularizations lead to the same family of self-adjoint extensions of the Hamiltonian. We regularize the Green function by subtracting its divergent part in the limit $\boldsymbol{q}' \to \boldsymbol{q}$.

$$G^{\mathrm{reg}}(\boldsymbol{q},\boldsymbol{q},E) = \lim_{\boldsymbol{q}'\to\boldsymbol{q}}\left[G(\boldsymbol{q},\boldsymbol{q}',E) - \frac{m}{\pi\hbar^2}\log(k_0|\boldsymbol{q}-\boldsymbol{q}'|)\right]$$

where k_0 is an arbitrary constant.

Relation between the wave function and Δ_1

We found

$$\Delta_1(E,\lambda,\boldsymbol{q}) = \Delta_0(E)\left[1-\lambda G_0^{\mathrm{reg}}(\boldsymbol{q},\boldsymbol{q},E)\right]$$

The effect that a perturbation by a point-like scatterer has on an energy level depends on the value of the wave function at this point. The semiclassical approach is based on this relation. Consider the determinant of the perturbed system, evaluated at the unperturbed energy $E = E_n$

$$\Delta_1(E_n,\lambda,\boldsymbol{q}) = -\lambda \lim_{E\to E_n} \Delta_0(E)\frac{|\psi_n(\boldsymbol{q})|^2}{E-E_n} = -\lambda\Delta_0'(E_n)|\psi_n(\boldsymbol{q})|^2$$

We take a derivative with respect to λ on both sides of this equation

$$|\psi_n(\boldsymbol{q})|^2 = -\left.\frac{\frac{\partial}{\partial\lambda}\Delta_1(E,\lambda,\boldsymbol{q})}{\frac{\partial}{\partial E}\Delta_1(E,\lambda,\boldsymbol{q})}\right|_{\substack{\lambda=0\\E=E_n}}$$

Inserting the semiclassical approximation for Δ_1 results in

$$|\psi_n(\boldsymbol{q})|^2 \approx \frac{\mathrm{Re}[\Delta_0(E_n)\, G^{\mathrm{reg}}(\boldsymbol{q},\boldsymbol{q},E_n)]^{\mathrm{sc,tr}}}{\mathrm{Re}\left[\Delta_0'(E_n)\right]^{\mathrm{sc,tr}}}$$

This is the result for the semiclassical approximation of $|\psi_n(\boldsymbol{q})|^2$.

Discussion of the result

We found

$$|\psi_n(\boldsymbol{q})|^2 \approx \frac{\mathrm{Re}[\Delta_0(E_n)\, G^{\mathrm{reg}}(\boldsymbol{q},\boldsymbol{q},E_n)]^{\mathrm{sc,tr}}}{\mathrm{Re}\left[\Delta_0'(E_n)\right]^{\mathrm{sc,tr}}}$$

Δ_0 and G_0 both have a semiclassical expansion in terms of trajectories. These sums are multiplied and cut off smoothly when the joint periods $\mathcal{T}_n + T_\gamma$ is half the Heisenberg time.

This result is independent of the choice of the regularisation of the Green function. If one considers only the zero-length contributions to the Green function one obtains for chaotic systems

$$|\psi_n(\boldsymbol{q})|^2 \approx \frac{\bar{d}(\boldsymbol{q},E_n)}{\bar{d}(E_n)} \approx \frac{\int \mathrm{d}^f p\, \delta(E-H(\boldsymbol{q},\boldsymbol{p}))}{\int \mathrm{d}^f q\, \mathrm{d}^f p\, \delta(E-H(\boldsymbol{q},\boldsymbol{p}))}.$$

When integrated over some small area this is consistent with the quantum ergodicity theorem, roughly speaking, states that almost all eigenstates are uniformly distributed on the energy shell in the semiclassical limit.

The result can applied for an examination of scars. If a small smoothing in $\boldsymbol{q}$ is applied, then the contribution comes from closed orbits near periodic orbits, and they can be described in terms of these periodic orbits.

Rank two perturbations

We consider also rank two perturbations which correspond to self-adjoint extensions of a Hamiltonian from whose domain two points are removed. They formally correspond to a perturbation by an operator of the form

$$\lambda_1 |\boldsymbol{q}_1\rangle\langle\boldsymbol{q}_1| + \mu |\boldsymbol{q}_1\rangle\langle\boldsymbol{q}_2| + \bar{\mu} |\boldsymbol{q}_2\rangle\langle\boldsymbol{q}_1| + \lambda_2 |\boldsymbol{q}_2\rangle\langle\boldsymbol{q}_2|$$

where λ_1 and λ_2 are real and $\mu = \mu_r + \mathrm{i}\mu_i$ is complex. Then

$$\Delta_2(E) = \Delta_0(E)\, \det \left[1 - \begin{pmatrix} G_0^{\mathrm{reg}}(\boldsymbol{q}_1, \boldsymbol{q}_1, E) & G_0(\boldsymbol{q}_1, \boldsymbol{q}_2, E) \\ G_0(\boldsymbol{q}_2, \boldsymbol{q}_1, E) & G_0^{\mathrm{reg}}(\boldsymbol{q}_2, \boldsymbol{q}_2, E) \end{pmatrix} \begin{pmatrix} \lambda_1 & \mu \\ \bar{\mu} & \lambda_2 \end{pmatrix} \right]$$

It is sufficient to consider the case $\lambda_1 = \lambda_2 = 0$ and $\mu = \mu_r + \mathrm{i}\mu_i$ is complex. Then

$$\Delta_2(E, \mu, \boldsymbol{q}_1, \boldsymbol{q}_2) = \Delta(E)\ [1 - \mu G_0(\boldsymbol{q}_2, \boldsymbol{q}_1, E) - \bar{\mu} G_0(\boldsymbol{q}_1, \boldsymbol{q}_2, E)\ + |\mu|^2 G_0(\boldsymbol{q}_1, \boldsymbol{q}_2, E)\, G_0(\boldsymbol{q}_2, \boldsymbol{q}_1, E)$$
$$- |\mu|^2 G_0^{\mathrm{reg}}(\boldsymbol{q}_1, \boldsymbol{q}_1, E) G_0^{\mathrm{reg}}(\boldsymbol{q}_2, \boldsymbol{q}_2, E)]$$

The determinant Δ_2 is again an entire function of E and the corresponding semiclassical approximation for Δ_2 has the form

$$\Delta_2(E, \mu, \boldsymbol{q}_1, \boldsymbol{q}_2) \approx 2\, \mathrm{Re}[\Delta_2(E, \mu, \boldsymbol{q}_1, \boldsymbol{q}_2)]^{\mathrm{sc,tr}}$$

Similarly to before one can show that

$$\Delta_0(E)\, G_0(\boldsymbol{q},\boldsymbol{q}',E) = -\frac{1}{2}\left[\frac{\partial}{\partial\mu_r} + \mathrm{i}\frac{\partial}{\partial\mu_i}\right] \Delta_2(E,\mu,\boldsymbol{q},\boldsymbol{q}')\big|_{\mu=0}\,,$$

from which the following semiclassical approximation is obtained

$$G_0(\boldsymbol{q},\boldsymbol{q}',E) \approx \frac{[\Delta_0(E)G_0(\boldsymbol{q},\boldsymbol{q}',E) + \overline{\Delta_0(E)G_0(\boldsymbol{q}',\boldsymbol{q},E)}]^{\mathrm{sc,tr}}}{2\,\mathrm{Re}[\Delta_0(E)]^{\mathrm{sc,tr}}}.$$

This can be interpreted as a resummation of numerator and denominator of

$$\frac{\Delta_0(E)\, G_0(\boldsymbol{q},\boldsymbol{q}',E)}{\Delta_0(E)}.$$

. Similarly for wave functions

$$\begin{aligned}\psi_m(\boldsymbol{q})\overline{\psi_m(\boldsymbol{q}')} &= -\left.\frac{\left[\frac{\partial}{\partial\mu_r} + \mathrm{i}\frac{\partial}{\partial\mu_i}\right]\Delta_2(E,\mu,\boldsymbol{q},\boldsymbol{q}')}{2\frac{\partial}{\partial E}\Delta_2(E,\mu,\boldsymbol{q},\boldsymbol{q}')}\right|_{\substack{\mu=0\\E=E_m}} \\ &\approx \frac{[\Delta_0(E_m)G_0(\boldsymbol{q},\boldsymbol{q}',E_m) + \overline{\Delta_0(E_m)G_0(\boldsymbol{q}',\boldsymbol{q},E_m)}]^{\mathrm{sc,tr}}}{2\,\mathrm{Re}[\Delta_0'(E_m)]^{\mathrm{sc,tr}}}\end{aligned}$$

Further applications

One can obtained resummed formulas for other quantities that are related to the Green function. For example, the Weyl transform of the Green function is

$$W(\boldsymbol{x},E)=\int \mathrm{d}^f q'\ \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\boldsymbol{q}'/\hbar}G(\boldsymbol{q}+\frac{1}{2}\boldsymbol{q}',\boldsymbol{q}-\frac{1}{2}\boldsymbol{q}',E)=h^f\sum_n\frac{W_n(\boldsymbol{x})}{E-E_n}$$

where $\boldsymbol{x}=(\boldsymbol{q},\boldsymbol{p})$ and $W_n(\boldsymbol{x})$ is the Wigner function of the n-th eigenstate with energy E_n. Using the result for the Green function and stationary phase approximation results in

$$W(\boldsymbol{x},E)\approx\frac{[\Delta(E)\ W(\boldsymbol{x},E)+\overline{\Delta(E)\ W(\boldsymbol{x},E)}]^{\mathrm{sc,tr}}}{2\ \mathrm{Re}\,[\Delta(E)]^{\mathrm{sc,tr}}}$$

where the semiclassical approximation to the function $W(\boldsymbol{x},E)$ is given by classical trajectories that satisfy the midpoint rule $\boldsymbol{x}=(\boldsymbol{x}_f+\boldsymbol{x}_i)/2$ where $\boldsymbol{x}_f$ and $\boldsymbol{x}_i$ are the final and initial points in phase space

Expectation values

A similar approach can be applied to expectation values of operators. Consider the perturbation of the Hamiltonian by a self-adjoint operator in the form $\hat{H} + \lambda \hat{A}$ and the corresponding spectral determinant $\Delta(E, \lambda)$. Then it follows from first-order perturbation theory that

$$\frac{\partial}{\partial \lambda} \Delta(E, \lambda) \Big|_{\substack{\lambda=0 \\ E=E_m}} = -\frac{\partial E_m(\lambda)}{\partial \lambda} \Big|_{\lambda=0} \frac{\Delta_0(E)}{E - E_m} \Big|_{E \to E_m} = -\langle \psi_m | A | \psi_m \rangle \, \Delta_0'(E_m).$$

Hence

$$\langle \psi_n | A | \psi_n \rangle = - \left. \frac{\frac{\partial}{\partial \lambda} \Delta(E, \lambda)}{\frac{\partial}{\partial E} \Delta(E, \lambda)} \right|_{\substack{\lambda=0 \\ E=E_n}}$$

The corresponding semiclassical approximation is given by

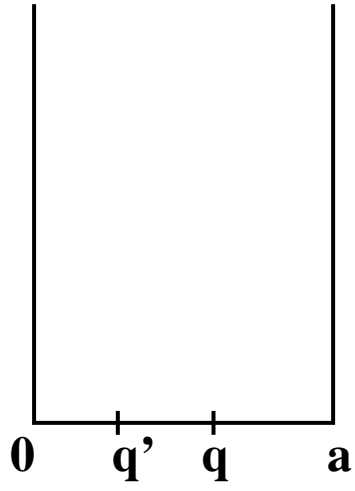
$$\langle \psi_n | A | \psi_n \rangle \approx - \left. \frac{\mathrm{Re} \left[\frac{\partial}{\partial \lambda} \Delta(E, \lambda) \right]^{\mathrm{sc,tr}}}{\mathrm{Re} \left[\frac{\partial}{\partial E} \Delta(E, \lambda) \right]^{\mathrm{sc,tr}}} \right|_{\substack{\lambda=0 \\ E=E_n}}$$

The contribution of the zero-length trajectories corresponds to an average of the classical $A(\boldsymbol{q}, \boldsymbol{p})$ over the energy shell.

A simple example

Particle in a one-dimensional box with Dirichlet b.c.s
($\hbar = 2m = 1$)

$$-\psi''(q) = E\psi(q)\,, \quad \psi(0) = \psi(a) = 0$$



Semiclassical Green function ($E = k^2$)

$$G(q, q', E) = \sum_{n=0}^{\infty} \frac{e^{2ink a}}{2ik} \left[e^{ik|q-q'|} - e^{ik(q+q')} - e^{ik(2a-q-q')} + e^{ik(2a-|q-q'|)} \right]$$

$$= \frac{\cos(ka - k|q-q'|) - \cos(ka - k(q+q'))}{2k \sin ka}$$

This is the exact Green function. The cut-off $T_{\rm H}/2$ corresponds to a length $L_H/2 = T_H/2v = a$.

A simple example

There is one periodic orbit of length $2a$ and its repetitions. This orbit is longer than the cut-off at a.

The mean spectral staircase is $\bar{N}(E) = ak/\pi - 1/2$.

Spectral determinant

$$\Delta(E) = \prod_{n=1}^{\infty}(1 - E/E_n) = \frac{\sin ka}{ka}$$

Semiclassical approximation

$$\Delta(E) = \frac{1}{2ka}\mathrm{e}^{-\mathrm{i}ka+\mathrm{i}\pi/2}\left(1 - \mathrm{e}^{2\mathrm{i}ka}\right)$$

Resummation of the spectral determinant

$$\Delta(E) = 2\,\mathrm{Re}[\Delta(E)]^{\mathrm{sc,tr}} = 2\,\mathrm{Re}\left\{\frac{1}{2ka}\mathrm{e}^{-\mathrm{i}ka+\mathrm{i}\pi/2}\right\} = \frac{\sin ka}{ka}$$

The resummation with a sharp cut-off is exact.

A simple example

The resummed expression for the Green function

$$G(q,q',E) = \frac{G(q,q',E)\ \Delta(E)}{\Delta(E)}$$

is (for the case $q + q' < a$)

$$\begin{aligned} G(q,q',E) &= \frac{2\,\mathrm{Re}[G(q,q',E)\Delta(E)]^{\mathrm{sc,tr}}}{2\,\mathrm{Re}[\Delta(E)]^{\mathrm{sc,tr}}} \\ &= \frac{\mathrm{Re}\left[\mathrm{e}^{-\mathrm{i}ka+\mathrm{i}\pi/2}\left(\mathrm{e}^{\mathrm{i}k|q-q'|-\mathrm{i}\pi/2} - \mathrm{e}^{\mathrm{i}k(q+q')-\mathrm{i}\pi/2}\right)\right]}{2k\,\mathrm{Re}\left[\mathrm{e}^{-\mathrm{i}ka+\mathrm{i}\pi/2}\right]} \\ &= \frac{\cos(ka-k|q-q'|)-\cos(ka-k(q+q'))}{2k\sin ka} \end{aligned}$$

Again the resummation with a sharp cut-off is exact.

Exercise 7

Continue with the simple example and obtain resummed expressions for the wave functions. Show that your result agrees with the exact normalised wave functions.

Bifurcations

Periodic orbits in mixed Systems

In mixed systems there are stable as well as unstable periodic orbits. The stability matrix M_p of a *stable periodic orbit p* has eigenvalues $\mathrm{e}^{\pm \mathrm{i}\alpha_p}$. In the linearised approximation the neighbouring orbits wind around the periodic orbit on tori. If α_p is a rational multiple of 2π

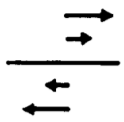
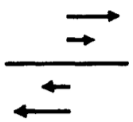
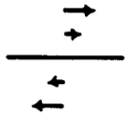
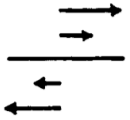
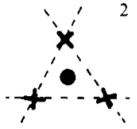
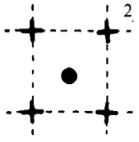
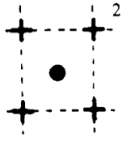
$$\alpha_p = 2\pi \frac{q}{r}$$

then the stability matrix for the r-th repetition of the periodic orbit, M_p^r, has an eigenvalue 1. This implies that the orbit is not isolated: a bifurcation occurs, in which two or more periodic orbits coalesce. The bifurcation is a period r-tupling bifurcation where p coalesces with one or more orbits which have r times the period of p. For any finite change of a parameter of a system an infinite number of bifurcations occur.

The bifurcations which occur if one parameter of the system is changed are bifurcations of codimension one. If more than one parameter of the system is varied, then the bifurcations can have more complicated forms which can involve a larger number of periodic orbits. In general, the codimension K is the number of parameters that are required to bring the participating periodic orbits into coalescence.

In addition to the codimension K, bifurcations are characterized by the repetition number r for which the bifurcation occurs. All generic bifurcations of codimension $K = 1$ and $K = 2$ have been completely classified for all r.

Bifurcations

Repetition number m	Linearised map $\mathbf{M}$ at resonance	Linearised map $\mathbf{M}^m$ at resonance	Fixed points of true $\mathbf{M}^m$ off resonance, $\varepsilon > 0$	Fixed points of true $\mathbf{M}^m$ off resonance, $\varepsilon < 0$	Normal form
1			 2	0	$\varepsilon q^2 + q^3 + p^2$
2			 2	1	$\varepsilon q^2 + q^4 + p^2$
3		Identity	 2	 2	$cq^2 + q^3 - qp^2$
4 ($\lvert c\rvert > \lvert a\rvert$)		Identity	 2	 2	$\varepsilon I + cI^2 + aI^2 \times \sin(4\phi)$
4 ($\lvert c\rvert < \lvert a\rvert$)		Identity	 3	 1	$\varepsilon I + cI^2 + aI^3 \times \sin(4\phi)$
5		Identity	 3	 1	$\varepsilon I + cI^2 + aI^{5/2} \times \sin(5\phi)$
>5	Natural extension of $m = 5$ case				

Bifurcating orbits are semiclassically more important than isolated orbits.

$$d_\gamma^{\mathrm{osc}}(E) \propto \frac{1}{\hbar^2} \int \mathrm{d}Q\,\mathrm{d}P\, G(Q,P)\, \mathrm{e}^{i\Phi(Q,P)/\hbar}$$

The normal form $\Phi(Q,P)$ describes the configuration of the periodic orbits that participate in the bifurcation.

Example saddle node bifurcation: $\Phi(Q,P) = P^2 + x_1 Q + Q^3$

Stationary points are at $(Q,P) = (\pm\sqrt{-x_1}, 0)$.

Contribution at bifurcation $\propto \hbar^{-\beta}$, where $\beta = 7/6$ for saddle node.

Away from the bifurcation ($-x_1$ large) we have contributions of isolated orbits $\propto \hbar^{-1}$. The two regimes are interpolated by an Airy function.

There is a different *diffraction integral* for every type of bifurcation. This makes semiclassical approximations in mixed systems very complicated!

Example: period-doubling pitchfork bifurcation

$$\begin{aligned} d_\xi(E) = \mathrm{Re}\ \Bigg[& \frac{1}{\pi\hbar} \left| \frac{\pi \Delta S}{2\hbar} \right|^{1/2} \exp\left(\frac{i}{\hbar}\bar{S} - \frac{i\pi}{2}\nu - \frac{i\pi}{4}\sigma \right) \\ & \times \Bigg\{ \left(\frac{A_1}{2} + \frac{A_0}{\sqrt{2}} \right) \left(\sigma_2 J_{1/4}\left(\frac{|\Delta S|}{\hbar} \right) e^{i\sigma_1 \pi/8} + J_{-1/4}\left(\frac{|\Delta S|}{\hbar} \right) e^{-i\sigma_1 \pi/8} \right) \\ & + \left(\frac{A_1}{2} - \frac{A_0}{\sqrt{2}} \right) \left(J_{3/4}\left(\frac{|\Delta S|}{\hbar} \right) e^{i\sigma_1 3\pi/8} + \sigma_2 J_{-3/4}\left(\frac{|\Delta S|}{\hbar} \right) e^{-i\sigma_1 3\pi/8} \right) \Bigg\} \Bigg] . \end{aligned}$$

Besides β there are further exponents that are important for the semiclassical influence of the bifurcation. They describes the size of the parameter intervals over which the bifurcation is semiclassically stronger than isolated periodic orbits. Consider

$$d_\gamma^{\mathrm{osc}}(E) \propto \frac{1}{\hbar^2} \int \mathrm{d}Q\, \mathrm{d}P\, G(Q,P)\, \mathrm{e}^{i\Phi(Q,P)/\hbar}$$

In the example $\Phi(Q,P) = P^2 + x_1 Q + Q^3$ we can make the exponent $\hbar$-independent by scaling

$$Q = \tilde{Q}\hbar^{1/3}\ , \quad P = \tilde{P}\hbar^{1/2}\ , \quad x_1 = \tilde{x}_1\hbar^{2/3}$$

Hence the relevant x_1 interval scales like $\hbar^{\sigma_1}$ where $\sigma_1 = 2/3$ in the example.
Bifurcations of higher codimension K have K parameters in their normal form, and there are K exponents σ_i that describe the relevant volume in parameter space. Because of this finite extension in parameter space, bifurcations of higher codimension cannot be neglected even if only one parameter is varied!

Billiard systems

Billiard systems

Billiard systems are popular model systems in quantum chaos. Let us first consider two-dimensional billiards. Some reasons for the popularity are

- Many standard examples of chaotic systems are billiard systems (stadium billiard, Sinai billiard, cardioid billiard, diamond billiard).
- Similarly, there are standard examples of integrable systems (rectangles, circle, ellipses, triangles (60-60-60, 90-60-30, 90-45-45), confocal parabolas).
- There are new types of systems like pseudo-integrable systems.
- Experiments in the field of quantum chaos are often done on systems that are modelled by billiard systems.
- There are special methods for numerical treatment and for analytical treatment.

Billiard systems

The Schrödinger equation for quantum billiards is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{q}) = E\,\psi_(\boldsymbol{q}) \qquad \text{or} \qquad (k^2+\nabla^2)\,\psi(\boldsymbol{q}) = 0, \qquad \boldsymbol{q}\in D,$$

where D is the domain of the billiard and $k=\sqrt{2mE}/\hbar$ is the wave number.

Possible boundary conditions are

$$\begin{aligned} \psi(\boldsymbol{q}) &= 0, && \boldsymbol{q}\in\partial D, && \text{Dirichlet b.c.s}\\ \boldsymbol{n}\cdot\nabla\psi(\boldsymbol{q}) &= 0, && \boldsymbol{q}\in\partial D, && \text{Neumann b.c.s}\\ \kappa\psi+\boldsymbol{n}\cdot\nabla\psi(\boldsymbol{q}) &= 0, && \boldsymbol{q}\in\partial D, && \text{Robin b.c.s} \end{aligned}$$

where ∂D is the boundary of the domain D, κ is the parameter of the Robin boundary conditions, and $\boldsymbol{n}$ is the outward pointing unit normal vector of the boundary. In the following we will abbreviate $\partial_{\boldsymbol{n}} = \boldsymbol{n}\cdot\nabla$.

For billiard systems it is convenient to use dimensionless coordinates in which $\hbar = 2m = 1$. Then $E = k^2$, and the semiclassical limit corresponds to $k\to\infty$. We will use dimensionless units in this section ($\hbar = 2m = 1$).

The mean density of states

For billiard systems higher-order corrections to Weyl's law for the mean density are known. Let $N(E)$ be the spectral staircase or spectral counting function

$$N(E) = \#\{E_n | E_n < E\} = \sum_n \theta(E - E_n),$$

with

$$d(E) = \frac{d}{dE} N(E) = \sum_n \delta(E - E_n).$$

For Dirichlet boundary conditions the result is

$$\bar{N}(E) \approx \frac{A}{4\pi} E - \frac{L}{4\pi} \sqrt{E} + \frac{1}{12\pi} \int_{\partial D} K(s)\, \mathrm{d}s + \sum_j \frac{1}{24} \left(\frac{\pi}{\alpha_j} - \frac{\alpha_j}{\pi} \right) \qquad \text{as} \qquad E \to \infty.$$

A is the area of the domain D, L is the length of the boundary ∂D, $K(s)$ is the curvature of the boundary at the coordinate s along the boundary. The sum over j runs over all corners of the billiard and α_j is the interior angle of a corner. For Robin boundary conditions the first two terms are

$$\bar{N}(E) \approx \frac{A}{4\pi} E - \frac{L}{4\pi} \sqrt{E} \left[1 - 2 \left(\sqrt{1 + \left(\frac{\kappa}{k} \right)^2} - \frac{\kappa}{k} \right) \right] \qquad \text{as} \qquad E \to \infty.$$

Boundary integral equation

We start by discussing a boundary integral equation that reduces the two-dimensional problem to a one-dimensional problem along the boundary. To derive this integral equation we consider

$$[E + \nabla^2] G_0(\boldsymbol{q}, \boldsymbol{q}', E) = \delta(\boldsymbol{q} - \boldsymbol{q}'), \qquad [E + \nabla^2]\psi(\boldsymbol{q}) = 0.$$

where $G_0(\boldsymbol{q}, \boldsymbol{q}', E)$ is the free Green function.

$$G_0(\boldsymbol{q}, \boldsymbol{q}', E) = -\frac{i}{4} H_0^{(1)}(k\,|\boldsymbol{q} - \boldsymbol{q}'|).$$

We multiply the first differential equation from the left with $\psi(\boldsymbol{q})$ and the second equation from the left with $G_0(\boldsymbol{q}, \boldsymbol{q}', E)$. The difference of the resulting equations is

$$\psi(\boldsymbol{q})\,[E + \nabla^2](G_0(\boldsymbol{q}, \boldsymbol{q}', E) - G_0(\boldsymbol{q}, \boldsymbol{q}', E)[E + \nabla^2]\psi(\boldsymbol{q}) = \psi(\boldsymbol{q})\,\delta(\boldsymbol{q} - \boldsymbol{q}').$$

This can be written in the form

$$\nabla\cdot[\psi(\boldsymbol{q})\nabla G_0(\boldsymbol{q}, \boldsymbol{q}', E) - G_0(\boldsymbol{q}, \boldsymbol{q}', E)\nabla\psi(\boldsymbol{q})] = \psi(\boldsymbol{q})\,\delta(\boldsymbol{q} - \boldsymbol{q}'),$$

We continue by integrating this equation over the domain D.

Boundary integral equation

We arrive at

$$\int_D \mathrm{d}^2 q\, \nabla\cdot[\psi(\boldsymbol{q})\nabla G_0(\boldsymbol{q},\boldsymbol{q}',E) - G_0(\boldsymbol{q},\boldsymbol{q}',E)\nabla\psi(\boldsymbol{q})] = \int_D \mathrm{d}^2 q\, \psi(\boldsymbol{q})\,\delta(\boldsymbol{q}-\boldsymbol{q}').$$

An application of the divergence theorem

$$\int_D \mathrm{d}^2 q\, \nabla\cdot\boldsymbol{F}(\boldsymbol{q}) = \int_{\partial D} \mathrm{d}s\, \boldsymbol{n}\cdot\boldsymbol{F}(\boldsymbol{q}),$$

results in

$$\int_{\partial D} \mathrm{d}s\, [\psi(\boldsymbol{q})\partial_{\boldsymbol{n}} G_0(\boldsymbol{q},\boldsymbol{q}',E) - G_0(\boldsymbol{q},\boldsymbol{q}',E)\partial_{\boldsymbol{n}}\psi(\boldsymbol{q})] = \begin{cases} 0 & \boldsymbol{q}' \notin D \\ \psi(\boldsymbol{q}')/2 & \boldsymbol{q}' \in \partial D, \\ \psi(\boldsymbol{q}') & \boldsymbol{q}' \in D/\partial D, \end{cases}$$

where $\partial_{\boldsymbol{n}} = \boldsymbol{n}\cdot\nabla$. The result on the boundary can be justified by potential theory.

We will consider Dirichlet boundary conditions $\psi(\boldsymbol{q}) = 0$ on ∂D in the following. One way to continue is to apply these conditions to the wave function in the integral equation.

Boundary integral equation

After applying Dirichlet boundary conditions to the function $\psi(\boldsymbol{q})$ we obtain for $\boldsymbol{q}' \in \partial D$

$$\int_{\partial D} \mathrm{d}s \; G_0(\boldsymbol{q}, \boldsymbol{q}', E)\, \partial_{\boldsymbol{n}} \psi(\boldsymbol{q}) = 0.$$

The free Green function G_0 has a logarithmic divergence in two dimensions as $\boldsymbol{q} \to \boldsymbol{q}'$

$$G_0(\boldsymbol{q}, \boldsymbol{q}', E) = -\frac{i}{4} H_0^{(1)}(k\,|\boldsymbol{q} - \boldsymbol{q}'|) \sim \frac{1}{2\pi} \log\left(\frac{k|\boldsymbol{q} - \boldsymbol{q}'|}{2}\right) + \frac{\gamma}{2\pi} - \frac{i}{4}$$

This is inconvenient for numerical and analytical applications. It is more appropriate to apply a normal derivative to the previous equation before applying the b.c.s, and we obtain

$$-\int_{\partial D} \mathrm{d}s \; \partial_{\boldsymbol{n}'} G_0(\boldsymbol{q}, \boldsymbol{q}', E) \partial_{\boldsymbol{n}} \psi(\boldsymbol{q}) = \frac{1}{2} \partial_{\boldsymbol{n}'} \psi(\boldsymbol{q}')$$

This result can again be justified by potential theory. This integral equation is now non-singular because $\partial_{\boldsymbol{n}'} G_0(\boldsymbol{q}, \boldsymbol{q}', E)$ stays finite if $\boldsymbol{q}$ approaches $\boldsymbol{q}'$ along the boundary. (We assume that the boundary is continuously differentiable.)

$$\partial_{\boldsymbol{n}'} G_0(\boldsymbol{q}, \boldsymbol{q}', E) = \frac{-ik}{4} H_1^{(1)}(k\,|\boldsymbol{q} - \boldsymbol{q}'|)\, \frac{\boldsymbol{n}' \cdot (\boldsymbol{q} - \boldsymbol{q}')}{|\boldsymbol{q} - \boldsymbol{q}'|}$$

Boundary integral equation

We define the integral operator

$$\hat{Q}u(s') = -2\int_{\partial D} \mathrm{d}s\; u(s)\,\partial_{\boldsymbol{n}'} G_0(\boldsymbol{q},\boldsymbol{q}',E)$$

With this definition the boundary integral equation has the form

$$(\mathbb{1}-\hat{Q})u(s') = 0.$$

This is a Fredholm integral equation of the second kind. Non-trivial solutions exit only if the Fredholm determinant vanishes

$$\Delta(E) = \det(\mathbb{1}-\hat{Q}) = 0.$$

By an application of Fredholm theory, $\Delta(E)$ can be represented by an absolutely convergent series which in the semiclassical approximation becomes a series over pseudo-orbits.

For $\mathrm{Im}\,k \geq 0$ all the zeros of the Fredholm determinant correspond to energies of the interior billiard with Dirichlet boundary conditions, $k = \pm\sqrt{E_n}$. For $\mathrm{Im}\,k < 0$ there can be further zeros. They correspond to resonances of the outside scattering problem with Neumann boundary conditions.

In the following we apply the boundary integral equation to derive the trace formula.

The spectral staircase is related to the spectral determinant by

$$N(E) = N_{\rm sm}(E) - \frac{1}{\pi} \lim_{\varepsilon \to 0} \operatorname{Im} \log \frac{\Delta(E + i\varepsilon)}{\Delta(0)}.$$

We expand the determinant in terms of traces of powers of $\hat{Q}$

$$\Delta(E) = \det(\mathbb{1} - \hat{Q}) = \exp\Big(\operatorname{Tr} \log(\mathbb{1} - \hat{Q})\Big) = \exp\left(-\sum_{n=1}^{\infty} \frac{1}{n} \operatorname{Tr} \hat{Q}^n\right),$$

and we arrive at the starting point for the derivation of the trace formula by

$$d(k) = \frac{d}{dk} N(E) = d_{sm}(k) + \frac{1}{\pi} \operatorname{Im} \sum_{n=1}^{\infty} \frac{1}{n} \frac{d}{dk} \operatorname{Tr} \hat{Q}^n(k),$$

where

$$\operatorname{Tr} \hat{Q}^n(k) = (-2)^n \int_{\partial \mathcal{D}} \mathrm{d}s_1 \ldots \mathrm{d}s_n \, \partial_{\boldsymbol{n}_n} G_0(\boldsymbol{q}_1, \boldsymbol{q}_n, E) \ldots \partial_{\boldsymbol{n}_2} G_0(\boldsymbol{q}_3, \boldsymbol{q}_2, E) \, \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q}_2, \boldsymbol{q}_1, E)$$

The trace formula can be obtained by evaluating all integrals in stationary phase approximation. The derivation can be significantly simplified by applying the multiple reflection expansion of Balian and Bloch (1970).

Multiple reflection expansion

This is a short excursion on the multiple reflection expansion of Balian and Bloch (1970).

We write the Green's function for the billiard with Dirichlet boundary condition in the form

$$G(\boldsymbol{q},\boldsymbol{q}',E) = G_0(\boldsymbol{q},\boldsymbol{q}',E) + G_1(\boldsymbol{q},\boldsymbol{q}',E).$$

Here G_0 is the free Green function and G_1 is a solution of

$$\begin{aligned} (E+\nabla^2)G_1(\boldsymbol{q},\boldsymbol{q}',E) &= 0 && \boldsymbol{q}\in D. \\ G_1(\boldsymbol{q},\boldsymbol{q}',E) &= -G_0(\boldsymbol{q},\boldsymbol{q}',E) && \boldsymbol{q}\in \partial D \end{aligned}$$

In the next step G_1 is represented by a double layer potential

$$G_1(\boldsymbol{q},\boldsymbol{q}',E) = \int_{\partial D} \mathrm{d}s_1 \; \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q},\boldsymbol{q}_1,E)\, \mu(\boldsymbol{q}_1,\boldsymbol{q}',E).$$

Potential theory provides the jump relation for this double layer potential. It is given by

$$G_1^{\uparrow}(\boldsymbol{q},\boldsymbol{q}',E) - \int_{\partial D} \mathrm{d}s_1 \; \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q},\boldsymbol{q}_1,E)\, \mu(\boldsymbol{q}_1,\boldsymbol{q}',E) = \frac{1}{2}\mu(\boldsymbol{q}_1,\boldsymbol{q}',E).$$

Multiple reflection expansion

Applying the boundary condition for G_1 results in

$$-G_0(\boldsymbol{q}_1, \boldsymbol{q}', E) - \int_{\partial D} \mathrm{d}s\, \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q}_1, \boldsymbol{q}_2, E)\, \mu(\boldsymbol{q}_2, \boldsymbol{q}', E) = \frac{1}{2}\mu(\boldsymbol{q}_1, \boldsymbol{q}', E)$$

Using this relation iteratively, one obtains the multiple reflection expansion of Balian and Bloch

$$\begin{aligned} G(\boldsymbol{q}, \boldsymbol{q}', E) &= G_0(\boldsymbol{q}, \boldsymbol{q}', E) + G_1(\boldsymbol{q}, \boldsymbol{q}', E) \\ &= G_0(\boldsymbol{q}, \boldsymbol{q}', E) + \int_{\partial D} \mathrm{d}s_1\ \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q}, \boldsymbol{q}_1, E)\, \mu(\boldsymbol{q}_1, \boldsymbol{q}', E) \\ &= G_0(\boldsymbol{q}, \boldsymbol{q}', E) + (-2) \int_{\partial D} \mathrm{d}s_1\ \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q}, \boldsymbol{q}_1, E)\, G_0(\boldsymbol{q}, \boldsymbol{q}', E) \\ &\quad + (-2) \int_{\partial D} \mathrm{d}s_1\, \mathrm{d}s_2\ \partial_{\boldsymbol{n}_2} G_0(\boldsymbol{q}, \boldsymbol{q}_2, E)\, \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q}_2, \boldsymbol{q}_1, E)\, \mu(\boldsymbol{q}_1, \boldsymbol{q}', E) \end{aligned}$$

We find

$$G(\boldsymbol{q}, \boldsymbol{q}', E) = \sum_{n=0}^{\infty} G^{(n)}(\boldsymbol{q}, \boldsymbol{q}', E),$$

where $G^{(n)}$ is the contribution from n reflections on the boundary to the Green function G.

Multiple reflection expansion

We found

$$G(\boldsymbol{q}, \boldsymbol{q}', E) = \sum_{n=0}^{\infty} G^{(n)}(\boldsymbol{q}, \boldsymbol{q}', E),$$

where

$$G^{(n)}(\boldsymbol{q}, \boldsymbol{q}', E) = (-2)^n \int_{\partial \mathcal{D}} ds_1 \dots ds_n \, \partial_{\boldsymbol{n}_n} G_0(\boldsymbol{q}, \boldsymbol{q}_n, E) \dots \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q}_2, \boldsymbol{q}_1, E) \; G_0(\boldsymbol{q}_1, \boldsymbol{q}', E)$$

From this form follows the composition rule

$$G^{(n+1)}(\boldsymbol{q}, \boldsymbol{q}', E) = (-2) \int_{\partial D} ds_1 \; \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q}, \boldsymbol{q}_1, E) \; G^{(n)}(\boldsymbol{q}_1, \boldsymbol{q}', E)$$

or more generally

$$G^{(m+n+1)}(\boldsymbol{q}, \boldsymbol{q}', E) = (-2) \int_{\partial D} ds_1 \; \partial_{\boldsymbol{n}_1} G^{(m)}(\boldsymbol{q}, \boldsymbol{q}_1, E) \; G^{(n)}(\boldsymbol{q}_1, \boldsymbol{q}', E)$$

We compare this to the formula for the traces of $\hat{Q}$

$$\mathrm{Tr}\, \hat{Q}^n(k) = (-2)^n \int_{\partial \mathcal{D}} \mathrm{d}s_1 \dots \mathrm{d}s_n \, \partial_{\boldsymbol{n}_n} G_0(\boldsymbol{q}_1, \boldsymbol{q}_n, E) \dots \partial_{\boldsymbol{n}_2} G_0(\boldsymbol{q}_3, \boldsymbol{q}_2, E) \; \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q}_2, \boldsymbol{q}_1, E)$$

Multiple reflection expansion

The comparison of the formulas shows

$$\mathrm{Tr}\,\hat{Q}^n = (-2)\int_{\partial D} \mathrm{d}s\,\partial_{\boldsymbol{n}'} G^{(n-1)}(\boldsymbol{q},\boldsymbol{q}',E)\Big|_{\boldsymbol{q}=\boldsymbol{q}'}$$

and hence

$$d(k) = d_{sm}(k) - \frac{2}{\pi}\frac{d}{dk}\,\mathrm{Im}\sum_{n=1}^{\infty}\frac{1}{n}\int_{\partial\mathcal{B}} ds\,\partial_{\boldsymbol{n}'} G^{(n-1)}(\boldsymbol{q},\boldsymbol{q}',E)|_{\boldsymbol{q}=\boldsymbol{q}'}$$

We want to derive the trace formula from this approach. Plan of proof

- First we show by induction that

$$G_{sc}^{(n)}(\boldsymbol{q},\boldsymbol{q}',E) = \sum_{\gamma_n}\frac{1}{\sqrt{8\pi k|\tilde{M}_{\gamma_n,12}|}}\exp\left(ikl_{\gamma_n} - i\frac{\pi}{2}\xi_{\gamma_n} - i\frac{3\pi}{4}\right)$$

  The sum runs over all trajectories with n reflections from $\boldsymbol{q}'$ to $\boldsymbol{q}$ and $\tilde{M}$ is the stability matrix at unit energy. The index ξ is given by the number of conjugate points plus twice the number of reflections at the boundary.

- Then the semiclassical approximation for the density of states follows from an evaluation of the above integral by the method of stationary phase.

Derivation of the semiclassical Green's function

We have the composition rule

$$G^{(n+1)}(\boldsymbol{q},\boldsymbol{q}',E) = (-2)\int_{\partial D} ds_1\ \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q},\boldsymbol{q}_1,E)\ G^{(n)}(\boldsymbol{q}_1,\boldsymbol{q}',E),$$

and we want to show by induction that

$$G^{(n)}_{sc}(\boldsymbol{q},\boldsymbol{q}',E) = \sum_{\gamma_n} \frac{1}{\sqrt{8\pi k|\tilde{M}_{\gamma_n,12}|}} \exp\left(ikl_{\gamma_n} - i\frac{\pi}{2}\xi_{\gamma_n} - i\frac{3\pi}{4}\right).$$

In the first step we show that the relation holds for $n = 0$.

$$G_0(\boldsymbol{q},\boldsymbol{q}',E) = -\frac{i}{4}H_0^{(1)}(k\,l) \sim \frac{1}{\sqrt{8\pi kl}} \exp\left(ikl - i\frac{3\pi}{4}\right) \quad \text{as} \quad k\to\infty.$$

where $l = |\boldsymbol{q}-\boldsymbol{q}'|$. This is correct, because $\tilde{M}_{12} = l$ and $\xi = 0$ for the direct trajectory. Next we need to approximate the above integral. We have in leading order.

$$\partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q},\boldsymbol{q}_1,E) \approx -i\,\boldsymbol{n}_1\cdot\boldsymbol{p}_1\ G^{(0)}_{sc}(\boldsymbol{q},\boldsymbol{q}_1,E) = ik\cos\alpha_1\ G^{(0)}_{sc}(\boldsymbol{q},\boldsymbol{q}_1,E)$$

were α_1 is the angle between $\boldsymbol{n}_1$ and momentum $\boldsymbol{p}_1$ and we used $\frac{\partial}{\partial \boldsymbol{q}_1} S(\boldsymbol{q},\boldsymbol{q}_1) = -\boldsymbol{p}_1$.

Derivation of the semiclassical Green function

With these results

$$(-2)\int_{\partial D} ds_1\ \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q},\boldsymbol{q}_1,E)\ G_{sc}^{(n)}(\boldsymbol{q}_1,\boldsymbol{q}',E)$$

$$=\sum_{\gamma_n}(-2)\int_{\partial\mathcal{D}} ds_1\ (ik\cos\alpha_1)\frac{\exp\left\{ik[l^{(0)}(\boldsymbol{q},\boldsymbol{q}_1)+l^{(n)}(\boldsymbol{q}_1,\boldsymbol{q}')]-i\frac{\pi}{2}\xi^{(n)}-i\frac{3\pi}{2}\right\}}{8\pi k\sqrt{|\tilde{M}_{12}^{(0)}\ \tilde{M}_{12}^{(n)}|}}$$

Stationary points are determined by

$$0=\frac{d}{ds_1}[l^{(0)}(\boldsymbol{q},\boldsymbol{q}_1)+l^{(n)}(\boldsymbol{q}_1,\boldsymbol{q}')]=\boldsymbol{t}_1\cdot[-\frac{\boldsymbol{p}_1^{(0)}}{k}+\frac{\boldsymbol{p}_1^{(n)}}{k}]=\sin\alpha_1^{(0)}-\sin\alpha_1^{(n)}.$$

From this follows that the angle of incidence and the angle of reflection are equal. It implies that $l^{(0)}$ and $l^{(n)}$ are parts of a longer trajectory with $(n+1)$ reflections.

The expansion up to second order is a bit lengthy and we give only the result

$$\frac{d^2}{ds_1^2}[l^{(0)}(\boldsymbol{q},\boldsymbol{q}_1)+l^{(n)}(\boldsymbol{q}_1,\boldsymbol{q}')]=-\frac{\cos^2\alpha_1\ \tilde{M}_{12}^{(n+1)}}{\tilde{M}_{12}^{(0)}\ \tilde{M}_{12}^{(n)}}.$$

Derivation of the semiclassical Green function

With this result we can evaluate

$$(-2)\int_{\partial D} ds_1\ \partial_{\boldsymbol{n}_1} G_0(\boldsymbol{q},\boldsymbol{q}_1,E)\ G_{sc}^{(n)}(\boldsymbol{q}_1,\boldsymbol{q}',E)$$

$$=\sum_{\gamma_{n+1}}\int_{\partial\mathcal{D}} ds_1\ \frac{\cos\alpha_1\ \exp\left\{ikl^{(n+1)}(\boldsymbol{q},\boldsymbol{q}')-i\frac{\pi}{2}\nu^{(n)}\right\}}{4\pi\sqrt{|\tilde{M}_{12}^{(0)}\,\tilde{M}_{12}^{(n)}|}}\int_{-\infty}^{\infty}\mathrm{d}s_1\ \exp\left(-ik\frac{\cos^2\alpha_1\,\tilde{M}_{12}^{(n+1)}}{2\,\tilde{M}_{12}^{(0)}\,\tilde{M}_{12}^{(n)}}s_1^2\right)$$

$$=\sum_{\gamma_{n+1}}\frac{1}{\sqrt{8\pi k\left|\tilde{M}_{12}^{(n+1)}\right|}}\ \exp\left(ikl^{(n+1)}-i\frac{\pi}{2}\nu^{(n+1)}-i\frac{3\pi}{4}\right)$$

where $\tilde{M}^{(n+1)}=\tilde{M}^{(0)}\tilde{M}_r\tilde{M}^{(n)}$ with

$$\tilde{M}^{(0)}=\begin{pmatrix}1 & l\\ 0 & 1\end{pmatrix},\qquad \tilde{M}_r=\begin{pmatrix}-1 & 0\\ \frac{2}{R\cos\alpha} & -1\end{pmatrix}.$$

and

$$\nu^{(n+1)}=\nu^{(n)}+2+\begin{cases}1 & \text{if}\quad \mathrm{sgn}(\tilde{M}_{12}^{(n+1)})=\mathrm{sgn}(\tilde{M}_{12}^{(n)}),\\ 0 & \text{if}\quad \mathrm{sgn}(\tilde{M}_{12}^{(n+1)})\neq\mathrm{sgn}(\tilde{M}_{12}^{(n)}).\end{cases}$$

Derivation of the trace formula

We obtained the correct rules for the composition of stability matrices and Maslov indices. In the final step we evaluate the following integral in stationary phase approximation.

$$d(k) = d_{sm}(k) - \frac{2}{\pi}\frac{d}{dk}\,\mathrm{Im}\sum_{n=1}^{\infty}\frac{1}{n}\int_{\partial\mathcal{B}} ds\;\partial_{\boldsymbol{n}'}\,G^{(n-1)}(\boldsymbol{q},\boldsymbol{q}',E)|_{\boldsymbol{q}=\boldsymbol{q}'}$$

The contribution of a periodic orbit with n reflections is obtained from the integral

$$d_{\gamma_n}(k) = -\frac{2}{\pi}\,\mathrm{Re}\,\frac{k}{n}\,\frac{l^{(n-1)}\cos\alpha}{\sqrt{8\pi k\,|\tilde{M}_{12}^{(n)}|}}\int_{\partial D}\mathrm{d}s\;\exp\left(ikl^{(n-1)}(\boldsymbol{q},\boldsymbol{q}) - i\frac{\pi}{2}\xi^{(n-1)} - i\frac{\pi}{4}\right).$$

From the stationary phase condition

$$0 = \frac{d}{ds}l^{(n-1)}(\boldsymbol{q},\boldsymbol{q}) = \boldsymbol{t}\cdot[-\frac{\boldsymbol{p}_i}{k} + \frac{\boldsymbol{p}_f}{k}]$$

follows that the angle of incidence is equal to the angle of reflection. That means that the orbit has to be periodic.

Derivation of the trace formula

We give only the result for the expansion up to second order

$$\frac{d^2}{ds^2} l^{(n-1)}(\boldsymbol{q}, \boldsymbol{q}) = -\frac{\cos^2(\mathrm{Tr}\, \tilde{M}_{po}^{(n)} - 2)}{(\tilde{M}_{po}^{(n)})_{12}},$$

and the result of the stationary phase approximation

$$d_{\gamma_n}(k) = \frac{l_{po}^{(n)}}{\pi r_{po} \sqrt{|\,\mathrm{Tr}\, \tilde{M}_{po}^{(n)} - 2|}} \cos\left\{ k l_{po}^{(n)} - \frac{\pi}{2} \mu_{po}^{(n)} \right\}.$$

Here $\tilde{M}_{po}^{(n)} = \tilde{M}_r \tilde{M}^{(n-1)}$ and

$$\mu_{po}^{(n)} = \xi^{(n-1)} + 2 + \begin{cases} 0 & \text{if} \quad (\tilde{M}_{po}^{(n)})_{12}/(\mathrm{Tr}\, \tilde{M}_{po}^{(n)} - 2) > 0, \\ 1 & \text{if} \quad (\tilde{M}_{po}^{(n)})_{12}/(\mathrm{Tr}\, \tilde{M}_{po}^{(n)} - 2) < 0. \end{cases}$$

Advantages of the derivation

- Only two stationary phase approximations needed.
- Derivation keeps track of the composition of Maslov indices and stability matrices.

Three-dimensional billiard systems

The same calculation can be done for three-dimensional billiard systems. Then $|\,\mathrm{Tr}\,M-2|$ is replaced by $|\det(M-1)|$ in the trace formula. In three dimensions one chooses a local coordinate system with one coordinate in the direction of a trajectory and two perpendicular to it. The stability matrix is four-dimensional

$$\begin{pmatrix} \mathrm{d}\boldsymbol{q}_\perp \\ \mathrm{d}\boldsymbol{p}_\perp \end{pmatrix} = M \begin{pmatrix} \mathrm{d}\boldsymbol{q}'_\perp \\ \mathrm{d}\boldsymbol{p}'_\perp \end{pmatrix} .$$

It is a symplectic matrix, $M^T J M = J$, and has 10 independent elements. It can be composed of three different types of matrices.

$$M = M_T^{b\leftarrow n} M_R^n M_S^n \ldots M_T^{3\leftarrow 2} M_R^2 M_S^2 M_T^{2\leftarrow 1} M_R^1 M_S^1 M_T^{1\leftarrow a}$$

Here M_T is the matrix for a part of the trajectory of length L between two reflections. M_S corresponds to a rotation of the local coordinate system around the trajectory such that the new coordinate with index 2 lies in the reflection plane that is spanned by the incoming and outgoing trajectory at a reflection point. M_T and M_S are given by

$$M_T = \begin{pmatrix} 1 & 0 & \frac{L}{p} & 0 \\ 0 & 1 & 0 & \frac{L}{p} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad M_S = \begin{pmatrix} \cos\theta & \sin\theta & 0 & 0 \\ -\sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & \cos\theta & \sin\theta \\ 0 & 0 & -\sin\theta & \cos\theta \end{pmatrix}$$

M_R is the matrix for a reflection

$$M_R = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \dfrac{2p}{R_a \cos\alpha} & \dfrac{2p}{R_c} & -1 & 0 \\ -\dfrac{2p}{R_c} & -\dfrac{2p\cos\alpha}{R_b} & 0 & 1 \end{pmatrix}$$

Here α is the angle of incidence. R_a and R_b are the radii of curvature in the reflection plane and perpendicular to it, respectively. R_a, R_b and R_c can be expressed in terms of the two main radii of curvature at the reflection point R_1 and R_2 and the angle β between the tangent lying in the reflection plane and the direction of the main curvature $1/R_1$.

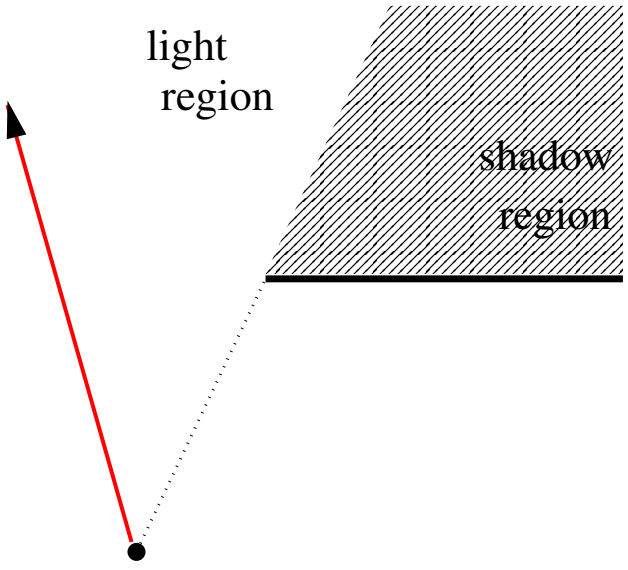
$$\frac{1}{R_a} = \frac{\cos^2\beta}{R_1} + \frac{\sin^2\beta}{R_2}, \quad \frac{1}{R_b} = \frac{\sin^2\beta}{R_1} + \frac{\cos^2\beta}{R_2}, \quad \frac{1}{R_c} = \frac{R_2 - R_1}{R_1 R_2}\cos\beta\,\sin\beta.$$

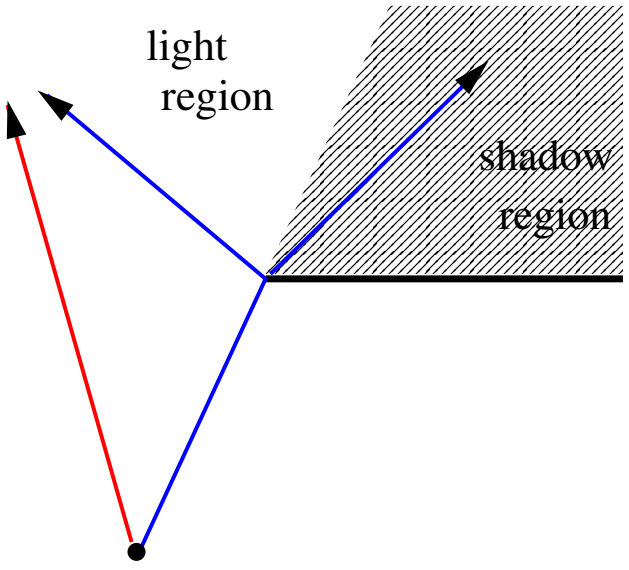
Explicit rules for calculating the Maslov index from the stability matrices can be given.

Diffraction

Diffraction

What are important corrections to semiclassics? Consider the example of a half-plane.





The usual semiclassical approach doesn't describe effects due to diffraction.

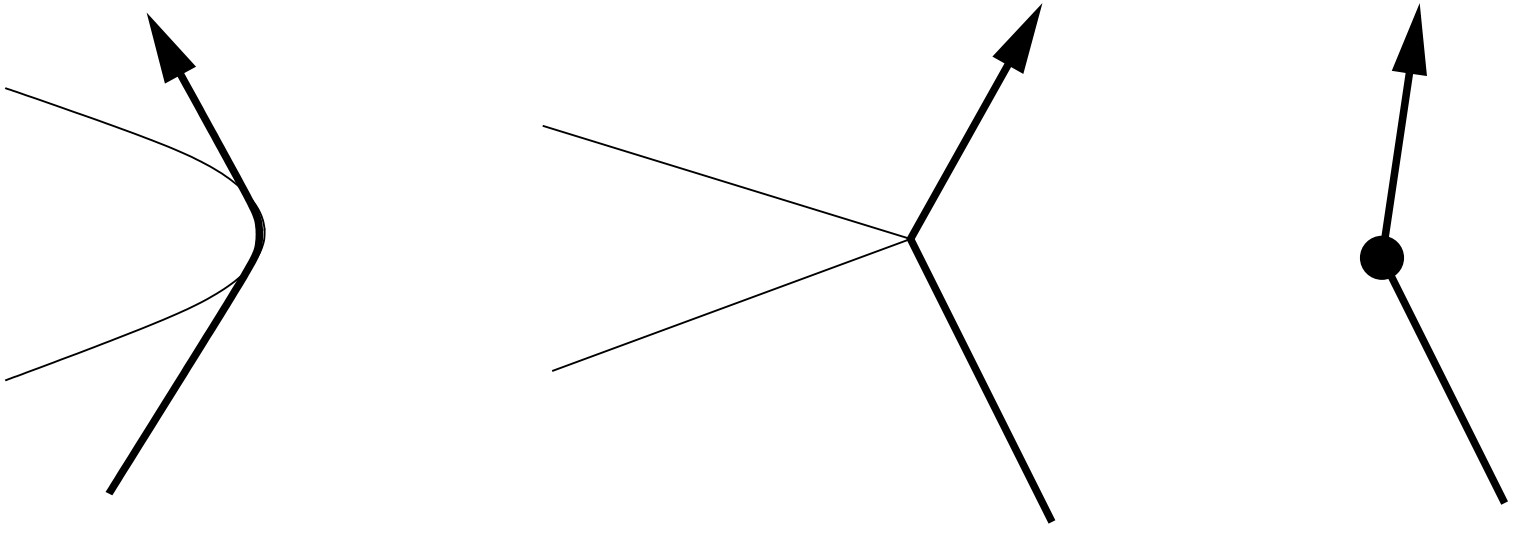
$\Longrightarrow$ Keller's geometrical theory of diffraction (GTD)

$$G(\boldsymbol{q}, \boldsymbol{q}', E) \approx G_0(\boldsymbol{q}, \boldsymbol{q}', E) + G_0(\boldsymbol{q}, \boldsymbol{q}_0, E)\, \mathcal{D}(\phi, \phi')\, G_0(\boldsymbol{q}_0, \boldsymbol{q}', E)$$

Diffractive rays have order $k^{-1/2}$ smaller amplitude than ordinary rays in 2D.

Geometrical theory of diffraction

Examples: surface diffraction, corner diffraction, point or flux line diffraction.



Case I (not discussed in this talk):

$$G(\boldsymbol{q}, \boldsymbol{q}', E) \approx G_0(\boldsymbol{q}, \boldsymbol{q}', E) + G_0(\boldsymbol{q}, \boldsymbol{q}_2, E)\, \mathcal{D}_2\, G_c(\boldsymbol{q}_2, \boldsymbol{q}_1, E)\, \mathcal{D}_1\, G_0(\boldsymbol{q}_1, \boldsymbol{q}', E)$$

Case II and III:

$$G(\boldsymbol{q}, \boldsymbol{q}', E) \approx G_0(\boldsymbol{q}, \boldsymbol{q}', E) + G_0(\boldsymbol{q}, \boldsymbol{q}_0, E)\, \mathcal{D}_0\, G_0(\boldsymbol{q}_0, \boldsymbol{q}', E)$$

Examples of diffraction coefficients

Diffraction on a corner with angle γ in two dimensions ($N = \gamma/\pi$)

$$\mathcal{D}(\phi, \phi') = -\frac{4}{N} \frac{\sin\frac{\pi}{N} \sin\frac{\phi}{N} \sin\frac{\phi'}{N}}{\left(\cos\frac{\pi}{N} - \cos\frac{\phi+\phi'}{N}\right)\left(\cos\frac{\pi}{N} - \cos\frac{\phi-\phi'}{N}\right)}.$$

Diffraction on a flux line with flux parameter α in two dimensions

$$\mathcal{D}(\phi, \phi') = \frac{2\sin(\alpha\pi)\, \exp\left\{\mathrm{i}\frac{\phi-\phi'}{2}\right\}}{\cos\left(\frac{\phi-\phi'}{2}\right)}.$$

Diffraction on a point-like scatterer with parameter a in two and dimensions

$$\mathcal{D} = \frac{2\pi}{i\frac{\pi}{2} - \gamma - \log\left(\frac{ka}{2}\right)}, \qquad \mathcal{D} = \frac{4\pi a}{1 + ika}.$$

In the first two cases the diffraction coefficients diverges for certain angles (at optical boundaries where ray contributions are discontinuous)

Multiple diffraction

General diffractive rays ξ can an arbitrary number of diffraction events, and an arbitrary number of reflections. They contribute to Green function

$$G_{\mathrm{d}}^{\xi}(\boldsymbol{q},\boldsymbol{q}',E) \approx G^{\xi}(\boldsymbol{q},\boldsymbol{q}_n,E)\,\mathcal{D}_n\,G^{\xi}(\boldsymbol{q}_n,\boldsymbol{q}_{n-1},E)\,\mathcal{D}_{n-1}\cdot\ldots\cdot\,\mathcal{D}_1\,G^{\xi}(\boldsymbol{q}_1,\boldsymbol{q}',E)$$

and to the density of eigenmodes

$$d^{\xi}(k) \approx \mathrm{Re}\left(\frac{L_\xi}{\pi}\prod_{j=1}^{n}\mathcal{D}_j\,G^{\xi}(\boldsymbol{q}_{j+1},\boldsymbol{q}_j,E)\right)$$

The contributions of the ray parts between diffraction events are of the form

$$G^{\xi}(\boldsymbol{q}_b,\boldsymbol{q}_a,E) \approx \frac{1}{\sqrt{8\pi k\,|\tilde{M}_{12}|}}\,\mathrm{e}^{\mathrm{i}kL-\mathrm{i}\pi\nu/2-\mathrm{i}3\pi/4}$$

For each diffraction event the amplitude decreases by an order $k^{-1/2}$

- Are these diffractive contributions important?
- How do contributions have to be modified at optical boundaries?

Exercise 8 (difficult)

Assume that the point $\boldsymbol{q}_0$ is at the corner point of a billiard. The contribution to the Green function from a trajectory that is diffracted once is given by

$$G^{(\xi_1,\xi_2)}(\boldsymbol{q},\boldsymbol{q}',E) \approx G^{\xi_2}(\boldsymbol{q},\boldsymbol{q}_0,E)\,\mathcal{D}\,G^{\xi_1}(\boldsymbol{q}_0,\boldsymbol{q}',E).$$

Here $\mathcal{D}$ is the diffraction coefficient of the corner, and the diffracted trajectory has the two parts ξ_1 and ξ_2. Calculate the contribution of a diffracted orbit to the density of states.

$$d(E) = -\frac{1}{\pi}\lim_{\varepsilon\to 0}\operatorname{Im}\int d^2q\, G(\boldsymbol{q},\boldsymbol{q},E+i\varepsilon).$$

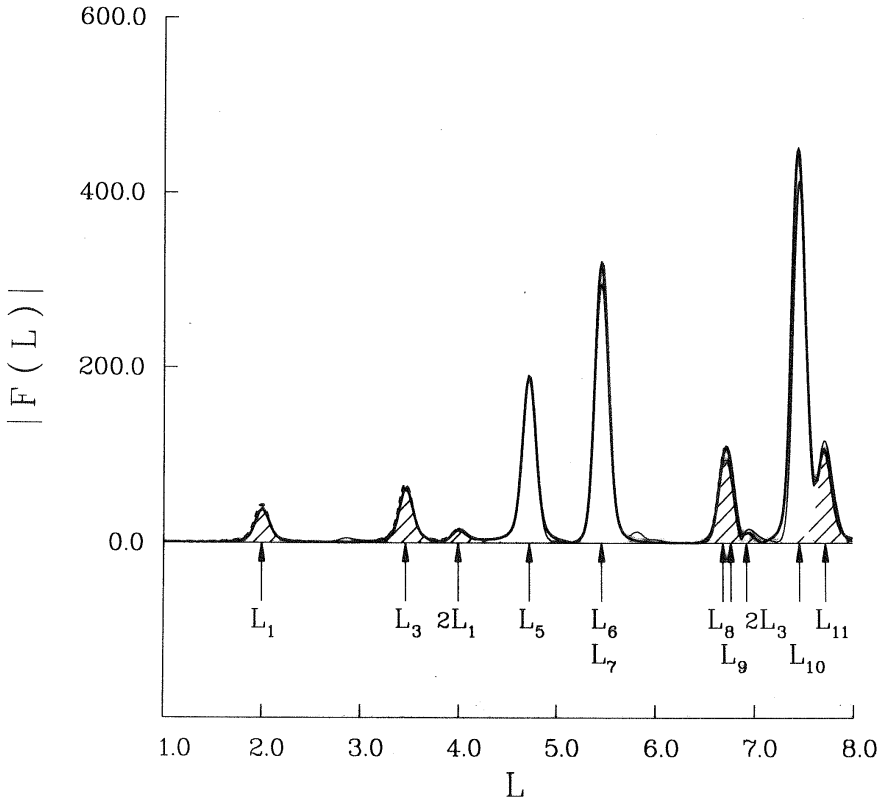
You should obtain

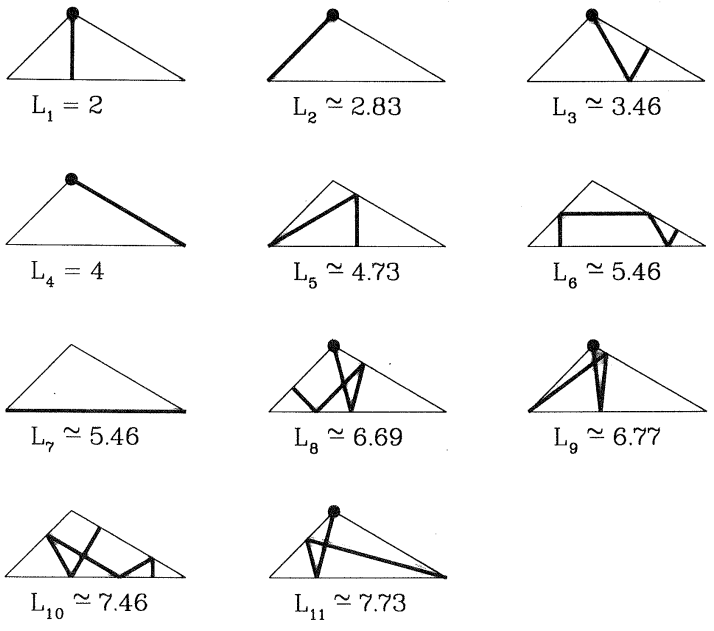
$$d^{\xi}(E) \approx \operatorname{Re}\left(\frac{T^{\xi}}{\pi}\mathcal{D}\,G^{\xi}(\boldsymbol{q}_0,\boldsymbol{q}_0,E)\right)$$

Here ξ is the trajectory that is obtained if ξ_2 and ξ_1 join smoothly to form a trajectory from $\boldsymbol{q}_0$ to $\boldsymbol{q}_0$.

Diffraction at a corner

Fourier transform of the density of eigenmodes for the triangle $\frac{7\pi}{12}, \frac{\pi}{4}, \frac{\pi}{6}$

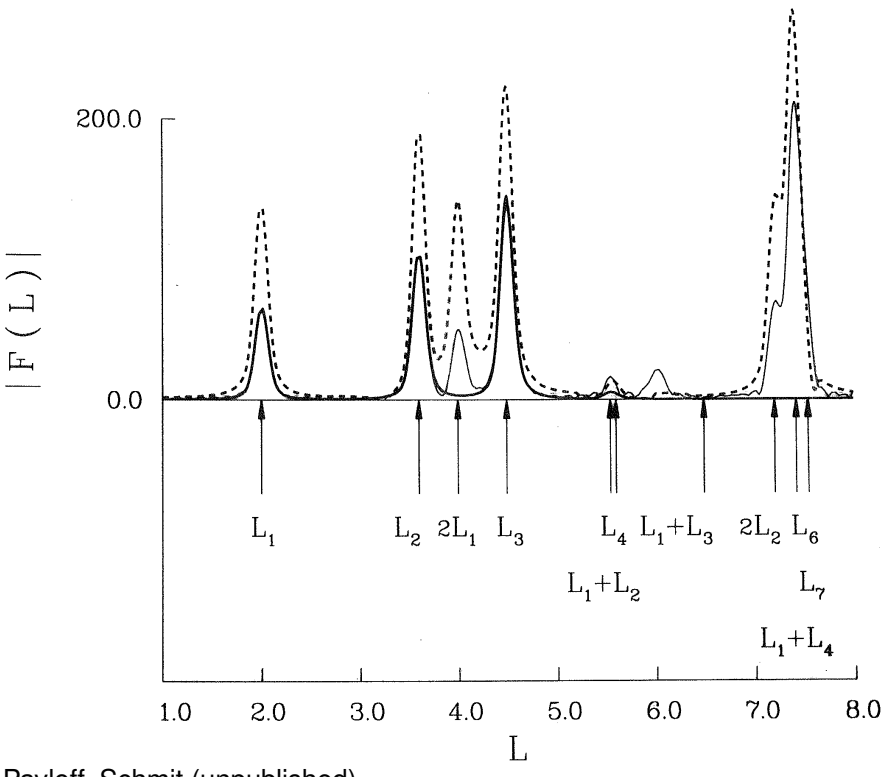


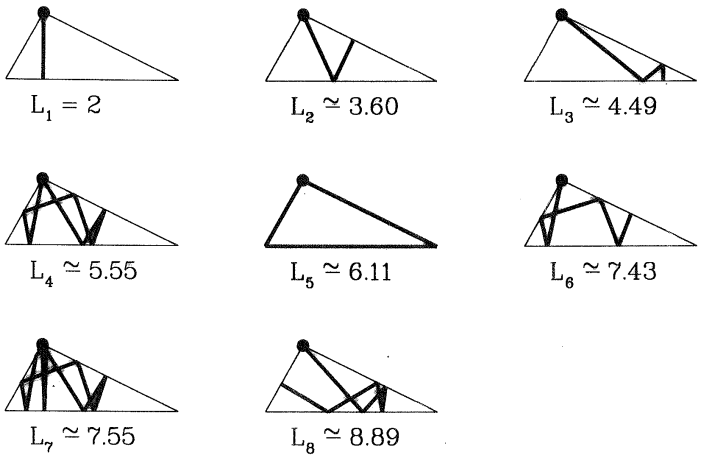


(Pavloff, Schmit)

Diffraction at a corner

Fourier transform of the density of eigenmodes for the triangle $\frac{11\pi}{21}, \frac{\pi}{3}, \frac{\pi}{7}$





Pavloff, Schmit (unpublished)

Uniform approximations needed $\Longrightarrow$ uniform geometrical theory of diffraction