Semiclassical Theory Approach in Quantum Chaos

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These lectures are intended to give a basic introduction to semiclassical methods in chaotic systems. These methods are valid in the semiclassical limit $\hbar \to 0$ where quantum mechanics is expected to reflect the underlying classical mechanics.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{q},t)+V(\boldsymbol{q})\psi(\boldsymbol{q},t)=i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{q},t).$$

The limit $\hbar \to 0$ is a singular limit, because the exact solution for small but finite $\hbar$ does not approach the solution of the unperturbed problem ($\hbar = 0$) as $\hbar \to 0$. It is a singular perturbation problem to which one applies methods of asymptotic analysis.

For example, one of the common problems is that of highly oscillatory integrals

$$\int_a^b \mathrm{d}y\, A(y)\,\mathrm{e}^{\frac{i}{\hbar}\phi(y)}.$$

They are approximated by stationary phase approximation.

Topics

- The semiclassical propagator
- Unitary operators
- Uniform approximations
- Green function and trace formula
- Wave functions
- Bifurcations
- Billiard systems
- Diffraction
- Spectral statistics
- Quantum transport

The semiclassical propagator

Classical mechanics

We start with a brief recap of classical mechanics. In the Lagrangian formulation of mechanics, the Lagrangian is defined as

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = T - V = \frac{m}{2}\dot{\boldsymbol{q}}^2 - V(\boldsymbol{q}).$$

where $\boldsymbol{q} = (q_1, \ldots, q_f)$ in f dimensions. The Euler-Lagrange equations of motion have the form

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\boldsymbol{q}}} - \frac{\partial L}{\partial \boldsymbol{q}} = 0.$$

Inserting the Lagrangian we obtain Newton's second law

$$0 = \frac{d}{dt} m\dot{\boldsymbol{q}} + \frac{\partial V(\boldsymbol{q})}{\partial \boldsymbol{q}} \qquad \Longrightarrow \qquad m\ddot{\boldsymbol{q}} = -\frac{\partial V(\boldsymbol{q})}{\partial \boldsymbol{q}}.$$

The momentum is obtained from

$$\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}} = m\dot{\boldsymbol{q}}.$$

Alternatively, one can define the Hamiltonian

$$H(\boldsymbol{q}, \boldsymbol{p}) = \dot{\boldsymbol{q}} \cdot \boldsymbol{p} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \frac{1}{2m}\boldsymbol{p}^2 + V(\boldsymbol{q}),$$

Classical mechanics

The Euler-Lagrange equations are equivalent to Hamilton's equations of motion

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{q}}, \qquad \dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}}.$$

Conservation of energy $E = H(\boldsymbol{q}, \boldsymbol{p})$ follows from

$$\frac{d}{dt} H(\boldsymbol{q}, \boldsymbol{p}) = \frac{\partial H}{\partial \boldsymbol{q}} \cdot \dot{\boldsymbol{q}} + \frac{\partial H}{\partial \boldsymbol{p}} \cdot \dot{\boldsymbol{p}} = \frac{\partial H}{\partial \boldsymbol{q}} \cdot \frac{\partial H}{\partial \boldsymbol{p}} - \frac{\partial H}{\partial \boldsymbol{p}} \cdot \frac{\partial H}{\partial \boldsymbol{q}} = 0.$$

Action principle

A central property of the Lagrangian formalism is that the equations of motion can be obtained from an action principle. Hamilton's principle function is defined for functions $\boldsymbol{q}(t)$ that run from $\boldsymbol{q}_a$ at time t_a to $\boldsymbol{q}_b$ at $t = t_b$

$$R[\boldsymbol{q}(t)](\boldsymbol{q}_b, t_b, \boldsymbol{q}_a, t_a) = \int_{t_a}^{t_b} L(\boldsymbol{q}, \dot{\boldsymbol{q}})\, dt.$$

The classical trajectories are those that make the functional $R[\boldsymbol{q}(t)]$ stationary with respect to infinitesimal variations $\boldsymbol{q}(t) \to \boldsymbol{q}(t) + \delta\boldsymbol{q}(t)$ that leave the end points invariant.

The variation of $R[\boldsymbol{q}(t)]$ is given by

$$0 = \delta R[\boldsymbol{q}] = R[\boldsymbol{q}+\delta\boldsymbol{q}] - R[\boldsymbol{q}] = \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial \dot{\boldsymbol{q}}}\delta\dot{\boldsymbol{q}} + \frac{\partial L}{\partial \boldsymbol{q}}\delta\boldsymbol{q}\right] dt$$

$$= \frac{\partial L}{\partial \dot{\boldsymbol{q}}}\delta\boldsymbol{q}\Big|_{t_a}^{t_b} - \int_{t_a}^{t_b} \left[\frac{d}{dt}\frac{\partial L}{\partial \dot{\boldsymbol{q}}} - \frac{\partial L}{\partial \boldsymbol{q}}\right] \delta\boldsymbol{q}\, dt,$$

where we integrated by parts. The first term in the last line vanishes, because $\delta\boldsymbol{q}(t_a) = 0$ and $\delta\boldsymbol{q}(t_b) = 0$. Hence the variation of $R[q(t)]$ vanishes if $\boldsymbol{q}(t)$ satisfies the Euler-Lagrange equations.

Note that there can be several different solutions $\boldsymbol{q}(t)$ that connect $\boldsymbol{q}_a$ at $t = t_a$ with $\boldsymbol{q}_b$ at $t = t_b$.

For a classical trajectory, Hamilton's principal function satisfies the relations

$$\frac{\partial R}{\partial \boldsymbol{q}_b} = \boldsymbol{p}_b, \qquad \frac{\partial R}{\partial \boldsymbol{q}_a} = -\boldsymbol{p}_a, \qquad \frac{\partial R}{\partial t_b} = -E.$$

Exercise 1

Show that Hamilton's principal function for a classical trajectory satisfies the relations

$$\frac{\partial R}{\partial \boldsymbol{q}_b} = \boldsymbol{p}_b, \qquad \frac{\partial R}{\partial \boldsymbol{q}_a} = -\boldsymbol{p}_a, \qquad \frac{\partial R}{\partial t_b} = -E.$$

Hint: There are different ways to prove this. For example, you can use the expression for $\delta R[\boldsymbol{q}(t)]$ to obtain the first two relations. The third relation is more tricky. One way is to fix a classical trajectory and follow it longer in time

$$\int_{t_a}^{t_b+\delta t_b} L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)\, dt = R[\boldsymbol{q}(t)](\boldsymbol{q}_b + \dot{\boldsymbol{q}}_b\, \delta t_b, t_b + \delta t_b, \boldsymbol{q}_a, t_a),$$

Then the required result can be extracted from a first order expansion of this expression.

Quantum mechanics

We consider conservative quantum systems with Hamiltonian

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{q}}).$$

The time evolution operator has the form

$$\hat{U}(t) = \exp\left(-\frac{i}{\hbar}\hat{H}t\right).$$

It propagates an initial state $|\psi_0\rangle$ at time $t = 0$ to a later state at time t

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi_0\rangle,$$

which is a solution of the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle, \qquad |\psi(0)\rangle = |\psi_0\rangle.$$

More generally

$$|\psi(t_b)\rangle = \hat{U}(t_b - t_a)\,|\psi(t_a)\rangle.$$

Alternatively, we can write this in position representation

$$\hat{\boldsymbol{q}}|\boldsymbol{q}\rangle = \boldsymbol{q}|\boldsymbol{q}\rangle, \qquad \langle \boldsymbol{q}|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q}-\boldsymbol{q}'), \qquad \int_{-\infty}^{\infty} \mathrm{d}^f q\, |\boldsymbol{q}\rangle\langle \boldsymbol{q}| = \mathbb{1}.$$

in the form

$$\psi(\boldsymbol{q},t) = \langle \boldsymbol{q}|\psi(t)\rangle = \int_{-\infty}^{\infty} \mathrm{d}^f q_0\, \langle \boldsymbol{q}|\hat{U}(t)|\boldsymbol{q}_0\rangle\, \langle \boldsymbol{q}_0|\psi_0\rangle = \int_{-\infty}^{\infty} \mathrm{d}^f q_0\, K(\boldsymbol{q},\boldsymbol{q}_0,t)\, \psi_0(\boldsymbol{q}_0),$$

where the propagator $K(\boldsymbol{q}_b,\boldsymbol{q}_a,t)$ is defined as

$$K(\boldsymbol{q}_b,\boldsymbol{q}_a,t) = \langle \boldsymbol{q}_b|\hat{U}(t)|\boldsymbol{q}_a\rangle.$$

In terms of eigenstates of the Hamiltonian $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ we have

$$K(\boldsymbol{q}_b,\boldsymbol{q}_a,t) = \sum_n \langle \boldsymbol{q}_b|\hat{U}(t)|\psi_n\rangle\langle\psi_n|\boldsymbol{q}_a\rangle = \sum_n \psi_n(\boldsymbol{q}_b)\, \psi_n^*(\boldsymbol{q}_a)\, \mathrm{e}^{-\frac{i}{\hbar}E_n t},$$

We want to obtain a semiclassical approximation for the propagator. This approximation will be given in by a sum over all classical trajectories from q_a to q_b in time t. This can be most clearly seen from the Feynman path integral. We consider first one-dimensional systems.

Exercise 2

Show that the propagator of the one-dimensional free particle is given by

$$K(q_b, q_a, t) = \left\langle q_b \left| \exp\left(-\frac{i}{\hbar} \frac{\hat{p}^2}{2m} t \right) \right| q_a \right\rangle = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(\frac{i}{\hbar} \frac{m(q_a - q_b)^2}{2t} \right).$$

Hint: Use the completeness of the momentum eigenstates

$$\hat{p}|p\rangle = p|p\rangle, \qquad \langle p|p'\rangle = \delta(p - p'), \qquad \int_{-\infty}^{\infty} \mathrm{d}p \; |p\rangle\langle p| = \mathbb{1}.$$

the amplitudes

$$\langle q|p\rangle = \frac{1}{\sqrt{2\pi i\hbar}} \mathrm{e}^{\frac{i}{\hbar}pq} = \langle p|q\rangle^*,$$

and the Gaussian integral

$$\int_{-\infty}^{\infty} \mathrm{d}x \; \exp(-ax^2 + bx) = \sqrt{\frac{\pi}{a}} \exp\left\{ \frac{b^2}{4a} \right\},$$

where $\mathrm{Re}\, a > 0$, or $\mathrm{Re}\, a,\ \mathrm{Re}\, b = 0$, $\mathrm{Im}\, a \neq 0$. Here and in the following $\sqrt{i} = \mathrm{e}^{i\frac{\pi}{4}}$, $\sqrt{-i} = \mathrm{e}^{-i\frac{\pi}{4}}$.

Exercise 2 (continued)

Show that the propagator of the free particle can be written in the form

$$K(q_b, q_a, t) = \sqrt{\frac{1}{2\pi\hbar}\left|\frac{\partial^2 R}{\partial q_b \partial q_a}\right|}\exp\left(\frac{i}{\hbar}R(q_b, q_a, t) - i\frac{\pi}{4}\right),$$

where $R(q_b, q_a, t)$ is Hamilton's principal function for the trajectory of the free particle from q_a to q_b in time t.

We return to general conservative systems. The time evolution can be split into parts

$$\hat{U}(t) = \mathrm{e}^{-i\hat{H}t/\hbar} = \mathrm{e}^{-i\hat{H}t_1/\hbar}\,\mathrm{e}^{-i\hat{H}t_2/\hbar} = \hat{U}(t_2)\hat{U}(t_1),$$

where $t = t_1 + t_2$. For the propagator, this correponds to the composition property

$$K(q_b, q_a, t) = \langle q_b|\hat{U}(t)|q_b\rangle = \langle q_b|\hat{U}(t_2)\hat{U}(t_1)|q_b\rangle = \int_{-\infty}^{\infty}\mathrm{d}q\, K(q_b, q, t_2)\, K(q, q_a, t_1).$$

The idea of the Feynman path integral is to split the time evolution into a large number of N parts and take the limit $N \to \infty$.

Propagator

We consider

$$\hat{U}(t) = \left[\hat{U}\left(\frac{t}{N}\right)\right]^N$$

A crucial step in the derivation is the factorisation of the propagator for small times

$$\hat{U}\left(\frac{t}{N}\right) = \exp\left(-\frac{it\hat{H}}{\hbar N}\right) = \mathrm{e}^{-\frac{\lambda(\hat{T}+\hat{V})}{N}} = \mathrm{e}^{-\frac{\lambda\hat{T}}{N}}\mathrm{e}^{-\frac{\lambda\hat{V}}{N}} + \mathcal{O}\left(\frac{\lambda^2}{N^2}\right).$$

where $\lambda = it/\hbar$. The error term can be obtained by a Taylor expansion. It can be neglected in the following calculation (Trotter formula).

$$\begin{aligned}
K(q, q_0, t) &= \langle q|[\mathrm{e}^{-\frac{\lambda}{N}(\hat{T}+\hat{V})}]^N|q_0\rangle \\
&= \lim_{N\to\infty}\langle q|[\mathrm{e}^{-\frac{\lambda}{N}\hat{T}}\mathrm{e}^{-\frac{\lambda\hat{V}}{N}}]^N|q_0\rangle \\
&= \lim_{N\to\infty}\int_{-\infty}^{\infty}\mathrm{d}q_1\ldots\mathrm{d}q_{N-1}\prod_{j=0}^{N-1}\langle q_{j+1}|\mathrm{e}^{-\frac{\lambda}{N}\hat{T}}\mathrm{e}^{-\frac{\lambda}{N}\hat{V}}|q_j\rangle \\
&= \lim_{N\to\infty}\int_{-\infty}^{\infty}\mathrm{d}q_1\ldots\mathrm{d}q_{N-1}\prod_{j=0}^{N-1}\langle q_{j+1}|\mathrm{e}^{-\frac{i}{\hbar}\frac{t}{N}\hat{T}}|q_j\rangle\,\mathrm{e}^{-\frac{i}{\hbar}\frac{t}{N}V(q_j)}
\end{aligned}$$

where $q_N = q$. In the final step we use the propagator of the free particle.

The result is

$$K(q,q_0,t) = \lim_{N\to\infty} \int_{-\infty}^{\infty} \mathrm{d}q_1 \ldots \mathrm{d}q_{N-1} \left(\sqrt{\frac{m}{2\pi i\hbar t}}\right)^N \exp\left(\frac{i}{\hbar}\varepsilon \sum_{j=0}^{N-1}\left[\frac{m}{2}\frac{(q_{j+1}-q_j)^2}{\varepsilon^2} - V(q_j)\right]\right)$$

where $\varepsilon = t/N$. In the exponent we have

$$\varepsilon \sum_{j=0}^{N-1}\left[\frac{m}{2}\frac{(q_{j+1}-q_j)^2}{\varepsilon^2} - V(q_j)\right] \underset{N\to\infty}{\Longrightarrow} \int_0^t \mathrm{d}t' \left[\frac{m}{2}\dot{q}^2(t') - V(q(t'))\right] = R(q,q_0,t).$$

This is the Feynman path integral. It is an integral over broken line paths as shown in the figure. It is interpreted as integral over all paths from q_0 to q in time t, written symbolically as

$$K(q,q_0,t) = \int_{\substack{q(t)=q \\ q(t_0)=q_0}} \mathcal{D}[q(t)] \exp\left\{\frac{i}{\hbar}R[q(t)]\right\}.$$

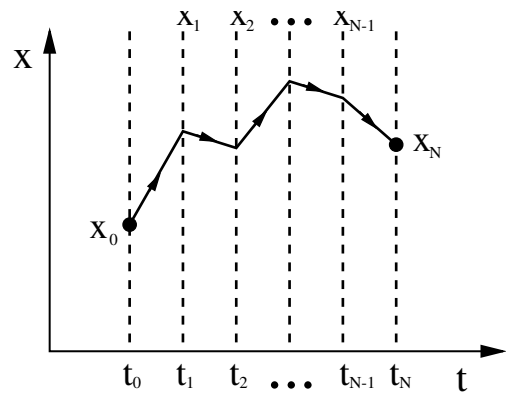


Figure: Broken line paths

The connection to classical mechanics is obtained in the limit $\hbar \to 0$ by stationary phase approximation.

Stationary phase approximation

The stationary phase approximation provides a leading order approximation in the limit $\eta \to \infty$ for the highly oscillatory integral

$$I(\eta) = \int_a^b \mathrm{d}y \; A(y)\, \mathrm{e}^{i\,\eta\,\phi(y)}.$$

Assume that ϕ has one non-degenerate stationary point $\phi'(y_0) = 0$, $\phi''(y_0) \neq 0$, for $a < y_0 < b$, and that $A(y_0) \neq 0$. Then the leading order approximation as $\eta \to \infty$ is obtained by expanding the phase up to second order about the stationary point

$$\phi(y) \approx \phi(y_0) + \frac{1}{2}\phi''(y_0)(y - y_0)^2$$

and evaluating the Gaussian integral

$$I(\eta) \sim \int_{-\infty}^{\infty} \mathrm{d}y \; A(y_0)\, \mathrm{e}^{i\eta\phi(y_0) + \frac{i\eta}{2}\phi''(y_0)\,(y-y_0)^2} = A(y_0)\sqrt{\frac{2\pi i}{\eta\phi''(y_0)}}\; \mathrm{e}^{i\eta\phi(y_0)} \qquad \text{as} \qquad \eta \to \infty$$

using

$$\int_{-\infty}^{\infty} \mathrm{d}y \; \mathrm{e}^{-ay^2} = \sqrt{\frac{\pi}{a}}.$$

Stationary phase approximation

- The main contribution to the integral comes from a region of order $\Delta y \propto \eta^{-1/2}$.
- If there are several stationary points in the interval (a, b) the contributions are added.
- For a stationary point at one of the endpoints, a or b, one gets half the contribution.
- If there is no stationary point in the interval $[a, b]$ then the leading order approximation (of order $1/\eta$) comes from the end points. It can be obtained by integration by parts.

Generalisation to f dimensions: consider the integral

$$I(\eta) = \int \mathrm{d}^f \boldsymbol{y}\, A(\boldsymbol{y})\, \exp\left(i\,\eta\,\phi(\boldsymbol{y})\right)$$

The contribution of a stationary point $\nabla\phi(\boldsymbol{y}_0) = 0$ to the integral is given by

$$I(\eta) \sim A(\boldsymbol{y}_0) \left(\frac{2\pi}{\eta}\right)^{n/2} \left|\det \frac{\partial^2 \phi}{\partial y_i \partial y_j}(\boldsymbol{y}_0)\right|^{-1/2} \mathrm{e}^{i\eta\phi(\boldsymbol{y}_0) + i\pi\nu/4},$$

where ν is the number of positive eigenvalues minus the number of negative eigenvalues of the matrix of second order derivatives, and it is assumed that this matrix does not have a vanishing determinant at $\boldsymbol{y}_0$.

The asymptotic relation $f(\eta) \sim g(\eta)$ as $\eta \to \eta_0$ means $\lim_{\eta\to\eta_0} f(\eta)/g(\eta) = 1$,

Semiclassical approximation for the path integral

We apply the stationary phase approximation to the path integral expression

$$\int_{-\infty}^{\infty} \mathrm{d}q_1 \ldots \mathrm{d}q_{N-1} \left(\sqrt{\frac{m}{2\pi i\hbar t}}\right)^N \exp\left(\frac{i}{\hbar}\varepsilon \sum_{j=0}^{N-1}\left[\frac{m}{2}\frac{(q_{j+1}-q_j)^2}{\varepsilon^2} - V(q_j)\right]\right).$$

Denoting the exponent by $i\Phi/\hbar$ we obtain the stationary points from

$$0 = \frac{\partial \Phi}{\partial q_j} = \varepsilon\left[-m\frac{(q_{j+1}-q_j)-(q_j-q_{j-1})}{\varepsilon^2} - \frac{\partial V(q_j)}{\partial q_j}\right] \qquad j = 1, \ldots, N-1.$$

This is a discretised form of Newton's equations and in the limit $\varepsilon \to 0$ we obtain

$$-m\ddot{q} - \frac{\partial V}{\partial q} = 0.$$

This shows is that in the semiclassical limit the propagator is given by a sum over all classical paths from q_a to q_b in time t

$$K(q_b, q_a, t) \approx \sum_{\gamma} F_{ba}\, \mathrm{e}^{\frac{i}{\hbar}R_{ba}}.$$

The semiclassical propagator

We obtained

$$K(q_b, q_a, t) \approx \sum_\gamma F_{ba}\, \mathrm{e}^{\frac{i}{\hbar} R_{ba}}.$$

The quantities F_{ba} and R_{ba} depend on the trajectory γ, and $R_{ba} = R(q_b, q_a, t)$. The prefactor F_{ba} can be obtained from the stationary phase approximation in $N-1$ dimensions. We won't do this calculation. Instead we ask: **What follows for F_{ba} from the composition property?**

$$K(q_c, q_a, t) = \int_{-\infty}^{\infty} \mathrm{d}q_b\, K(q_c, q_b, t_2)\, K(q_b, q_a, t_1).$$

where $t = t_2 + t_1$. We evaluate this integral in stationary phase approximation. The stationary phase condition is

$$0 = \frac{\partial R_{cb}}{\partial q_b} + \frac{\partial R_{ba}}{\partial q_b} = -p^i_{cb} + p^f_{ba}.$$

We find that the stationary point $q_b = \bar{q}_b$ is determined by the condition that the final momentum of the trajectory from q_a to $\bar{q}_b$ is equal to the initial momentum of the trajectory from $\bar{q}_b$ to q_c. This means that the two partial trajectories join smoothly and form a classical trajectory from q_a to q_c in time t. At $q_b = \bar{q}_b$

$$R_{ca} = R_{cb} + R_{ba}.$$

The semiclassical propagator

Performing the stationary phase approximation results in

$$F_{ca}\,\mathrm{e}^{\frac{i}{\hbar}R_{ca}} = F_{cb}\,\mathrm{e}^{\frac{i}{\hbar}R_{cb}}F_{ba}\,\mathrm{e}^{\frac{i}{\hbar}R_{ba}}\sqrt{\frac{2\pi i\hbar}{\left[\frac{\partial^2 R_{cb}}{\partial q_b^2}+\frac{\partial^2 R_{ba}}{\partial q_b^2}\right]_{q_b=\bar{q}_b}}}.$$

A classical calculation shows that

$$\left[\frac{\partial^2 R_{cb}}{\partial q_b^2}+\frac{\partial^2 R_{ba}}{\partial q_b^2}\right]_{q_b=\bar{q}_b} = -\frac{\frac{\partial^2 R_{cb}}{\partial q_c \partial q_b}\,\frac{\partial^2 R_{ba}}{\partial q_b \partial q_a}}{\frac{\partial^2 R_{ca}}{\partial q_c \partial q_a}}.$$

This implies

$$F_{ca} = F_{cb}\,F_{ba}\sqrt{\frac{2\pi\hbar}{i}\,\frac{\frac{\partial^2 R_{ca}}{\partial q_c \partial q_a}}{\frac{\partial^2 R_{cb}}{\partial q_c \partial q_b}\,\frac{\partial^2 R_{ba}}{\partial q_b \partial q_a}}}.$$

It suggests that

$$F_{ca} \propto \sqrt{\frac{1}{2\pi\hbar}\left|\frac{\partial^2 R_{ca}}{\partial q_c \partial q_a}\right|}\,\tilde{F}_{ca}.$$

The question is what is the factor $\tilde{F}_{ca}$. It depends on the signs of the mixed partial derivatives.

We have

$$\frac{\partial^2 R_{ba}}{\partial q_b \partial q_a} = -\left.\frac{\partial p_a}{\partial q_b}\right|_{q_a} \qquad \text{or} \qquad \left[\frac{\partial^2 R_{ba}}{\partial q_b \partial q_a}\right]^{-1} = -\left.\frac{\partial q_b}{\partial p_a}\right|_{q_a}$$

The last term involves minus the change δq_b in the final position q_b of a trajectory that starts at q_a with momentum $p_a + \delta p_a$. The mixed partial derivative changes sign when this quantity is zero.

We need to consider trajectories in the neighbourhood of a classical trajectory which satisfies Newton's second law

$$m\frac{d^2}{dt^2}q = -\frac{\partial V(q)}{\partial q}.$$

We replace $q(t)$ by $q(t) + \delta q(t)$ and obtain a differential equation for $\delta q(t)$

$$m\frac{d^2}{dt^2}\delta q = -V''(q(t))\,\delta q.$$

This is the **Jacobi equation**. It is a homogeneous second order linear equation for $\delta q(t)$. According to the **Sturm Separation Theorem**, the zeros of any two linearly independent solutions are alternating (and simple).

The semiclassical propagator

Let n_{ba} denote the number of zeros of a solution of the Jacobi equation of length t_1 that starts with $\delta q(0) = 0$, $\delta \dot{q}(0) \neq 0$. Then

$$\left(\frac{\partial^2 R_{ba}}{\partial q_b \partial q_a} \right) = \left| \frac{\partial^2 R_{ba}}{\partial q_b \partial q_a} \right| (-1)^{1+n_{ba}}.$$

There is an additional (-1) because for small times the mixed partial derivative approaches that of a free particle and is negative. The *ac* and *bc* cases are defined correspondingly. We define

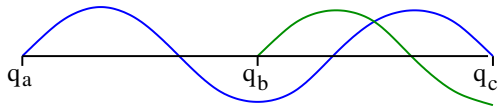
$$F_{ca} = \sqrt{\frac{1}{2\pi\hbar} \left| \frac{\partial^2 R_{ca}}{\partial q_c \partial q_a} \right|} \, \tilde{F}_{ca}$$

Then

$$\tilde{F}_{ca} = \tilde{F}_{cb} \, \tilde{F}_{ba} \sqrt{i \, (-1)^{n_{ca} - n_{ba} - n_{cb}}} \, .$$

It follows from the Sturm Separation Theorem that there are only two posibilities

$$n_{ca} - n_{ba} - n_{cb} = \begin{cases} 0 \\ 1 \end{cases} \, .$$



The semiclassical propagator

For both cases we obtain

$$\tilde{F}_{ca} = \tilde{F}_{cb}\,\tilde{F}_{ba}\,\sqrt{i\,(-1)^{n_{ca}-n_{ba}-n_{cb}}}$$

$$= \tilde{F}_{cb}\,\tilde{F}_{ba}\,\exp\left(i\frac{\pi}{4} - i\frac{\pi}{2}(n_{ca}-n_{ba}-n_{cb})\right).$$

This leads to our final result

$$F_{ca} = \sqrt{\frac{1}{2\pi\hbar}\left|\frac{\partial^2 R_{ca}}{\partial q_c \partial q_a}\right|}\,\exp\left(-i\frac{\pi}{4} - i\frac{\pi}{2}n_{ca}\right).$$

Strictly speaking, there could be an additional factor f_{ca} with $f_{ca} = f_{cb}\,f_{ba}$, but this factor is one.

In summary, we obtained the following result for the semiclassical propagator

$$K_{sc}(q_b, q_a, t) = \sum_{\gamma} \sqrt{\frac{1}{2\pi\hbar}\left|\frac{\partial^2 R}{\partial q_b \partial q_a}\right|}\,\exp\left(\frac{i}{\hbar}R(q_b, q_a, t) - i\frac{\pi}{4} - i\frac{\pi}{2}n_{ba}\right).$$

This is the Van Vleck propagator or the Van Vleck-Gutzwiller propagator.

Exercise 3

For the harmonic oscillator with potential

$$V(q) = \frac{m}{2}\omega^2 q^2,$$

the semiclassical approximation is identical to the exact result.

Determine the propagator of the harmonic oscillator, valid for all times $t > 0$. This formula is known as Feynman-Souriau formula.

The semiclassical propagator in f dimensions

In f dimensions the semiclassical propagator is given by

$$K_{sc}(\boldsymbol{q}_b, \boldsymbol{q}_a, t) = \sum_{\gamma} \frac{1}{(2\pi\hbar)^{f/2}} \sqrt{\left|\det\left(\frac{\partial^2 R}{\partial \boldsymbol{q}_b \, \partial \boldsymbol{q}_a}\right)\right|} \exp\left\{\frac{i}{\hbar} R(\boldsymbol{q}_b, \boldsymbol{q}_a, t) - if\frac{\pi}{4} - i\nu\frac{\pi}{2}\right\}$$

where the sum runs over all classical trajectories γ that go from $\boldsymbol{q}_a$ to $\boldsymbol{q}_b$ in time t.

For the determination of ν consider the matrix

$$A = \left(\frac{\partial^2 R}{\partial \boldsymbol{q}_b \, \partial \boldsymbol{q}_a}\right)^{-1} = -\frac{\partial \boldsymbol{q}_b}{\partial \boldsymbol{p}_a}.$$

The **Morse index** ν increases by one for every reduction of the rank of A by one if one follows the trajectory for time t.

This happens at conjugate points. At these points neighbouring trajectories that start at the same position with infinitesimally different momentum intersect the original trajectory. This typically occurs at caustics. At these points the semiclassical propagator diverges.

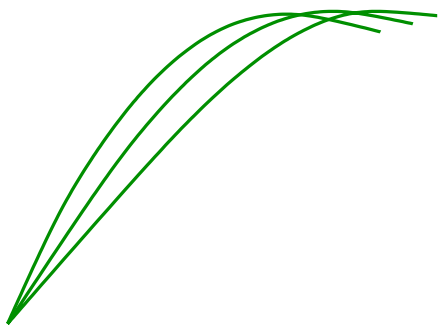


Figure: Caustic

Unitary transformations

Unitary transformations

The form of the semiclassical transformation of the propagator is familiar from a different context. For simplicity, let us consider one-dimensional systems.

Short review of canonical transformations

Consider a Hamiltonian $H(q,p)$ with equations of motion

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q},.$$

A transformation $(q,p) \to (Q,P)$ is canonical if it preserves the Hamilton's equations

$$\dot{Q} = \frac{\partial H}{\partial P}, \qquad \dot{P} = -\frac{\partial H}{\partial Q}, \qquad \text{where} \qquad H(q,p) = H(q(Q,P),p(Q,P)).$$

Canonical transformations are produced by generating functions that depend on one of the old and one of the new coordinates (see e.g. Goldstein). For example, after choosing a function $F_1(q,Q)$ the transformation

$$p = \frac{\partial F_1(q,Q)}{\partial q}, \qquad P = -\frac{\partial F_1(q,Q)}{\partial Q}$$

is canonical.

Unitary transformations

Alternatively, one may define a function $F_2(q,P)$. It is related to $F_1(q,Q)$ by

$$F_2(q,P) = F_1(q,Q) + PQ,$$

where $Q = Q(q,P)$ and satisfies

$$\frac{\partial F_2}{\partial q} = \frac{\partial F_1}{\partial q} + \frac{\partial F_1}{\partial Q}\frac{\partial Q}{\partial q} + \frac{\partial Q}{\partial q}P = p, \qquad \frac{\partial F_2}{\partial P} = \frac{\partial F_1}{\partial Q}\frac{\partial Q}{\partial P} + \frac{\partial Q}{\partial P}P + Q = Q.$$

Altogether there are four different cases

$$\begin{aligned}
&F_1(q,Q) && p = \frac{\partial F_1(q,Q)}{\partial q} && P = -\frac{\partial F_1(q,Q)}{\partial Q},\\
&F_2(q,P) = F_1(q,Q) + PQ && p = \frac{\partial F_2(q,P)}{\partial q} && Q = \frac{\partial F_2(q,P)}{\partial P},\\
&F_3(p,Q) = F_1(q,Q) - pq && q = -\frac{\partial F_3(p,Q)}{\partial p} && P = -\frac{\partial F_3(p,Q)}{\partial Q},\\
&F_4(p,P) = F_1(q,Q) + PQ - pq && q = -\frac{\partial F_4(p,P)}{\partial p} && Q = \frac{\partial F_4(p,P)}{\partial P}.
\end{aligned}$$

Unitary transformations

In quantum mechanics, canonical transformations correspond to unitary transformations (change of bases). They are defined by the transition amplitudes

$$\langle q|Q\rangle, \qquad \langle q|P\rangle, \qquad \langle p|Q\rangle, \qquad \langle p|P\rangle.$$

Unitarity implies, for example,

$$\int_{-\infty}^{\infty} \mathrm{d}Q\, \langle q|Q\rangle\langle Q|q'\rangle = \delta(q-q') \qquad \text{and} \qquad \int_{-\infty}^{\infty} \mathrm{d}q\, \langle Q|q\rangle\langle q|Q'\rangle = \delta(Q-Q').$$

Miller (1974) derived semiclassical approximations for the transition amplitudes. The transition amplitudes are written in the form

$$\langle q|Q\rangle = A_1(q,Q)\,\exp\left(\frac{i}{\hbar}f_1(q,Q)\right), \qquad \langle q|P\rangle = A_2(q,P)\,\exp\left(\frac{i}{\hbar}f_2(q,P)\right),$$
$$\langle p|Q\rangle = A_3(p,Q)\,\exp\left(\frac{i}{\hbar}f_3(p,Q)\right), \qquad \langle p|P\rangle = A_4(p,P)\,\exp\left(\frac{i}{\hbar}f_4(p,P)\right).$$

It is assumed that transformations between canonically conjugate variables take the form

$$\langle q|p\rangle = \frac{1}{\sqrt{2\pi i\hbar}}\,\mathrm{e}^{\frac{i}{\hbar}pq} = \overline{\langle p|q\rangle}, \qquad \langle Q|P\rangle = \frac{1}{\sqrt{2\pi i\hbar}}\,\mathrm{e}^{\frac{i}{\hbar}PQ} = \overline{\langle P|Q\rangle}.$$

Unitary transformations

Unitary transformations are performed in stationary phase approximation

$$\langle q|Q\rangle = \int_{-\infty}^{\infty} \mathrm{d}p \, \langle q|p\rangle \, \langle p|Q\rangle.$$

Inserting the previous expressions

$$A_1(q,Q) \, \exp\left(\frac{i}{\hbar} f_1(q,Q)\right) \approx \int_{-\infty}^{\infty} \mathrm{d}p \, \frac{A_3(p,Q)}{\sqrt{2\pi i\hbar}} \, \exp\left(\frac{i}{\hbar} pq + \frac{i}{\hbar} f_3(p,Q)\right).$$

The stationary phase condition is

$$q + \frac{\partial f_3(p,Q)}{\partial p} = 0,$$

and at the stationary point

$$f_1(q,Q) = pq + f_3(p,Q).$$

These relations agree with those of the generating functions for the canonical transformations. All the other relations for the generating functions are obtained by consider the seven other possible unitary transformations. This leads to the identification of the functions f_i with the generating functions F_i.

The amplitudes are determined by further using the unitarity relations.

Unitary transformations

Altogether the result is

$$\langle q|Q\rangle = \left[\frac{-1}{2\pi i\hbar}\frac{\partial^2 F_1}{\partial q\partial Q}\right]^{1/2}\exp\left(\frac{i}{\hbar}F_1(q,Q)\right), \quad \langle q|P\rangle = \left[\frac{1}{2\pi i\hbar}\frac{\partial^2 F_2}{\partial q\partial P}\right]^{1/2}\exp\left(\frac{i}{\hbar}F_2(q,P)\right),$$

$$\langle p|Q\rangle = \left[\frac{1}{2\pi i\hbar}\frac{\partial^2 F_3}{\partial p\partial Q}\right]^{1/2}\exp\left(\frac{i}{\hbar}F_3(p,Q)\right), \quad \langle p|P\rangle = \left[\frac{-1}{2\pi i\hbar}\frac{\partial^2 F_4}{\partial p\partial P}\right]^{1/2}\exp\left(\frac{i}{\hbar}F_4(p,P)\right),$$

If there are several stationary points then one adds the contributions.

Comparison to the semiclassical propagator

$$K_{sc}(q_b,q_a,t) = \sum_\gamma \sqrt{\frac{1}{2\pi\hbar}\left|\frac{\partial^2 R}{\partial q_b\partial q_a}\right|}\exp\left(\frac{i}{\hbar}R(q_b,q_a,t) - i\frac{\pi}{4} - i\frac{\pi}{2}n_{ba}\right).$$

The propagator can be considered as a unitary transformation because

$$K(q_b,q_a,t_b-t_a) = \langle q_b|U(t_b-t_a)|q_a\rangle = \langle q_b,t_b|q_a,t_a\rangle.$$

In classical mechanics the coordinates (q_a,p_a) at time t_a are related to (q_b,p_b) at time t_b by a canonical transformation, whose generating function is the principal function $R(q_b,q_a,t_b-t_a)$.

Unitary transformations, example

Let us consider a transformation from (q, p) to new variables (Q, P) where P is equal to the energy $E = p^2/2m + V(q)$. We are interested in the amplitude $\langle q|P\rangle$ which corresponds to the wave function of an energy eigenstate. The generating function $F_2(q, P)$ of the transition satisfies

$$\frac{\partial F_2(q,P)}{\partial q} = p, \qquad \frac{\partial F_2(q,P)}{\partial P} = Q.$$

Since $P = E$ we have from the first equation

$$\frac{F_2(q,E)}{\partial q} = p = \pm\sqrt{2m(E - V(q))}$$

from which follows

$$F_2(q,E) = \pm \int \mathrm{d}q\, \sqrt{2m(E - V(q))} + C(E).$$

$C(E)$ leads to an irrelevant phase that can be neglected. For the amplitude we need

$$\frac{\partial^2 F_2}{\partial q \partial E} = \pm\left(\frac{2}{m}[E - V(q)]\right)^{-1/2} = \pm\frac{1}{v(q)}.$$

The final result agrees with the WKB approximation

$$\langle q|E\rangle = \frac{1}{\sqrt{2\pi\hbar v(q)}}\left[\exp\left(\frac{i}{\hbar}\int p\,dq - i\frac{\pi}{4}\right) + \exp\left(-\frac{i}{\hbar}\int p\,dq + i\frac{\pi}{4}\right)\right].$$

Uniform approximations

We found that the semiclassical propagator diverges at conjugate points. Does the exact propagator diverge as well? Generally not (an exception is the harmonic oscillator). The reason for the divergence is a coalescence of two stationary points at a caustic. Near the caustic the stationary phase approximation becomes inaccurate and has to be replaced by a uniform approximation.

Uniform approximations occur in various contexts in semiclassics (caustics, bifurcations, diffraction, break-up of tori). We discuss a basic example. Consider

$$I(\eta) = \int \mathrm{d}x \; g(x)\, \mathrm{e}^{i\eta f(x)}$$

Assume that $f(x)$ has two (non-degenerate) stationary points, $f'(x_1) = f'(x_2) = 0$. We evaluate the integral in stationary phase approximation and obtain in leading order for $\eta \to \infty$

$$I(\eta) \approx \sum_{i=1}^{2} g(x_i) \sqrt{\frac{2\pi i}{\eta f''(x_i)}}\, \mathrm{e}^{i\eta f(x_i)} = \sum_{i=1}^{2} A(x_i)\, \mathrm{e}^{i\eta f(x_i)}.$$

If for a fixed value of η the stationary points are too close together, they cannot be considered separately but give a joint contribution to the integral. We then apply a coordinate transformation $x \to y$ that maps $f(x)$ onto a simpler form with two stationary points

$$F(y, \xi) = \frac{1}{3} y^3 - \xi y + c\,.$$

Uniform approximation

The mapping $x \to y$ results in

$$f(x) = F(y, \xi) = \frac{1}{3} y^3 - \xi y + c.$$

The function $F(y, \xi)$ has two stationary points

$$0 = \frac{\partial}{\partial y} F(y, \xi) = y^2 - \xi \qquad \Longrightarrow \qquad y = \pm\sqrt{\xi}.$$

For the mapping $x \to y$ to be one-to-one the two stationary points have to map onto each other

$$f(x_1) = F(-\sqrt{\xi}, \xi) = \frac{2}{3}\xi^{3/2} + c, \qquad f(x_2) = F(\sqrt{\xi}, \xi) = -\frac{2}{3}\xi^{3/2} + c,$$

(w.l.o.g. x_1 is the maximum and x_2 the minimum.) This determines the values of ξ and c

$$c = \frac{1}{2}(f(x_1) + f(x_2)), \qquad \xi = \left[\frac{3}{4}(f(x_1) - f(x_2))\right]^{2/3}.$$

We arrive at the integral

$$I(\eta) = \int \mathrm{d}y \; G(y)\, \mathrm{e}^{i\eta F(y,\xi)}, \qquad \text{where} \qquad G(y) = g(x)\, \frac{dx}{dy}.$$

Uniform approximation

So far everything has been exact. Now we write $G(y)$ in the form

$$G(y) = G_0 + G_1 \frac{\partial}{\partial \xi} F(y,\xi) + h(y) \frac{\partial}{\partial y} F(y,\xi).$$

The last term vanishes at the stationary points. It is neglected because it leads to a higher order contribution. This can be seen by an integration by parts. The constants G_0 and G_1 are determined by the value of $G(y)$ at the stationary points.

For the last step we need the value of the Jacobian at the stationary points. It is obtained by differentiating

$$f(x) = \frac{1}{3} y^3 - \xi y + c$$

twice with the result

$$f''(x) \left(\frac{\partial x}{\partial y} \right)^2 + f'(x) \frac{\partial^2 x}{\partial y^2} = 2y\,.$$

Hence

$$G_0 = \frac{g(x_1)\,\xi^{1/4}}{\sqrt{-2f''(x_1)}} + \frac{g(x_2)\,\xi^{1/4}}{\sqrt{2f''(x_2)}}, \qquad G_1 = \frac{g(x_1)\,\xi^{-1/4}}{\sqrt{-2f''(x_1)}} - \frac{g(x_2)\,\xi^{-1/4}}{\sqrt{2f''(x_2)}}$$

It remains to evaluate the integrals

$$I(\eta) \approx \int \mathrm{d}y\; G_0\, \mathrm{e}^{i\eta(y^3/3-\xi y+c)} - \frac{i}{\eta}\frac{\partial}{\partial \xi}\int \mathrm{d}y\; G_1\, \mathrm{e}^{i\eta(y^3/3-\xi y+c)}$$
$$= \frac{2\pi G_0}{\eta^{1/3}}\mathrm{e}^{i\eta c}\mathrm{Ai}(-\eta^{2/3}\xi) + \frac{2\pi i G_1}{\eta^{2/3}}\mathrm{e}^{i\eta c}\mathrm{Ai}'(-\eta^{2/3}\xi)$$

where we used the integral representation of the Airy function

$$\mathrm{Ai}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}z\,\mathrm{e}^{iz^3/3+xz}.$$

With the asymptotic relations

$$\mathrm{Ai}(-z) \sim \frac{1}{\sqrt{\pi}z^{1/4}}\cos\left(\frac{2}{3}z^{3/2}-\frac{\pi}{4}\right), \qquad \mathrm{Ai}'(-z) \sim \frac{z^{1/4}}{\sqrt{\pi}}\sin\left(\frac{2}{3}z^{3/2}-\frac{\pi}{4}\right)$$

We obtain

$$I(\eta) \approx g(x_1)\sqrt{\frac{2\pi i}{\eta f''(x_1)}}\,\mathrm{e}^{i\eta f(x_1)} + g(x_2)\sqrt{\frac{2\pi i}{\eta f''(x_2)}}\,\mathrm{e}^{i\eta f(x_2)}.$$

The uniform approximation interpolates between two asymptotic regimes. In the opposite limit

$$I(\eta) \approx \frac{2\pi g(x_0)\,2^{1/3}}{[\eta\, f'''(x_0)]^{1/3}}\mathrm{Ai}(0)\,\mathrm{e}^{i\eta f(x_0)}.$$

Uniform approximation

Co-dim.	Type	Unfoldings	Singularity index
1	Fold	$\frac{x^3}{3} + \xi_1 x$	$\frac{1}{6}$
2	Cusp	$\frac{x^4}{4} + \xi_1 \frac{x^2}{2} + \xi_2 x$	$\frac{1}{4}$
3	Swallow-tail	$\frac{x^5}{5} + \xi_1 \frac{x^3}{3} + \xi_2 \frac{x^2}{2} + \xi_3 x$	$\frac{3}{10}$
4	Butterfly	$\frac{x^6}{6} + \xi_1 \frac{x^4}{4} + \xi_2 \frac{x^3}{3} + \xi_3 \frac{x^2}{2} + \xi_4 x$	$\frac{1}{3}$
3	Elliptic umbilic	$x^3 - 3xy^2 + \xi_1(x^2 + y^2) + \xi_2 x + \xi_3 y$	$\frac{1}{3}$
3	Hyperbolic umbilic	$x^3 + y^3 + \xi_1 xy + \xi_2 x + \xi_3 y$	$\frac{1}{3}$
4	Parabolic umbilic	$x^2 y + y^4 + \xi_1 x^2 + \xi_2 y^2 + \xi_3 x + \xi_4 y$	$\frac{3}{8}$

Table: Elementary catastrophes

Green functions, Gutzwiller trace formula and spectral determinants

Green function

For an investigation of the energy domain we consider the Green function

$$G(\boldsymbol{q}, \boldsymbol{q}', E) = \left\langle \boldsymbol{q} \left| \frac{1}{E - \hat{H}} \right| \boldsymbol{q}' \right\rangle ,$$

the kernel of the resolvent operator $(E - \hat{H})^{-1}$. It satisfies the differential equation

$$\left(E + \frac{\hbar^2}{2m} \nabla^2 - V(\boldsymbol{q}) \right) G(\boldsymbol{q}, \boldsymbol{q}', E) = \delta(\boldsymbol{q} - \boldsymbol{q}') ,$$

In terms of the eigenstates of the Hamiltonian

$$\hat{H} \, |\psi_n\rangle = E_n \, |\psi_n\rangle, \qquad \langle \psi_m | \psi_n \rangle = \delta_{mn}, \qquad \sum_n |\psi_n\rangle \langle \psi_n| = \mathbb{1}.$$

it is repesented by

$$G(\boldsymbol{q}, \boldsymbol{q}', E) = \sum_n \frac{\psi_n(\boldsymbol{q}) \, \psi_n^*(\boldsymbol{q}')}{E - E_n} .$$

The Green function is related to the propagator by the transform

$$G(\boldsymbol{q}, \boldsymbol{q}', E) = \frac{1}{i\hbar} \lim_{\varepsilon \to 0} \int_0^\infty \mathrm{d}t \, K(\boldsymbol{q}, \boldsymbol{q}', t) \, \exp\left(\frac{i}{\hbar} (E + i\varepsilon) \, t \right) .$$

Exercise 4

Consider the one-dimensional particle in a box, $q \in [0, a]$.

$$-\frac{\hbar^2}{2m}\psi''(q) = E\psi(q), \quad \psi(0) = 0, \quad \psi(a) = 0.$$

The Green function for a particle in a box satisfies

$$\left(E + \frac{\hbar^2}{2m}\frac{d^2}{dq^2}\right) G(q, q', E) = \delta(q - q'), \quad G(0, q', E) = G(a, q', E) = 0,$$

Show that it can be obtained from the general formula

$$G(q, q', E) = \frac{2m}{\hbar^2}\,\frac{\psi_l(q_<)\,\psi_r(q_>)}{W(q')}.$$

Here $q_<$ and $q_>$ are the smaller and larger of q and q', respectively. ψ_l is a solution of the Schrödinger equation that satisfies the boundary condition on the left-hand side, and ψ_r correspondingly on the right-hand side. The Wronskian W is defined as

$$W(q) = \psi_l(q)\psi_r'(q) - \psi_l'(q)\psi_r(q).$$

Exercise 4 (continued)

This requires you to show that the Green function satisfies both boundary conditions, and that it satisfies the differential equation in the regions $q < q'$ and $q > q'$. The delta-function can be verified by integrating the differential equation from $q = q' - \varepsilon$ to $q = q' + \varepsilon$ and letting ε go to zero.

What is the result for the Green function?

Green function

With the propagator of the free particle we obtain the free Green function in f dimensions

$$G_{\text{free}}(\boldsymbol{q},\boldsymbol{q}',E) = \frac{m}{2i\hbar^2}\left(\frac{1}{2\pi\hbar}\,\frac{\sqrt{2mE}}{|\boldsymbol{q}-\boldsymbol{q}'|}\right)^{f/2-1} H^{(1)}_{f/2-1}\left(\frac{\sqrt{2mE}}{\hbar}|\boldsymbol{q}-\boldsymbol{q}'|\right).$$

Here $H^{(1)}_l(z) = J_l(z) + iN_l(z)$ denotes the Hankel function of the first kind.

We want to obtain a semiclassical approximation for the Green function. For this purpose we insert the semiclassical propagator

$$K(\boldsymbol{q},\boldsymbol{q}',t) \approx \sum_\gamma \frac{1}{(2\pi\hbar)^{f/2}}\sqrt{\left|\det\frac{\partial^2 R_\gamma}{\partial\boldsymbol{q}\,\partial\boldsymbol{q}'}\right|}\exp\left\{\frac{i}{\hbar}R_\gamma(\boldsymbol{q}',\boldsymbol{q},t) - i\,f\frac{\pi}{4} - i\nu_\gamma\frac{\pi}{2}\right\}$$

into the transform

$$G(\boldsymbol{q},\boldsymbol{q}',E) = \frac{1}{i\hbar}\lim_{\varepsilon\to 0}\int_0^\infty \mathrm{d}t\,K(\boldsymbol{q},\boldsymbol{q}',t)\,\exp\left(\frac{i}{\hbar}(E+i\varepsilon)\,t\right).$$

and evaluate the integral in stationary phase approximation. The stationary phase condition is

$$\left.\frac{\partial R_\gamma(\boldsymbol{q},\boldsymbol{q}',t)}{\partial t}\right|_{t=t_0} + E = 0 \qquad \text{or} \qquad -E_\gamma(t_0) + E = 0.$$

Green function

The stationary phase condition selects the time t_0 for which the energy E_γ of the trajectory γ that runs from $\boldsymbol{q}'$ to $\boldsymbol{q}$ in time t_0 is equal to E. We introduce a new action function

$$S(\boldsymbol{q},\boldsymbol{q}',E) = R(\boldsymbol{q},\boldsymbol{q}',t_0) + Et_0 = \int_0^{t_0} L\,\mathrm{d}t + \int_0^{t_0} H\,\mathrm{d}t = \int_0^{t_0} \boldsymbol{p}\cdot\dot{\boldsymbol{q}}\,\mathrm{d}t = \int_{\boldsymbol{q}'}^{\boldsymbol{q}} \boldsymbol{p}\cdot\mathrm{d}\boldsymbol{q}.$$

where t_0 is determined by the condition

$$\left.\frac{\partial R(\boldsymbol{q},\boldsymbol{q}',t)}{\partial t}\right|_{t=t_0} = -E.$$

The action satisfies the relations

$$\frac{\partial S}{\partial \boldsymbol{q}'} = -\boldsymbol{p}', \qquad \frac{\partial S}{\partial \boldsymbol{q}} = \boldsymbol{p}, \qquad \frac{\partial S}{\partial E} = t_0.$$

For the stationary phase approximation we expand in the exponent

$$R_\gamma(\boldsymbol{q}',\boldsymbol{q},t) + Et \approx R(\boldsymbol{q},\boldsymbol{q}',t_0) + Et_0 + \frac{1}{2}\left.\frac{\partial^2 R_\gamma(\boldsymbol{q}',\boldsymbol{q},t)}{\partial t^2}\right|_{t=t_0} (t-t_0)^2,$$

and we evaluate the Gaussian integral over time t.

Green function

The stationary phase approximation results in

$$G(\boldsymbol{q},\boldsymbol{q}',E) \approx \sum_\gamma \frac{2\pi}{(2\pi i\hbar)^{(f+1)/2}} \frac{\sqrt{\left|\det \frac{\partial^2 R_\gamma}{\partial \boldsymbol{q}\,\partial \boldsymbol{q}'}\right|}}{\sqrt{\left|\frac{\partial^2 R_\gamma}{\partial t^2}\right|}} \exp\left\{\frac{i}{\hbar} S_\gamma(\boldsymbol{q},\boldsymbol{q}',E) - i\frac{\pi}{2}\xi_\gamma\right\}$$

where

$$\xi = \begin{cases} \nu, & \frac{\partial^2 R}{\partial t^2} > 0, \\ \nu+1, & \frac{\partial^2 R}{\partial t^2} < 0. \end{cases}$$

ξ is the number of conjugate points for constant energy. It can differ from the number of conjugate points for constant time by one. In the next step we replace the principal function R_γ by the action S_γ. The calculations are quite technical and we only state the result. It is conveniently expressed in a local coordinate system in which the first coordinate is along the trajectory and the remaining $(f-1)$ coordinates are perpendicular to the trajectory.

$$G(\boldsymbol{q},\boldsymbol{q}',E) = \sum_\gamma \frac{2\pi}{(2\pi i\hbar)^{(f+1)/2}} \sqrt{\left|\frac{1}{\dot q_1 \dot q_1'} \det{}'\left(-\frac{\partial^2 S_\gamma}{\partial \boldsymbol{q}\,\partial \boldsymbol{q}'}\right)\right|} \exp\left(\frac{i}{\hbar} S_\gamma(\boldsymbol{q},\boldsymbol{q}',E) - i\frac{\pi}{2}\xi_\gamma\right).$$

The prime at the determinant indicates that it is taken w.r.t. the $(f-1)$ perpendicular coordinates.

Exercise 5

Show that the Green function for a particle in a box, that you obtained in Exercise 4, can be written as a sum over all trajectories from q' to q. The formula for a geometric series is helpful. Convergence problems can be avoided by assuming that E has a small positive imaginary part.

Green function

Our next step is to derive the Gutzwiller trace formula. For simplicity we will consider two-dimensional systems, although it is not difficult to generalise the result to f dimensions. The previous result then has the form

$$G(\boldsymbol{q},\boldsymbol{q}',E)=\sum_{\gamma}\frac{2\pi}{(2\pi i\hbar)^{3/2}}\sqrt{\left|\frac{1}{\dot{q}_1\dot{q}_1'}\;\frac{\partial^2 S_\gamma}{\partial q_2\,\partial q_2'}\right|}\exp\left(\frac{i}{\hbar}S_\gamma(\boldsymbol{q},\boldsymbol{q}',E)-i\frac{\pi}{2}\xi_\gamma\right).$$

The coordinate q_1 is along the trajectory and q_2 is perpendicular to it. We also use $q_\perp$ for q_2.

The result can be expressed in terms of the stability matrix. This matrix describes the linearised motion in the neighbourhood of the trajectory. It provides deviations $\delta q_\perp$ and $\delta p_\perp$ at the end point of a trajectory in terms of the deviations $\delta q_\perp'$ and $\delta p_\perp'$ at the starting point.

$$\begin{pmatrix}\delta q_\perp\\ \delta p_\perp\end{pmatrix}=M\begin{pmatrix}\delta q_\perp'\\ \delta p_\perp'\end{pmatrix}.$$

M is a symplectic matrix. It satisfies $M^TJM=J$ where J denotes the matrix $J=\begin{pmatrix}0 & I\\ -I & 0\end{pmatrix}$. In two dimensions this is equivalent to $\det M=1$.

The stability matrix

The stability matrix can be expressed in terms of the action function $S(\boldsymbol{q}, \boldsymbol{q}', E)$. We have

$$p_2 = \frac{\partial S}{\partial q_2}, \qquad p_2' = -\frac{\partial S}{\partial q_2'}.$$

It then follows

$$\delta p_2 = \frac{\partial^2 S}{\partial q_2 \partial q_2}\delta q_2 + \frac{\partial^2 S}{\partial q_2' \partial q_2}\delta q_2',$$
$$\delta p_2' = -\frac{\partial^2 S}{\partial q_2 \partial q_2'}\delta q_2 - \frac{\partial^2 S}{\partial q_2' \partial q_2'}\delta q_2'.$$

Solving for δq_2 and δp_2 leads to

$$\delta q_2 = \left(\frac{\partial^2 S}{\partial q_2 \partial q_2'}\right)^{-1}\left[-\frac{\partial^2 S}{\partial q_2' \partial q_2'}\delta q_2' - \delta p_2'\right]$$
$$\delta p_2 = \left(\frac{\partial^2 S}{\partial q_2 \partial q_2'}\right)^{-1}\left[\left(\frac{\partial^2 S}{\partial q_2 \partial q_2'}\frac{\partial^2 S}{\partial q_2' \partial q_2} - \frac{\partial^2 S}{\partial q_2 \partial q_2}\frac{\partial^2 S}{\partial q_2' \partial q_2'}\right)\delta q_2' - \frac{\partial^2 S}{\partial q_2 \partial q_2}\delta p_2'\right]$$

The elements of the stability matrix can be read off. One can check that $\det M = 1$.

Trace formula

The density of states is defined by

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

It is related to the Green function by

$$\begin{aligned} d(E) &= -\frac{1}{\pi} \lim_{\varepsilon \to 0} \operatorname{Im} \operatorname{Tr} G(E + i\varepsilon) \\ &= -\frac{1}{\pi} \lim_{\varepsilon \to 0} \operatorname{Im} \int d^2q \sum_n \frac{\psi(\boldsymbol{q})\psi^*(\boldsymbol{q})}{E + i\varepsilon - E_n} \\ &= \frac{1}{\pi} \lim_{\varepsilon \to 0} \sum_n \frac{\varepsilon}{(E - E_n)^2 + \varepsilon^2} \end{aligned}$$

The stationary phase condition

$$0 = \left. \frac{\partial S_\gamma(\boldsymbol{q}, \boldsymbol{q}', E)}{\partial \boldsymbol{q}} \right|_{\boldsymbol{q}'=\boldsymbol{q}} + \left. \frac{\partial S_\gamma(\boldsymbol{q}, \boldsymbol{q}', E)}{\partial \boldsymbol{q}'} \right|_{\boldsymbol{q}'=\boldsymbol{q}} = \boldsymbol{p} - \boldsymbol{p}'.$$

requires trajectories to be periodic. The further evaluation depends on whether the periodic orbits are unstable, stable or neutral.

Periodic orbits in two dimensions

Let λ_1 and λ_2 be the eigenvalues of the stability matrix. Then

$$\det M = \lambda_1 \lambda_2 = 1, \qquad \mathrm{Tr}\, M = \lambda_1 + \lambda_2 \in \mathbb{R}, \qquad \lambda_{1,2} = \frac{1}{2}\left(\mathrm{Tr}\, M \pm \sqrt{(\mathrm{Tr}\, M)^2 - 4}\right).$$

We consider the cases

- $\mathrm{Tr}\, M = 2$, $\lambda_1 = \lambda_2 = 1$:
  Periodic orbits are not isolated. This is typical for integrable systems where periodic orbits form families. $\mathrm{Tr}\, M = 2$ happens also at bifurcations of periodic orbits.

- $|\mathrm{Tr}\, M| < 2$, $\lambda_1 = \mathrm{e}^{iv}$, $\lambda_2 = \mathrm{e}^{-iv}$,:
  Periodic orbits are stable. This typically occurs in mixed systems. if v is a rational multiple of 2π, $v = 2\pi n/m$ then the m-th repetition of the orbit bifurcates $\lambda_1^m = \mathrm{e}^{2\pi n\, i} = 1$. This requires uniform approximations.

- $\mathrm{Tr}\, M = -2$, $\lambda_1 = \lambda_2 = -1$,:
  Limiting case of (2).

- $|\mathrm{Tr}\, M| > 2$, $\lambda_1 = \pm\mathrm{e}^{u}$, $\lambda_2 = \pm\mathrm{e}^{-u}$,: Periodic orbits are unstable. This is typical for chaotic systems.

Trace formula

We continue with the evaluation of the integral

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

for chaotic systems. The semiclassical approximation for the Green function is

$$G(\boldsymbol{q}, \boldsymbol{q}', E) = \sum_{\gamma} \frac{1}{\sqrt{2\pi\hbar^3 \dot{q}_1 \dot{q}'_1 \, |M_{\gamma,12}|}} \exp\left(\frac{i}{\hbar} S_\gamma(\boldsymbol{q}, \boldsymbol{q}', E) - i\frac{\pi}{2}\xi_\gamma - i\frac{3\pi}{4} \right).$$

and the stationary phase condition is

$$0 = \left. \frac{\partial S_\gamma(\boldsymbol{q}, \boldsymbol{q}', E)}{\partial \boldsymbol{q}} \right|_{\boldsymbol{q}'=\boldsymbol{q}} + \left. \frac{\partial S_\gamma(\boldsymbol{q}, \boldsymbol{q}', E)}{\partial \boldsymbol{q}'} \right|_{\boldsymbol{q}'=\boldsymbol{q}} = \boldsymbol{p} - \boldsymbol{p}'.$$

The action S_γ does not change if one moves the starting point of a trajectory along a periodic orbit. The stationary phase approximation is applied only in the direction perpendicular to the periodic orbit. We assume that the periodic orbit is isolated.

Trace formula

We expand

$$S_\gamma(\boldsymbol{q}, \boldsymbol{q}, E) \approx S_\gamma(E) + \frac{1}{2}\sigma q_2^2,$$

where $S_\gamma(E)$ is the action of the periodic orbit and

$$\sigma = \frac{\partial^2 S_\gamma}{\partial q_2 \partial q_2} + 2\frac{\partial^2 S_\gamma}{\partial q_2 \partial q_2'} + \frac{\partial^2 S_\gamma}{\partial q_2' \partial q_2'} = \frac{\partial^2 S_\gamma}{\partial q_2 \partial q_2'}(2 - \operatorname{Tr} M) = -\frac{1}{M_{12}}(2 - \operatorname{Tr} M).$$

The evaluation of the integral

$$\begin{aligned} d_\gamma(E) &= \operatorname{Re} \int \mathrm{d}q_1\, \mathrm{d}q_2\, \frac{1}{\sqrt{2\pi^3\hbar^3 \dot{q}_1^2\, |M_{\gamma,12}|}} \exp\left(\frac{i}{\hbar}S_\gamma(E) + \frac{i}{2\hbar}\sigma q_2^2 - i\frac{\pi}{2}\xi_\gamma - i\frac{\pi}{4}\right) \\ &= \operatorname{Re} \int \frac{\mathrm{d}q_1}{\dot{q}_1}\, \frac{1}{\pi\hbar\sqrt{|\operatorname{Tr} M_\gamma - 2|}} \exp\left(\frac{i}{\hbar}S_\gamma(E) - i\frac{\pi}{2}\mu_\gamma\right) \end{aligned}$$

where

$$\mu = \begin{cases} \xi, & \sigma > 0, \\ \xi + 1, & \sigma < 0. \end{cases}$$

The index ξ can change along a periodic orbit between two values that differ by one. The Maslov index μ is the larger of these two values.

Trace formula, zero length contribution

The direct trajectory γ_0 from $\boldsymbol{q}'$ to $\boldsymbol{q}$ in the limit $\boldsymbol{q}' \to \boldsymbol{q}$ approaches that of a free particle with energy E replaced by $E - V((\boldsymbol{q}+\boldsymbol{q}')/2)$. Its contribution to the Green function is approximated by the free Green function

$$G_{\gamma_0}(\boldsymbol{q}, \boldsymbol{q}', E) \approx \frac{m}{2i\hbar^2} H_0^{(1)}\left(\frac{\sqrt{2m(E-V)}}{\hbar}|\boldsymbol{q}-\boldsymbol{q}'|\right) .$$

Here $H_0^{(1)}(z) = J_0(z) + iN_0(z)$ and $V = V((\boldsymbol{q}+\boldsymbol{q}')/2)$. Its contribution to the density of states is

$$\bar{d}(E) \approx -\frac{1}{\pi} \lim_{\varepsilon \to 0} \operatorname{Im} \int_{A(E)} \mathrm{d}^2 q \, G_0(\boldsymbol{q}, \boldsymbol{q}, E + i\varepsilon) = \frac{m}{2\pi\hbar^2} \int_{A(E)} \mathrm{d}^2 q = \frac{mA(E)}{2\pi\hbar^2}.$$

Here $A(E)$ is the area in which $E > V(\boldsymbol{q})$ and we used $J_0(0) = 1$.This can be recognised as the Thomas-Fermi approximation for the density of states

$$\bar{d}(E) \approx \frac{1}{(2\pi\hbar)^2} \int \mathrm{d}^2 q \, \mathrm{d}^2 p \, \delta\left(E - \frac{p^2}{2m} - V(\boldsymbol{q})\right) .$$

Trace formula

The final result is the Gutzwiller trace formula

$$d(E) \approx \bar{d}(E) + \sum_{\gamma} \frac{T_\gamma}{\pi\hbar\, r_\gamma \sqrt{|\operatorname{Tr} M_\gamma - 2|}} \cos\left(\frac{1}{\hbar} S_\gamma(E) - \frac{\pi}{2}\mu_\gamma\right)$$

The sum is over all periodic orbits. T_γ is the period and r_γ is the repetition number if γ is a repetition of a shorter orbit. In higher dimensions $|\operatorname{Tr} M_\gamma - 2|$ has to be replaced by $|\det(M - \mathbb{1})|$.

- Formula can be made convergent by considering other functions $\sum_n f(E_n)$ instead of $d(E)$.
- Requires orbits up to the Heisenberg time $T_H = 2\pi\hbar\bar{d}(E)$ to resolve neighbouring levels.
- This leads to an exponentially increasing effort for higher energy levels.
- Exact version in Selberg trace formula. Analogies to Riemann zeta function.
- For integrable systems one has to integrate over tori of periodic orbits (Berry-Tabor formula).
- For mixed systems one has to deal with bifurcations of periodic orbits and break-up of tori.

Fourier transform

The Fourier transform of the density of states has peaks at the periods of the periodic orbits

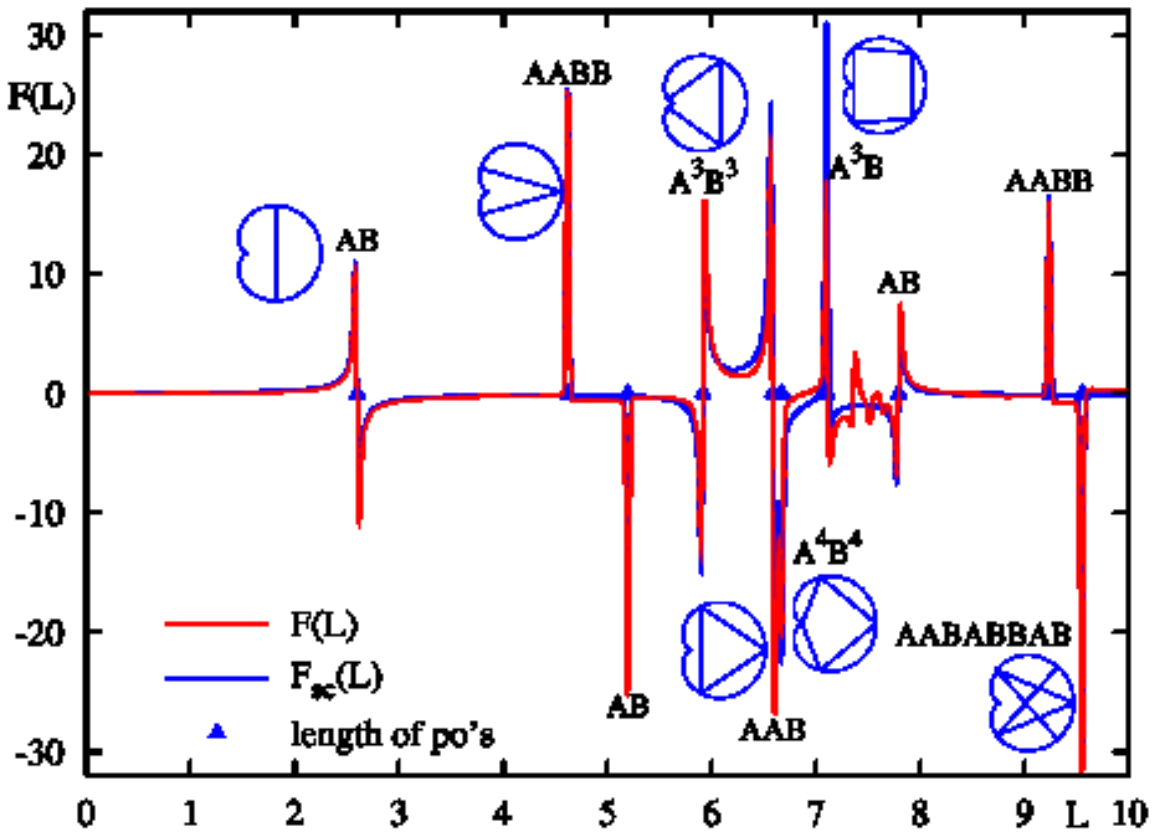
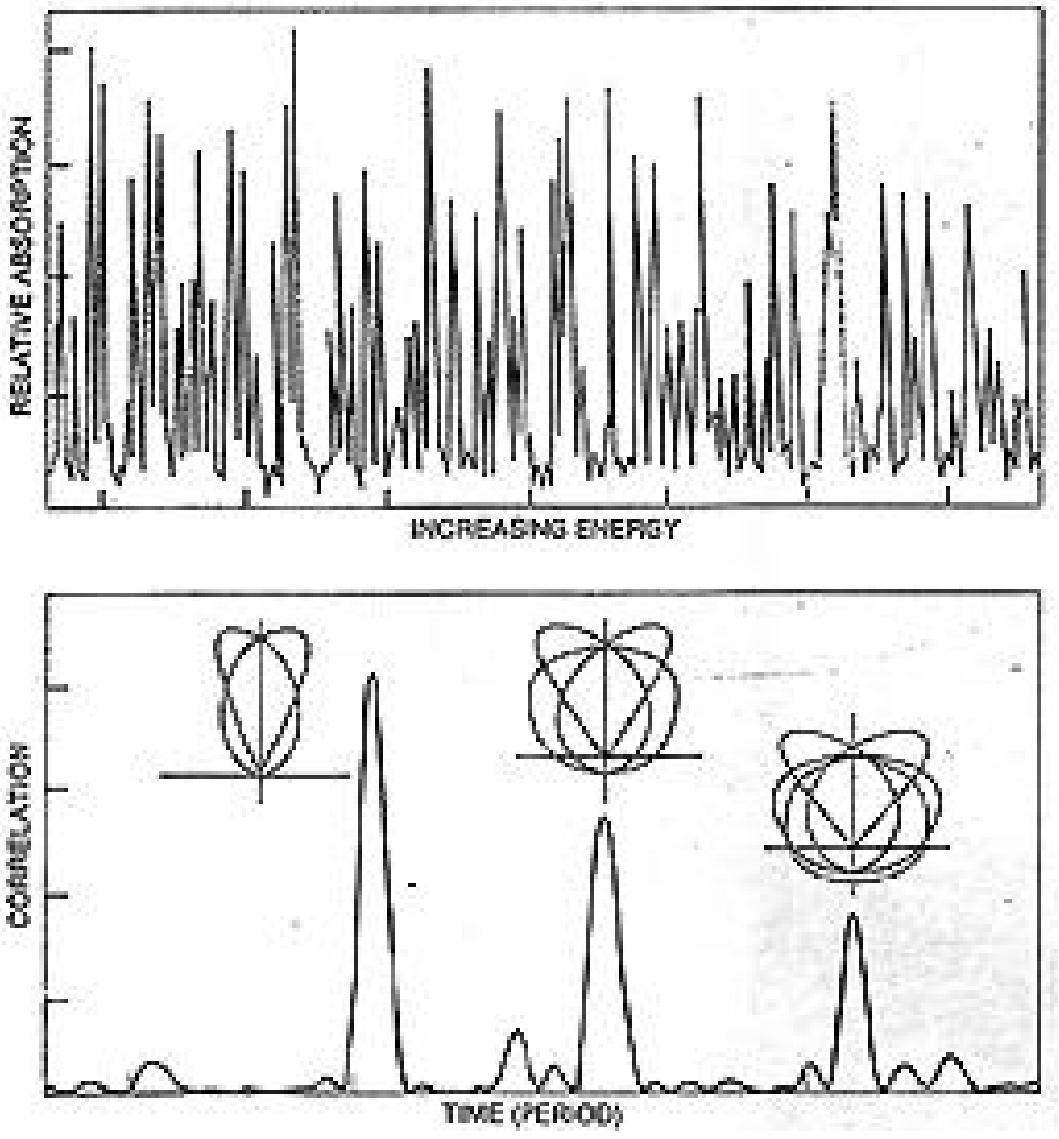


Figure: Arnd Bäcker

Hydrogen atom in a magnetic field



Example: billiard systems

Billiard systems are common model systems. It is convenient to use dimensionless units $\hbar = 2m = 1$. Then $E = k^2$ and the semiclassical limit corresponds to $k \to \infty$. The trace formula for $d(k) = 2kd(E)$ has the form

$$d(k) = \sum_n \delta(k - k_n) \approx \bar{d}(k) + \sum_\gamma \frac{l_\gamma \cos\left(\mathrm{i}kl_\gamma - \mathrm{i}\frac{\pi}{2}\mu_\gamma\right)}{\pi r_\gamma \sqrt{|\operatorname{Tr} M_\gamma - 2|}}, \qquad \text{where} \qquad \bar{d}(k) \approx \frac{Ak}{2\pi}.$$

The stability matrices are composed of two types of matrices, $M = \ldots M_r^3 M_t^{3\leftarrow 2} M_r^2 M_t^{2\leftarrow 1}$, one for every reflection, M_r, and one for every path between two reflections, M_t,

$$M_t = \begin{pmatrix} 1 & \frac{l}{k} \\ 0 & 1 \end{pmatrix}, \qquad M_r = \begin{pmatrix} -1 & 0 \\ \frac{2k}{R\cos\alpha} & -1 \end{pmatrix}$$

l is the length of the path and α is the angle of reflection (angle between normal to boundary and trajectory). R is the radius of curvatures. It is negative for concave boundaries (e.g. Sinai billiard).

The Maslov index has an additional contribution of twice the number of reflections at walls with Dirichlet boundary conditions. For concave billiards there are no conjugate points.

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 $C_0 = 1$.