Path integrals in quantum mechanics & Semiclassical approximation

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Topics of the presentation

Topics of the presentation

Definitions from classical mechanics

Physical system of interest

Non-relativistic 1D quantum particle in time-independent potential

- Classical **Lagrangian**

$$L(\dot{x}, x) = \frac{m}{2}\dot{x}^2 - V(x)$$

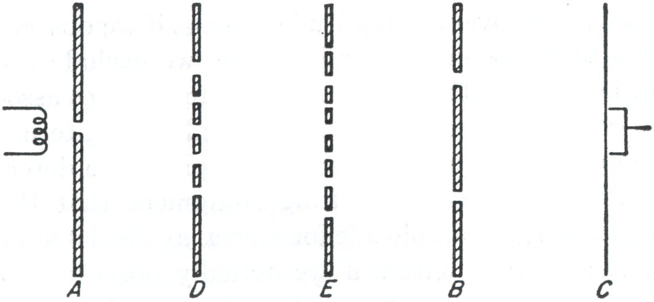
- Classical **action**

$$S[x(t)] = \int_{t_a}^{t_b} L(\dot{x}(t), x(t))\mathrm{d}t$$

- **Boundary conditions**

$$\begin{cases} x(t_a) = x_a \\ x(t_b) = x_b \\ T = t_b - t_a \end{cases}$$

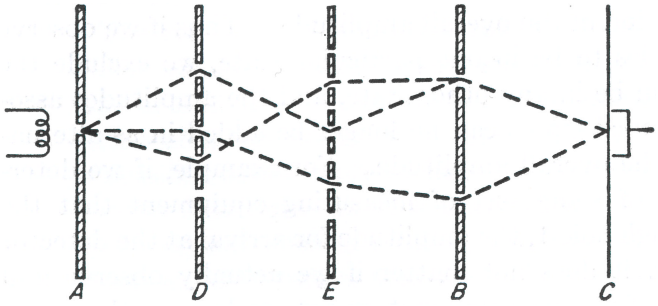
Feynman's thought experiment 1



Event: a particle initially at A moves to C
Method: a path between A and C

Events are observed/measured, methods are not

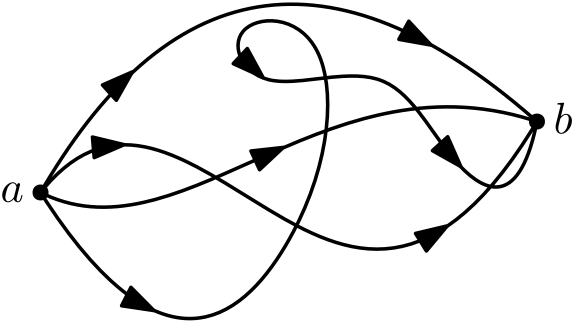
Feynman's thought experiment 2



- **Event** can happen in different **methods** $i = 1, 2, \dots$
- **Amplitude** $\phi_i \in \mathbb{C}$ associated to method i
- **Total amplitude** $\phi = \phi_1 + \phi_2 + \dots$
- **Total probability** $P = |\phi|^2 = |\phi_1 + \phi_2 + \dots|^2$

Feynman's thought experiment 3

In the limit of infinitely many screens and holes



Event: a particle initially at $a = (x_a, t_a)$ moves to $b = (x_b, t_b)$
Method: a path between $a = (x_a, t_a)$ and $b = (x_b, t_b)$

Feynman's postulates

The amplitude assigned to a method is

Transition amplitude

$$\phi[x(t)] \sim \exp\left(\frac{i}{\hbar} S[x(t)]\right)$$

The total amplitude of the event is the sum over all methods

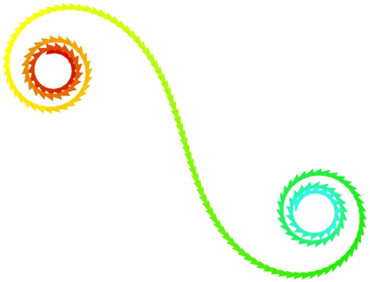
Probability transition amplitude

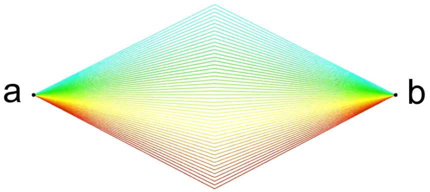
$$K(b,a) = \sum_{\substack{\text{all paths} \\ a \to b}} \phi[x(t)]$$

Convergence of the path integral

Path integral

$$K(b,a) = \int \exp\left(\frac{i}{\hbar} S[x(t)]\right) \mathrm{D}x(t)$$





Topics of the presentation

Useful formulas for Schrödinger $\Rightarrow$ Feynman

- **Trotter's formula** (omit limit)

$$e^{\hat{A}+\hat{B}} = \lim_{N\to\infty} \prod_{k=1}^{N} e^{\hat{A}/N} e^{\hat{B}/N}$$

- **Time evolution operator**

$$\hat{U}(t_b, t_a) = \exp\left(-\frac{i}{\hbar}(t_b - t_a)\hat{H}\right)$$

- Position-momentum sandwich

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

- **Identity operator**

$$1 = \int \mathrm{d}x \, |x\rangle \langle x| = \int \mathrm{d}p \, |p\rangle \langle p|$$

Schrödinger $\Rightarrow$ Feynman 1

We expect the **propagator** to be equivalent to the path integral

Proposition to prove

$$\left\langle x_b \middle| \hat{U}(t_b, t_a) \middle| x_a \right\rangle \stackrel{?}{=} K(b, a)$$

Denote time-step $\varepsilon = T/N$, let $N \to \infty$, apply Trotter's formula

$$\begin{aligned}
\left\langle x_b \middle| \hat{U}(t_b, t_a) \middle| x_a \right\rangle &= \left\langle x_b \middle| e^{-iT(\hat{T}+\hat{V})/\hbar} \middle| x_a \right\rangle \\
&= \left\langle x_b \middle| \prod_{k=1}^{N} e^{-i\varepsilon\hat{T}/\hbar} e^{-i\varepsilon\hat{V}/\hbar} \middle| x_a \right\rangle \\
&= \ddots
\end{aligned}$$

Schrödinger $\Rightarrow$ Feynman 2

Insert $N-1$ identity operators ($x_b = x_N$ and $x_a = x_0$)

$$\ddots = \int \mathrm{d}x_1 \cdots \int \mathrm{d}x_{N-1} \prod_{k=1}^{N} \left\langle x_k \,\middle|\, e^{-i\varepsilon \hat{T}/\hbar} e^{-i\varepsilon V(x_{k-1})/\hbar} \,\middle|\, x_{k-1} \right\rangle = \ddots$$

Compute the sandwich with the position-momentum braket

$$\begin{aligned}
&\left\langle x_k \,\middle|\, e^{-i\varepsilon \hat{T}/\hbar} \,\middle|\, x_{k-1} \right\rangle = \\
&= \frac{1}{2\pi\hbar} \int \mathrm{d}p \exp\left(\frac{ipx_k}{\hbar}\right) \exp\left(-\frac{i\varepsilon p^2}{2m\hbar}\right) \exp\left(-\frac{ipx_{k-1}}{\hbar}\right) \\
&= \frac{1}{2\pi\hbar} \int \mathrm{d}p \exp\left(-\frac{i\varepsilon p^2}{2m} + \frac{ip(x_k - x_{k-1})}{\hbar}\right) \\
&= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \exp\left(\frac{im}{2\hbar\varepsilon}(x_k - x_{k-1})^2\right)
\end{aligned}$$

Schrödinger $\Rightarrow$ Feynman 3

With the following **normalization constant**

$$A^{-1} = \sqrt{\frac{m}{2\pi i\hbar\varepsilon}}$$

we stick everything together to get

$$\ddots = \left\langle x_b \middle| \hat{U}(t_b, t_a) \middle| x_a \right\rangle =$$

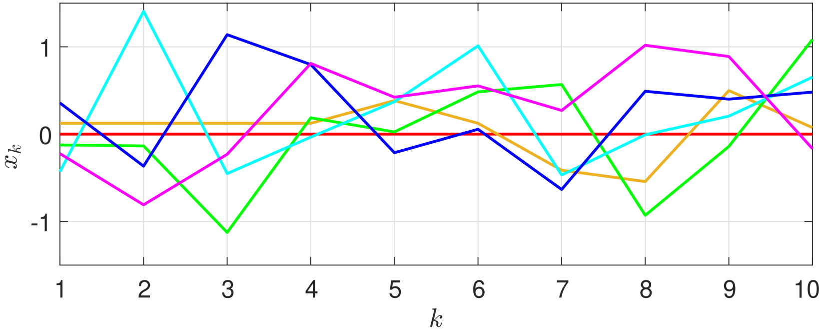
$$= \frac{1}{A^N} \int \mathrm{d}x_1 \cdots \int \mathrm{d}x_{N-1} \exp\left(\sum_{k=1}^{N} \left[\frac{im}{2\hbar\varepsilon}(x_k - x_{k-1})^2 - i\frac{\varepsilon}{\hbar} V(x_{k-1}) \right] \right)$$

$$= \int \frac{\mathrm{d}x_1}{A} \cdots \int \frac{\mathrm{d}x_{N-1}}{A} \frac{\exp}{A} \left(\frac{i\varepsilon}{\hbar} \sum_{k=1}^{N} \left[\frac{m}{2} \left(\frac{x_k - x_{k-1}}{\varepsilon} \right)^2 - V(x_{k-1}) \right] \right)$$

Schrödinger ⇒ Feynman 4

Interpreting the **red** and **blue** parts

$$\int \frac{\mathrm{d}x_1}{A} \cdots \int \frac{\mathrm{d}x_{N-1}}{A} \frac{\exp}{A} \left(\frac{i}{\hbar} \varepsilon \sum_{k=1}^{N} \left[\frac{m}{2} \left(\frac{x_k - x_{k-1}}{\varepsilon} \right)^2 - V(x_{k-1}) \right] \right)$$



Schrödinger $\Rightarrow$ Feynman 5

We end up with a **cumbersome definition**

$$\left\langle x_b \,\middle|\, \hat{U}(t_b, t_a) \,\middle|\, x_a \right\rangle = \lim_{N\to\infty}$$

$$\int \frac{\mathrm{d}x_1}{A} \cdots \int \frac{\mathrm{d}x_{N-1}}{A} \frac{\exp}{A} \left(\frac{i}{\hbar} \varepsilon \sum_{k=1}^{N} \left[\frac{m}{2} \left(\frac{x_k - x_{k-1}}{\varepsilon} \right)^2 - V(x_{k-1}) \right] \right)$$

$$= \int \mathrm{D}x(t)\, \exp\left(\frac{i}{\hbar} S[x(t)] \right) = K(b, a)$$

We have indeed shown that

Propagator

$$\left\langle x_b \,\middle|\, \hat{U}(t_b, t_a) \,\middle|\, x_a \right\rangle = K(b, a)$$

Schrödinger ⇒ Feynman 6

Why is it called the propagator?

$$\begin{aligned}\psi(x_b, t_b) &= \langle x_b \,|\, \psi(t_b)\rangle = \left\langle x_b \middle| \hat{U}(t_b, t_a) \middle| \psi(t_a) \right\rangle \\ &= \int \mathrm{d}x_a \, \left\langle x_b \middle| \hat{U}(t_b, t_a) \middle| x_a \right\rangle \langle x_a \,|\, \psi(t_a)\rangle \\ &= \int \mathrm{d}x_a \, K(b, a)\psi(x_a, t_a)\end{aligned}$$

Wavefunction time evolution

$$\psi(x_b, t_b) = \int K(b, a)\psi(x_a, t_a)\mathrm{d}x_a$$

K is called the **kernel** (of the convolution)

Topics of the presentation

Link with statistical physics

Consider the **canonical ensemble** with **density matrix**

$$\hat{\rho} = e^{-\beta \hat{H}}$$

The **partition function** is

$$Z = \mathrm{Tr}(\hat{\rho}) = \int \mathrm{d}x' \, \langle x' | e^{-\beta \hat{H}} | x' \rangle$$

We recognise the path integral

$$K(b,a) = \left\langle x_b \middle| e^{-i(t_b - t_a)/\hbar \hat{H}} \middle| x_a \right\rangle$$

with paths respecting

- **Periodic boundary conditions** $x_a = x_b = x'$
- **Time-temperature identification**

$$-\beta = -\frac{i}{\hbar}(t_b - t_a)$$

Wick rotation

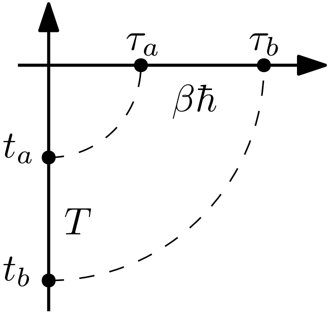
Time-temperature identification

$$\beta\hbar = i(t_b - t_a) = iT$$

suggests a **Wick rotation**

$$t \to it = \tau \in \mathbb{R}$$

to **imaginary time**



Euclidean action 1

How does the path integral change under Wick rotation?

$$\langle x'|e^{-\beta \hat{H}}|x'\rangle = \int \exp\left(\frac{i}{\hbar} S[x(t)]\right) \mathrm{D}x(t)$$

$$= \int \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t \left[\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x(t))\right]\right) \mathrm{D}x(t) = \ddots$$

Change of variable $it = \tau$, $\mathrm{d}t = -i\mathrm{d}\tau$ yields

$$\ddots = \int \exp\left(-\frac{1}{\hbar}\int_{\tau_a}^{\tau_b} \mathrm{d}\tau \left[\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + V(x(\tau))\right]\right) \mathrm{D}x(\tau)$$

Euclidean action 2

We recognize the classical **Hamiltonian**

$$H(\dot{x}, x) = \frac{m}{2}\dot{x}^2 + V(x)$$

Therefore we define

Euclidean action

$$S_E[x(\tau)] = \int_{\tau_a}^{\tau_b} H(\dot{x}(\tau), x(\tau))\mathrm{d}\tau$$

Finally

$$\langle x'|e^{-\beta\hat{H}}|x'\rangle = \int \exp\left(-\frac{1}{\hbar}S_E[x(\tau)]\right) \mathrm{D}x(\tau)$$

Euclidean action 3

The partition function becomes

Partition function ⇔ Path integral

$$Z = \int \mathrm{d}x' \int \exp\left(-\frac{1}{\hbar} S_E[x(\tau)]\right) \mathrm{D}x(\tau)$$

provided PBCs and $\beta\hbar = iT$

- Integration over x' ensures all possible paths are considered
- Practically one computes

$$\langle x | e^{-\beta \hat{H}} | x \rangle = K(b, a)|_{T=-i\beta\hbar}$$

Harmonic oscillator 1

Remember!

$$K(b,a) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} \cdot \exp\left(\frac{im\omega}{2\hbar\sin(\omega T)}\left[(x_a^2 + x_b^2)\cos(\omega T) - 2x_a x_b\right]\right)$$

We want to substitute $T = -i\hbar\beta$. Use properties

$$\begin{cases} \sin(ix) = i\sinh(x) \\ \cos(ix) = \cosh(x) \end{cases}$$

Harmonic oscillator 2

We obtain

$$\langle x|e^{-\beta\hat{H}}|x\rangle = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}}\exp\left(-\frac{m\omega x^2}{\hbar\sinh(\beta\hbar\omega)}\left[\cosh(\beta\hbar\omega)-1\right]\right)$$

We compute the integral

$$\begin{aligned} Z &= \int \mathrm{d}x\,\langle x|e^{-\beta\hat{H}}|x\rangle = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}}\sqrt{\frac{\pi\hbar\sinh(\beta\hbar\omega)}{m\omega(\cosh(\beta\hbar\omega)-1)}} \\ &= \cdots \\ &= \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} = \sum_{n=0}^{\infty}\exp\left(-\beta\hbar\omega\left(n+\frac{1}{2}\right)\right) \end{aligned}$$

Harmonic oscillator 3

Indeed we obtain

$$Z = \sum_{n=0}^{\infty} \exp\left(-\beta\hbar\omega\left(n+\frac{1}{2}\right)\right) = \sum_{n=0}^{\infty} e^{-\beta E_n}$$

with the **energy spectrum**

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right)$$

Remember!

$$Z = \mathrm{Tr}(\hat{\rho}) = \sum_n \langle n| e^{-\beta\hat{H}} |n\rangle = \sum_n e^{-\beta E_n} \qquad \hat{H}\,|n\rangle = E_n\,|n\rangle$$

Topics of the presentation

Topics of the presentation

Initial definitions

Physical system of interest

Particle of energy E in a 1D time-independent potential $V(x)$

- **Local momentum** (squared)

$$p(x)^2 = 2m(E - V(x))$$

- **Local wavevector**

$$k(x) = \frac{p(x)}{\hbar}$$

- **Local de Broglie wavelength**

$$\lambda(x) = \frac{2\pi}{k(x)} = \frac{2\pi\hbar}{p(x)}$$

Criterion of validity

We will show that it must be

WKB criterion 1

$$\lambda(x) \ll L$$

L characteristic length scale for $V(x)$ variation

or equivalently

WKB criterion 2

$$\left|\frac{\mathrm{d}\lambda}{\mathrm{d}x}\right| = 2\pi\hbar\left|\frac{p'(x)}{p(x)}\right| \sim \lambda\left|\frac{V'(x)}{E - V(x)}\right| \ll 1$$

Topics of the presentation

Derivation of the WKB wavefunction 1

Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\psi(x)=E\psi(x)$$

put in the form

$$\hbar^2\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2}+p(x)^2\right]\psi(x)=0$$

Remember!

$$p(x)^2=2m(E-V(x))$$

Derivation of the WKB wavefunction 2

Eikonal $S(x)$ defined such that

$$\psi(x) = e^{iS(x)/\hbar}$$

Schrödinger equation becomes

$$\left(\frac{\mathrm{d}S}{\mathrm{d}x}\right)^2 - i\hbar\frac{\mathrm{d}^2 S}{\mathrm{d}x^2} = p(x)^2$$

Semiclassical expansion of eikonal

$$S(x) = \sum_{j=0}^{\infty} \hbar^j S_j(x) = S_0 + \hbar S_1 + \hbar^2 S_2 + \ldots$$

Derivation of the WKB wavefunction 3

Group orders of $\hbar^j$ to get tower of ODEs

$$\hbar^0 : \qquad \left(\frac{\mathrm{d}S_0}{\mathrm{d}x}\right)^2 = p(x)^2$$

$$\hbar^1 : \qquad 2\frac{\mathrm{d}S_0}{\mathrm{d}x}\frac{\mathrm{d}S_1}{\mathrm{d}x} = i\frac{\mathrm{d}^2 S_0}{\mathrm{d}x^2}$$

$$\hbar^2 : \qquad 2\frac{\mathrm{d}S_0}{\mathrm{d}x}\frac{\mathrm{d}S_2}{\mathrm{d}x} = -\left(\frac{\mathrm{d}S_1}{\mathrm{d}x}\right)^2 + i\frac{\mathrm{d}^2 S_1}{\mathrm{d}x^2}$$

$$\hbar^{j\geq 3} : \qquad \ldots$$

(A recurrence relation can be derived)

Derivation of the WKB wavefunction 4

Solutions for each ODE are

$$\hbar^0 : \qquad S_0(x) = \pm \int_{x_0}^{x} p(y)\mathrm{d}y$$

$$\hbar^1 : \qquad S_1(x) = \frac{1}{i} \ln \left(\frac{1}{\sqrt{p(x)}} \right) + \text{const.}$$

$$\hbar^2 : \qquad S_2(x) = \int_{x_0}^{x} \frac{3p'(x)^2 - 2p(y)p''(y)}{8p(y)^3} \mathrm{d}y = O\left(\frac{\lambda}{L}\right)$$

WKB criterion 1

At second order in $\hbar$, WKB valid only when $\lambda(x) \ll L$

The WKB wavefunction 1

WKB wavefunction

$$\psi_\pm(x) = e^{i(S_0(x)+\hbar S_1(x))/\hbar} = \frac{1}{\sqrt{p(x)}} \exp\left(\pm\frac{i}{\hbar}\int_{x_0}^{x} p(y)\mathrm{d}y\right)$$

Approximation breaks down at **turning points** x^*

$$p(x^*) = \sqrt{2m(E - V(x^*))} = 0 \quad \Leftrightarrow \quad V(x^*) = E$$

WKB criterion 2

$$\lambda\left|\frac{V'(x)}{E - V(x)}\right| \ll 1$$

The WKB wavefunction 2

- If $E > V(x)$

$$\psi_{\pm}(x) = \frac{1}{\sqrt{p(x)}} \exp\left(\pm \frac{i}{\hbar} \int_{x_0}^{x} p(y)\mathrm{d}y\right)$$

- If $E < V(x)$

$$\psi_{\pm}(x) = \frac{1}{\sqrt{|p(x)|}} \exp\left(\pm \frac{1}{\hbar} \int_{x_0}^{x} |p(y)|\mathrm{d}y\right)$$

Remember!

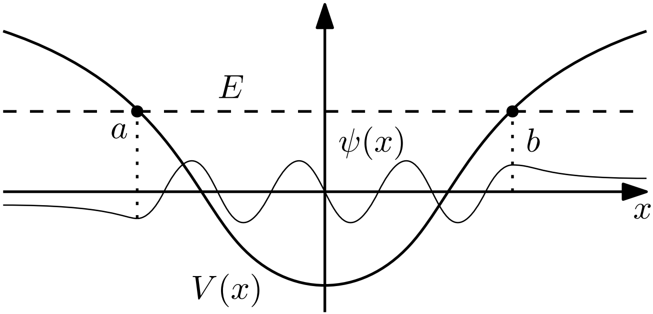
If $E < V(x)$ then

$$p(x) = \sqrt{2m(E - V(x))} = \sqrt{-2m|E - V(x)|} = \pm i|p(x)|$$

Topics of the presentation

Stitching solutions together 1

- $a < x < b$: oscillatory solution
- $x < a$ or $x > b$: exponential decay



Focus on turning point $b = x_0$, can get a by analogy

Stitching solutions together 2

We have two cases

- If $x < b$

$$\psi(x) = \frac{C_1}{\sqrt{p}} \exp\left(\frac{i}{\hbar}\int_b^x p(y)\mathrm{d}y\right) + \frac{C_2}{\sqrt{p}} \exp\left(-\frac{i}{\hbar}\int_b^x p(y)\mathrm{d}y\right)$$

- If $x > b$

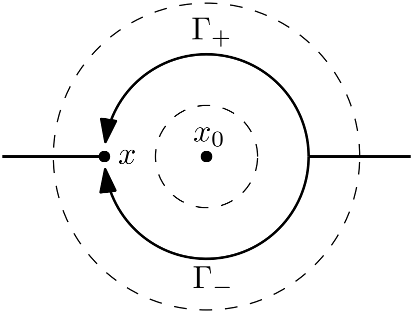
$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar}\int_b^x |p(y)|\mathrm{d}y\right)$$

with $C, C_1, C_2 \in \mathbb{C}$

Contouring the turning point

Can't just match C, C_1, C_2 at $x_0 = b$

- Allow $x, x_0 \in \mathbb{C}$
- Analytically extend $p(x), V(x)$ on complex plane
- Linearly approximate $E - V(x)$



Contouring the turning point 3

We find

$$|p(x)| \xrightarrow{\Gamma_\pm} p(x)e^{\pm i\pi/2}$$

Remember!

- If $x > b$

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar}\int_b^x |p(y)|\mathrm{d}y\right)$$

- If $x < b$

$$\psi(x) = \frac{C_1}{\sqrt{p}} \exp\left(\frac{i}{\hbar}\int_b^x p(y)\mathrm{d}y\right) + \frac{C_2}{\sqrt{p}} \exp\left(-\frac{i}{\hbar}\int_b^x p(y)\mathrm{d}y\right)$$

Contouring the turning point 4

Therefore

$$\begin{aligned} \Gamma_+ &\quad \rightarrow \quad C_2 = Ce^{-i\pi/4} \\ \Gamma_- &\quad \rightarrow \quad C_1 = Ce^{i\pi/4} \end{aligned}$$

and finally for $x < b$

$$\begin{aligned} \psi(x) &= \frac{C_1}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar}\int_b^x p(y)\mathrm{d}y\right) + \frac{C_2}{\sqrt{p(x)}} \exp\left(-\frac{i}{\hbar}\int_b^x p(y)\mathrm{d}y\right) \\ &= \frac{2C}{\sqrt{p(x)}} \cos\left(\int_b^x \frac{p(y)}{\hbar}\mathrm{d}y + \frac{\pi}{4}\right) \end{aligned}$$

Connection rules 1

At turning point $x_0 = b$ we have

Connection rules at $x_0 = b$

- If $x < b$

$$\psi(x) = \frac{2C}{\sqrt{p(x)}} \cos\left(\int_b^x \frac{p(y)}{\hbar} \mathrm{d}y + \frac{\pi}{4}\right)$$

- If $x > b$

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar} \int_b^x |p(y)| \mathrm{d}y\right)$$

Connection rules 2

By analogy, at turning point $x_0 = a$ we have

Connection rules at $x_0 = a$

- If $x > a$

$$\psi(x) = \frac{2C}{\sqrt{p(x)}} \cos\left(\int_a^x \frac{p(y)}{\hbar} \mathrm{d}y - \frac{\pi}{4}\right)$$

- If $x < a$

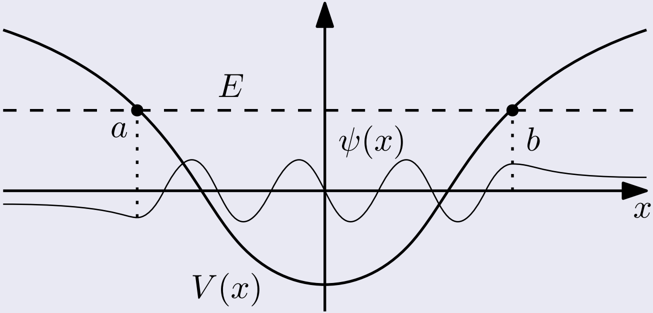
$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} \exp\left(+\frac{1}{\hbar} \int_a^x |p(y)| \mathrm{d}y\right)$$

Topics of the presentation

Derivation of the Born-Sommerfeld quantization rule 1

Let's apply the connection rules to a potential well

Remember!



Derivation of the Born-Sommerfeld quantization rule 2

- If $x > a$ at $x_0 = a$

$$\psi(x) = \frac{2C}{\sqrt{p(x)}} \cos\left(\int_a^x \frac{p(y)}{\hbar}\mathrm{d}y - \frac{\pi}{4}\right)$$

- If $x < b$ at $x_0 = b$

$$\psi(x) = \frac{2C}{\sqrt{p(x)}} \cos\left(\int_b^x \frac{p(y)}{\hbar}\mathrm{d}y + \frac{\pi}{4}\right)$$

$$\cos\left(\int_a^x \frac{p(y)}{\hbar}\mathrm{d}y - \frac{\pi}{4}\right) = \pm\cos\left(\int_b^x \frac{p(y)}{\hbar}\mathrm{d}y + \frac{\pi}{4}\right)$$

Therefore for $n \in \mathbb{N}$

$$\int_a^x \frac{p(y)}{\hbar}\mathrm{d}y - \frac{\pi}{4} = \int_b^x \frac{p(y)}{\hbar}\mathrm{d}y + \frac{\pi}{4} + n\pi$$

Born-Sommerfeld quantization rule

Born-Sommerfeld quantization rule

$$\int_a^b p(x)\mathrm{d}x = \pi\hbar\left(n+\frac{1}{2}\right)$$

n number of half-waves $\Leftrightarrow$ n number of nodes of ψ

- WKB criterion implies $n \gg 1$
- For example, harmonic oscillator gives exact result

$$\begin{cases} V(x) = \dfrac{1}{2}m\omega^2x^2 \\ b = -a = \sqrt{\dfrac{2E}{m\omega^2}} \end{cases} \quad \Rightarrow \quad E = \hbar\omega\left(n+\frac{1}{2}\right)$$

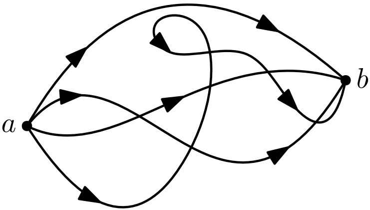
Topics of the presentation

End of the presentation 1

In this presentation we learned about

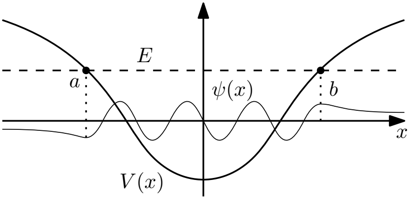
Path integrals

$$\int \exp\left(\frac{i}{\hbar}S[x(t)]\right)\, \mathrm{D}x(t)$$



Semiclassical approximation

$$\psi(x) = \exp\left(\frac{i}{\hbar}S(x)\right)$$



End of the presentation 2

Thank you for your attention!

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