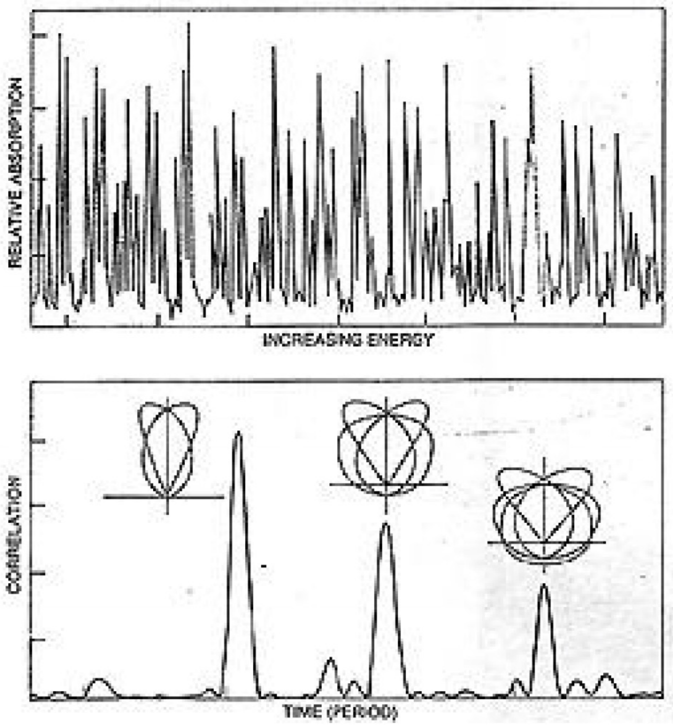
10. Semiclassics

Hydrogen atom in magnetic field

light absorption



energy

Fourier-transform

time

motivation: q.m. properties (spectrum, eigenfunctions)

from classical dynamics

→ helpful if more intuitive than q.m. calculation

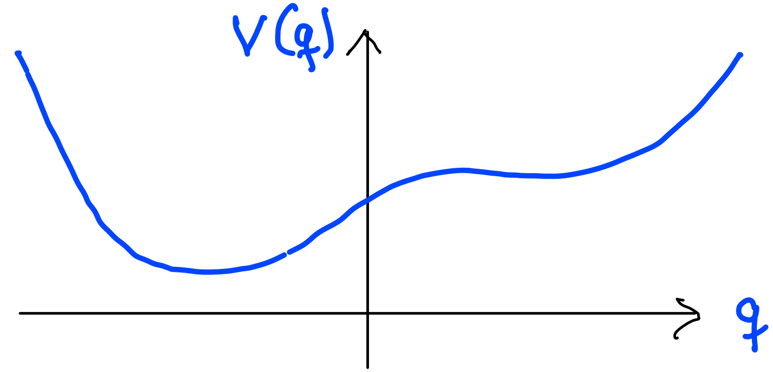
→ quantum-classical correspondence

10.1. Integrable Systems

1D: WKB (Wentzel, Kramers, Brillouin) - approximation

Schrödinger eq.:
(time-indep., q)

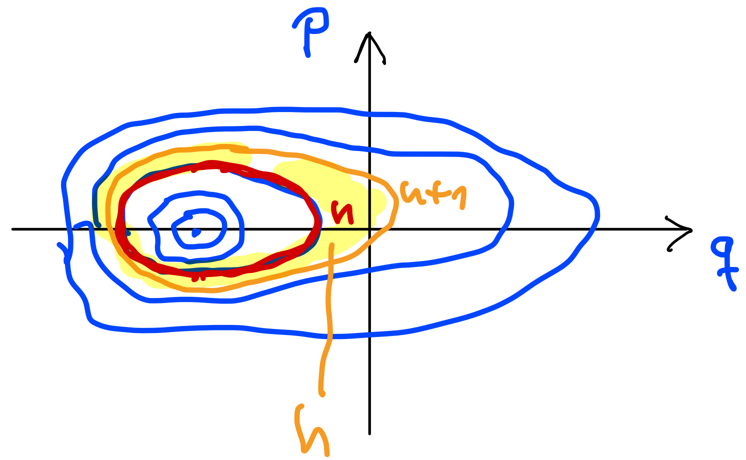
$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + V(q)\right)\psi(q) = E\,\psi(q)$$



$$\psi_{WKB}(q) = \frac{1}{\sqrt{p(q)}}\, e^{\pm\frac{i}{\hbar}\int^{q} dq'\, p(q')}$$

cl. phase space: $\frac{p^2}{2m} + V(q) = E$

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



validity: De-Broglie wave length $\lambda = \frac{h}{p(q)}$ changes slowly

$\Rightarrow$ invalid at turning point $p(q) = 0$ (momentum repr., $\tilde{\Psi}_{WKB}(p)$)

$\Rightarrow \ldots \Rightarrow$ WKB quantization:

$$\oint p \, dq = \left(n + \frac{1}{2}\right) h \quad ; \quad n = 0, 1, 2, \ldots$$

remarks:
- periodic orbit
- $\frac{1}{2}$ from turning points: corrects Bohr-Sommerfeld quantization
- area h between quantized orbits
- energy spacing: $E_{n+1} - E_n = \frac{h}{\tau(E)}$ ← classical period

f D: EBK (Einstein, Brillouin, Keller) - quantization for integrable system

f dim. torus: $\oint_{\gamma_i} p \, dq = \left(n_i + \frac{\nu_i}{4}\right) h \quad ; \quad i = 1, \ldots, f \quad ; \quad n_i = 0, 1, 2, \ldots$

fundamental orbit → γ_i

Einstein 1917: What happens for non-integrable systems?

10.2. Propagator, Green function, Density of States

aim: general q.m. quantities and relations for time-indep. H

- propagator (time-evolution operator $\mathcal{U}$ in position representation):

$$K(q,q',t) := \langle q|\,\mathcal{U}(t,0)\,|q'\rangle = \langle q|\, e^{-\frac{i}{\hbar}Ht} \underset{\uparrow}{} |q'\rangle$$

$$\sum_n |n\rangle\langle n|$$

properties:

- $\psi(q,t) = \int_{-\infty}^{\infty} dq'\, K(q,q',t)\, \psi(q',0)$

- $\lim_{t\to 0^+} K(q,q',t) = \delta(q-q')$

- representation using eigenfunctions: $K(q,q',t) = \sum_n \psi_n(q)\, \psi_n^*(q')\, e^{-\frac{i}{\hbar}E_n t}$ $\quad(+)$

- free particle: $H = \frac{p^2}{2}$ $(m=1)$

$$\Rightarrow \quad K(q,q',t) = \dots = \left(\frac{1}{2\pi i\hbar t}\right)^{\frac{f}{2}} e^{\frac{i}{\hbar}\frac{(q-q')^2}{2t}}$$

- Green function (energy dependent)

$$G(q, q', E+i\varepsilon) := \frac{1}{i\hbar}\int_0^\infty dt\, K(q, q', t)\, e^{\frac{i}{\hbar}(E+i\varepsilon)t}$$

- one-sided FT
- $\varepsilon > 0$ for convergence

properties:

- $(H-E)\, G(q, q', E) = -\delta(q-q')$
- representation with eigenfunctions: $G(q, q', E+i\varepsilon) \overset{(+)}{=} \sum_n{}' \frac{\psi_n(q)\, \psi_n^*(q')}{E - E_n + i\varepsilon}$

  $\Rightarrow$ eigenenergies are poles!

- $\mathrm{Tr}\, G(q, q', E) = \int dq\, G(q, q, E+i\varepsilon) = \sum_n \frac{1}{E - E_n + i\varepsilon}$

- density of states

$$d(E) = \sum_n \delta(E-E_n) = -\frac{1}{\pi} \lim_{\varepsilon\to 0^+} \mathrm{Im} \sum_n \frac{1}{E-E_n+i\varepsilon} = -\frac{1}{\pi} \lim_{\varepsilon\to 0^+} \mathrm{Im}\, \mathrm{Tr}\, G(q,q';E+i\varepsilon)$$

representation of δ-function:

$$\delta(x) = -\frac{1}{\pi} \lim_{\varepsilon\to 0^+} \mathrm{Im} \underbrace{\frac{1}{x+i\varepsilon}}_{\mathrm{Im}\frac{x-i\varepsilon}{x^2+\varepsilon^2} = -\frac{\varepsilon}{x^2+\varepsilon^2}} = \frac{1}{\pi} \lim_{\varepsilon\to 0^+} \frac{\varepsilon}{x^2+\varepsilon^2}$$

10.3. Semiclassical Propagator

Van Vleck 1926, Gutzwiller 1967

$$K_{sc}(q,q',t) = \left(\frac{1}{2\pi i\hbar}\right)^{\frac{f}{2}} \sum_{\substack{j \\ \text{cl. traj.}}} \left| \det \frac{\partial^2 S_j(q,q',t)}{\partial q\, \partial q'} \right|^{\frac{1}{2}} e^{\frac{i}{\hbar} S_j(q,q',t) - i\frac{\pi \nu_j}{2}}$$

f: d.o.f.

$\sum_j$: sum over cl. trajectories j from q' to q within time t

S_j: action of cl. trajectory j from q' to q within time t

$$S_j(q,q',t) = \int_0^t dt'\, \mathcal{L}(q_j(t'), \dot{q}_j(t')) = \int_0^t dt' \left(p_j(t') \cdot \dot{q}_j(t') - E_j \right)$$

$$= \int_{q'}^{q} p_j(q'')\, dq'' - E_j t$$

free particle: $S(q,q',t) = p(q-q') - \frac{p^2}{2}t \overset{p=\frac{q-q'}{t}}{=} \frac{(q-q')^2}{2t}$

What is relation of final phase space point (q,p) to initial (q',p')?

use action as generator of canonical transformation:

$$\frac{\partial S(q,q',t)}{\partial q} = p$$

$$\frac{\partial S(q,q',t)}{\partial q'} = -p'$$

$$\frac{\partial S(q,q',t)}{\partial t} = -E$$

$$K_{sc}(q,q',t) = \left(\frac{1}{2\pi i\hbar}\right)^{\frac{f}{2}} \sum_{\substack{j \\ \text{cl. traj.}}} \left| \det \frac{\partial^2 S_j(q,q',t)}{\partial q\, \partial q'} \right|^{\frac{1}{2}} e^{\frac{i}{\hbar} S_j(q,q',t) - i\frac{\pi \nu_j}{2}}$$

$$\left(\frac{1}{2\pi\hbar}\right)^f \left| \det \frac{\partial^2 S_j(q,q',t)}{\partial q\, \partial q'} \right| = \text{cl. probability density of trajectory } j$$

initial point (q', p') surrounded by phase space density one per Planck cell

$$w(q',p') = \frac{1}{h^f}$$

$\Rightarrow$ prob. density in (q,q'):

$$P(q,q',t) = \int dp'\, w(q',p')\, \delta\big(q - q_t(q',p')\big) \qquad \int \delta(f(x))\,dx = \frac{1}{\left|\frac{df}{dx}\right|_{f(x)=0}}$$

$$= \frac{1}{h^f} \cdot \frac{1}{\left|\det \frac{\partial q_t}{\partial p'}\right|_{q_t = q}} \underset{\substack{\text{matrix}\\ \text{invertible}}}{=} \frac{1}{h^f}\left|\det \frac{\partial p'}{\partial q}\right| = \frac{1}{(2\pi\hbar)^f}\left|\det \frac{\partial^2 S}{\partial q'\, \partial q}\right| \checkmark$$

$f \times f$ matrix

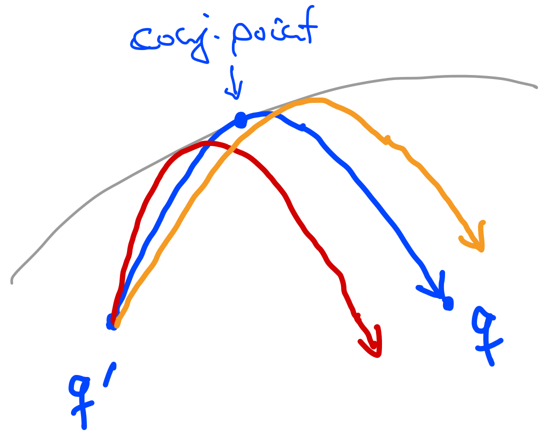
free particle: $\dfrac{\partial^2 S}{\partial q\, \partial q'} = -\dfrac{1}{t} \quad \Rightarrow \quad \left|\det \dfrac{\partial^2 S}{\partial q\, \partial q'}\right| = \dfrac{1}{t^f}$

$$K_{sc}(q,q',t) = \left(\frac{1}{2\pi i\hbar}\right)^{\frac{f}{2}} \sum_{\substack{j \\ \text{cl. traj.}}} \left| \det \frac{\partial^2 S_j(q,q',t)}{\partial q\, \partial q'} \right|^{\frac{1}{2}} e^{\frac{i}{\hbar} S_j(q,q',t) - i\frac{\pi \nu_j}{2}}$$

ν_j : number of conjugated points along trajectory j

Def.: matrix $\frac{\partial q}{\partial p'}$ has at least one eigenvalue 0

e.g. at caustic



determinant diverges → change to momentum repr. → $e^{-i\frac{\pi}{2}}$

free particle: $K_{sc} = \left(\frac{1}{2\pi i\hbar t}\right)^{\frac{f}{2}} e^{\frac{i}{\hbar}\frac{(q-q')^2}{2t}} = K_{qm}$ no approx.

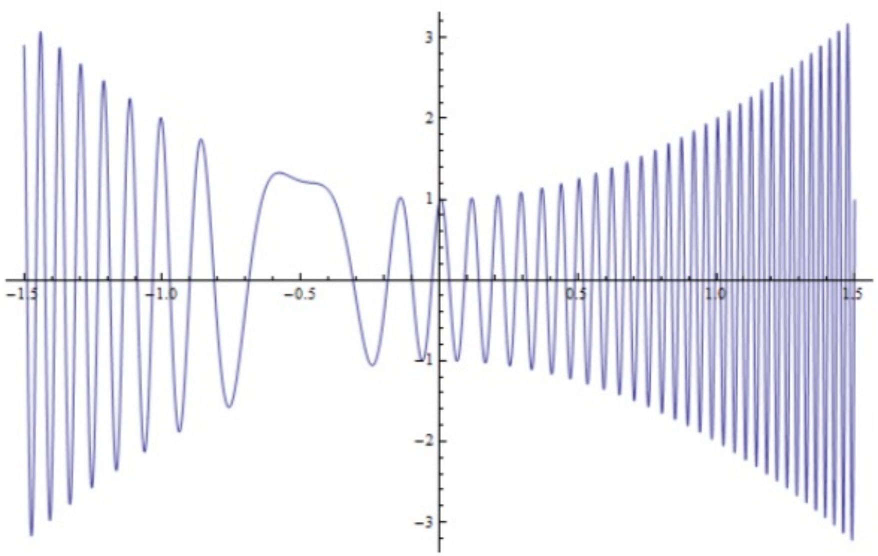
10.3.1. Stationary Phase Approximation

$$I = \int_{-\infty}^{\infty} dx \; A(x) \; e^{\frac{i}{\hbar} W(x)}$$

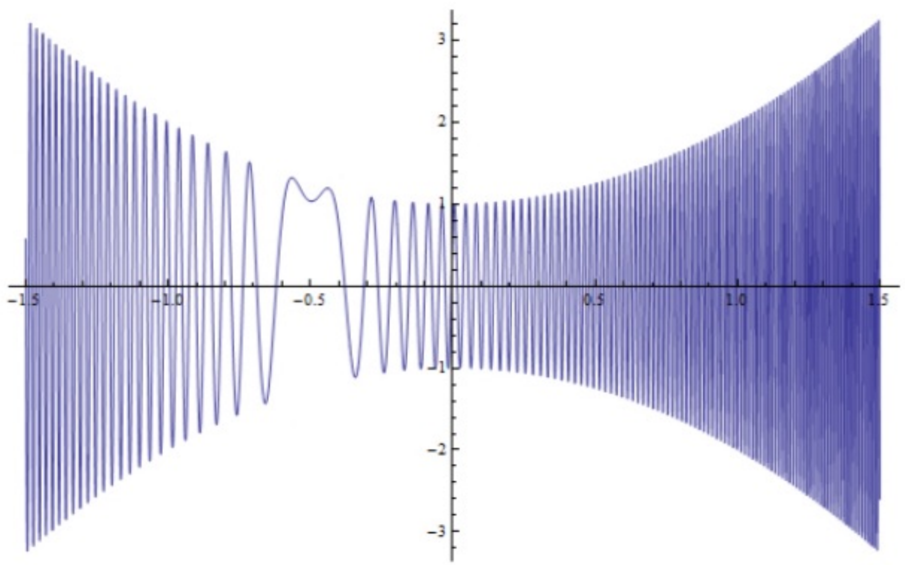
- $A(x)$ slowly varying
- $\frac{W(x)}{\hbar} \gg 1$ phase

$\Rightarrow$ averages to zero ! ?

$\text{Re}\,(1+x^2)\, e^{i(1+x+x^2)50}$



$\text{Re}\,(1+x^2)\, e^{i(1+x+x^2)150}$



exception: stationary point x_s : $\left.\frac{\partial}{\partial x} W(x)\right|_{x=x_s} = 0$

Taylor expansion at x_s: $W(x) = W(x_s) + \frac{1}{2}(x-x_s)^2 W''(x_s) + \dots$

$$I \approx \int_{-\infty}^{\infty} dx\, A(x)\, e^{\frac{i}{\hbar}\left(W(x_s) + \frac{1}{2}(x-x_s)^2 W''(x_s)\right)} \qquad y = x - x_s$$

$$= e^{\frac{i}{\hbar} W(x_s)} \underbrace{\int_{-\infty}^{\infty} dy\, \underbrace{A(y+x_s)}_{\approx A(x_s)}\, e^{\frac{i}{\hbar} \frac{y^2}{2} W''(x_s)}}_{A(x_s)\sqrt{\frac{2\pi i\hbar}{W''(x_s)}}}$$

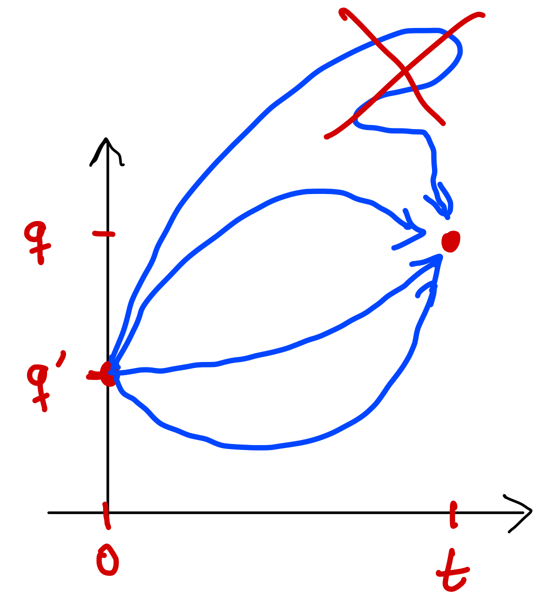
$$\boxed{\int d^f x\; A(\vec{x})\, e^{\frac{i}{\hbar} W(\vec{x})} \approx (2\pi i \hbar)^{\frac{f}{2}} \left(\det \frac{\partial^2 W}{\partial x_n \partial x_m}\right)^{-\frac{1}{2}} A(\vec{x}_s)\, e^{\frac{i}{\hbar} W(\vec{x}_s)}}$$

10.3.2. Derivation of K_{sc} from Feynman path integral

$$K(q, q', t) = \int \mathcal{D}(q) \; e^{\frac{i}{\hbar} \int_0^t \mathcal{L}(q, \dot{q})\, dt'}$$

integration over all paths $q(t)$ from q' to q in t

many more than the solutions of Hamilton's equation of motion



Semiclassical approximation with stationary phase approx.:

cl. action $\int_0^t L\,dt' \gg \hbar$

- contributions average to zero
- at stationary points: $\delta \int_0^t L\,dt' \overset{!}{=} 0$ Hamilton's principle $\Rightarrow$ cl. traj.

$$\Rightarrow K_{sc}(q,q',t) = \sum_j A_j\, e^{\frac{i}{\hbar} S_j(q,q',t)}$$

Van Vleck 1926, Gutzwiller 1967

with $$A_j = \left(\frac{1}{2\pi i \hbar}\right)^{\frac{f}{2}} \left| \det \frac{\partial^2 S(q,q',t)}{\partial q\, \partial q'} \right|^{\frac{1}{2}} e^{-i\frac{\pi}{2}\nu_j}$$

from stationary phase and probability of contribution

- valid for arbitrary times (number of trajectories increases)