

Title: PSI 2019/2020 - Quantum Theory (Dupuis) - Lecture 10

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Propagator as PI on the configuration space

Starting point: time-evolution operator in the position rep.

Schrödinger picture $=$ propagator $= \langle x'' | U(\tau'', \tau) | x' \rangle$
 $= K(x'', \tau''; x', \tau)$

$\boxed{V=0}$ $K(x'', \tau''; x', \tau) = \left(\frac{m}{2\pi\hbar(\tau'' - \tau)} \right)^{1/2} e^{-\frac{(x'' - x')^2 m}{2\hbar(\tau'' - \tau)}}$

— H time independent $U(z'', z') = e^{-\frac{(z'' - z')H}{\hbar}}$
→ Wick rotation ($t \rightarrow -i\tau$)

$$\psi(x, \tau) = e^{-\frac{(\tau - \tau')}{\hbar} H} \psi(x, \tau')$$

$$H = \frac{p^2}{2m} + \alpha V(x).$$

$$\boxed{V \neq 0}$$

General strategy? $\rightarrow$ divide the time interval into N steps

use two properties

- time-evolution eq for H

$$U(\tau'', \tau') = U(\tau'', \tau) U(\tau, \tau')$$
- Convolution property of the propagator

al into N equal subintervals: $\varepsilon = \frac{\tau'' - \tau'}{N}$ ($N \rightarrow \infty, \varepsilon \rightarrow 0$)

eg for H time independent

$$K(\tau') = U(\tau'', \tau) U(\tau, \tau') \quad \tau' < \tau < \tau''$$

property of the kernel/propagator

$$K(x'', \tau''; x', \tau') = \int_{-\infty}^{\infty} dx K(x'', \tau''; x, \tau) K(x, \tau; x', \tau')$$

$$U = e^{\frac{-(a+b)\hbar}{\hbar}} = e^{-a\hbar} e^{-b\hbar}$$

$$H = \frac{p^2}{2m} + \alpha V(x)$$

dependent $U(z'', z') = e^{\frac{-(z'' - z')\hbar}{\hbar}}$
 on $(t \rightarrow -i\tau)$

any time interval $(z'' - z')$

nal strategy? $\rightarrow$ divide the time interval into N equal subintervals: $\varepsilon = \frac{\tau'' - \tau'}{N}$

use two properties

- time-evolution op for H time independent

$$U(\tau'', \tau') = U(\tau'', \tau) U(\tau, \tau') \quad \tau' < \tau < \tau''$$
- convolution property of the kernel/propagator $K(x'', \tau''; x', \tau')$

$$\rightarrow K(x'', \tau''; x', \tau') = \int \prod_{i=1}^{N-1} dx_i \left(K(x_i, \tau_i, x_{i-1}, \tau_{i-1}) \right) K(x'', \tau'', x_{N-1}, \tau_{N-1})$$

$$U(z'', z') = U(z'', z) U(z, z') \quad z' > z > z''$$

• Convolution property of the kernel/propagator $K(x'', z''; x', z')$

$$K(x'', z''; x', z') = \int \frac{dx_i}{i\hbar} \underbrace{K(x_i, z_i; x_{i-1}, z_{i-1})}_{\rightarrow \langle x_i | e^{-\frac{\epsilon}{\hbar} H} | x_{i-1} \rangle} K(x'', z'', x_{N-1}, z_{N-1})$$

$$K(x'', z''; x', z') = \int_{-\infty}^{\infty} dx K(x'', z''; x, z) K(x, z; x', z')$$

$$(x'', z'', x_{N-1}, z_{N-1})$$

- ① study $K(x_n, z_n; x_{n-1}, z_{n-1})$.
- ② take limit $N \rightarrow \infty$?

$$\textcircled{1} \quad K(x_n, \tau_n; x_{n-1}, \tau_{n-1}) = \langle x_n | e^{-\frac{\epsilon}{\hbar} \left(\frac{p^2}{2m} + V(x) \right)}$$

$$= \langle x_n | 1 - \frac{i}{\hbar} \left(\frac{\hat{p}^2}{2m} + V(x) \right) | x_{n-1} \rangle$$

$$= \delta(x_n - x_{n-1}) - \frac{i}{\hbar} \langle x_n | \frac{\hat{p}^2}{2m} + V | x_{n-1} \rangle$$

$$= \int dp \langle x_n | \frac{p^2}{2m} + V | p \rangle \langle p | x_{n-1} \rangle$$

$$\left(\frac{\hat{p}^2}{2m} + V(x) \right) |x_{n-1}\rangle$$

$$= \frac{1}{2\pi\hbar} \int dp \langle x_n | \frac{p^2}{2m} + V(x) | p \rangle \langle p | x_{n-1} \rangle$$

$$= \frac{1}{2\pi\hbar} \int dp \left(\frac{p^2}{2m} + V(x_n) \right) e^{\frac{i}{\hbar}(x_n - x_{n-1})p}$$

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

$$\left(\frac{\hat{p}^2}{2m} + V(x) \right) |x_{n-1}\rangle + O(\epsilon^2)$$

$$- \frac{\epsilon}{\hbar} \langle x_n | \frac{\hat{p}^2}{2m} + V | x_{n-1} \rangle$$

$$= \int dp \langle x_n | \frac{\hat{p}^2}{2m} + V | p \rangle \langle p | x_{n-1} \rangle$$

$$= \frac{1}{2\pi\hbar} \int dp \left(\frac{p^2}{2m} + V(x_n) \right) e^{\frac{i}{\hbar}(x_n - x_{n-1})p}$$

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

$$\begin{aligned}
 \langle x_n | \hat{U} | x_{n-1} \rangle &= \langle x_n | 1 - \frac{\varepsilon}{\hbar} \left(\frac{\hat{p}^2}{2m} + V(x) \right) | x_{n-1} \rangle + \mathcal{O}(\varepsilon^2) \\
 &= \delta(x_n - x_{n-1}) - \frac{\varepsilon}{\hbar} \underbrace{\langle x_n | \frac{\hat{p}^2}{2m} + V | x_{n-1} \rangle}_{= \int dp \langle x_n | \frac{\hat{p}^2}{2m} + V(x) | p \rangle \langle p | x_{n-1} \rangle} \\
 &= \frac{1}{2\pi\hbar} \int dp \left(\frac{\hat{p}^2}{2m} + V(x_n) \right) e^{-\frac{ip(x_n - x_{n-1})}{\hbar}} \\
 &= \frac{1}{2\pi\hbar} \int dp \left(\frac{p^2}{2m} + V(x_n) \right) e^{-\frac{ip(x_n - x_{n-1})}{\hbar}} + \mathcal{O}(\varepsilon^2)
 \end{aligned}$$

$$K(x_n, \tau_n; x_{n-1}, \tau_{n-1}) = \frac{1}{2\pi\hbar} \int dp e^{ip/\hbar (x_n - x_{n-1})} \left[e^{-\frac{\epsilon}{\hbar} \left(\frac{p^2}{2m} + V(x_n) \right)} \right]$$

$$\begin{aligned}
 &= \frac{1}{2\pi\hbar} \int dp \, e^{ip/\hbar(x_n - x_{n-1})} \left[e^{-\frac{\epsilon}{\hbar} \left(\frac{p^2}{2m} + V(x_n) \right)} + \mathcal{O}(\epsilon^2) \right] \\
 &= \left(\frac{m}{2\pi\hbar\epsilon} \right)^{1/2} e^{-\frac{(x_n - x_{n-1})^2 m}{2\hbar\epsilon} - \frac{\epsilon}{\hbar} V(x_n) + \mathcal{O}(\epsilon^2)}.
 \end{aligned}$$

V indpt of p
 $\downarrow$

$$K(x_n, \tau_n; x_{n-1}, \tau_{n-1}) = \frac{1}{2\pi\hbar} \int dp e^{ip/\hbar (x_n - x_{n-1})} \left[e^{-\frac{\epsilon}{\hbar} \left(\frac{p}{2m} \right)^2} \right]$$

$$K(x_n, \tau_n; x_{n-1}, \tau_{n-1}) = \left(\frac{m}{2\pi\hbar\epsilon} \right)^{1/2} e^{-\frac{(x_n - x_{n-1})^2 m}{2\hbar\epsilon} - \frac{\epsilon}{\hbar}}$$

$$e^{-\frac{1}{\hbar} S_E(x, \varepsilon)}$$

"Euclidean" $\leftrightarrow$ Wick rotation.

$$S_E(x, \varepsilon) = \sum_{k=1}^N \frac{m}{2} \frac{(x_k - x_{k-1})^2}{\varepsilon} + \varepsilon V(x_k).$$

$\hookrightarrow$ factorize by ε , take $\varepsilon \rightarrow 0$

$$\lim_{\varepsilon \rightarrow 0} S_E(x, \varepsilon) = \int_{\tau}^{\tau''} d\tau \left(\frac{m}{2} \left(\frac{dx(\tau)}{d\tau} \right)^2 + V(x(\tau)) \right) := S_E(x).$$

Euclidean
action.

$$\textcircled{2} \quad \left[K(x'', \tau''; x', \tau') = \lim_{N \rightarrow \infty} \int \left(\frac{m}{2\pi \hbar \epsilon} \right)^{N/2} \prod_{n=1}^{N-1} dx_n \cdot e^{-\frac{1}{\hbar} S} \right]$$

$\rightarrow$ factorize

• Propagator as P I on the configuration space

"formal" limit
 $\Rightarrow$

$$K(x'', z'', x', z') = \int_{\substack{x(z'') = x'' \\ x(z') = x'}} dx[z]$$

in space

$$U(x', x'') = \int_{\substack{x(\tau'') = x'' \\ x(\tau') = x'}} dx[\tau] \cdot e^{\frac{i}{\hbar} S_E(x)}$$

Configuration
path integral

$$x_{n-1}, x_{n-1}, x_{n-1} = (2\pi\hbar\epsilon)$$

$$(\tau; x, \tau) = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\hbar\epsilon} \right)^N \prod_{n=1}^N dx_n e^{-\frac{m}{2\hbar\epsilon} \sum_{n=1}^N (x_n - x_{n-1})^2}$$

Euclidean $\leftarrow$

$$S_E(x, \epsilon) = \sum_{k=1}^N \frac{m}{2} \dot{x}_k^2$$

! entering
in $dx[\tau]$

factorize by ϵ , take ϵ

$$\lim_{\epsilon \rightarrow 0} S_E(x, \epsilon)$$

$\ominus$ divergent when $N \rightarrow \infty$
 $\oplus$ undpt of V $\leftarrow$ normalization by dividing $\frac{1}{\int dx} \int dx V=0$

$$-aH - bH.$$

$$e^{-bH}.$$

configuration

with integral.

inverse Wick rotation

$$\langle x'' | U(t'', t') | x' \rangle = \int d\alpha[t] e^{\frac{i}{\hbar} S(x)}$$

$$H = \frac{p^2}{2m} + \alpha V(x).$$

$$S(x) = \int_{t'}^{t''} dt \left[\frac{1}{2} m \left(\frac{dx}{dt} \right)^2 - V(x) \right]$$

$\oplus$ undpt of $V \leftarrow$ norm

ex. Free particle. $V=0$

$$K(x'', \tau'', x', \tau') = \lim_{N \rightarrow \infty} \int \left(\frac{m}{2\pi\hbar\epsilon} \right)^{N/2}$$

normalization
 condition $\int |\psi|^2 dx = 1$

$$\left(\frac{m}{2\pi\hbar\epsilon} \right)^{N/2} \prod_{n=1}^{N-1} dx_n e^{-\frac{1}{\hbar} \sum_{k=1}^N \frac{m(x_k - x_{k-1})^2}{2\epsilon}}$$

$$\sum_{k=1}^N \frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon}$$

$$x_0 = x'$$

$$x_N = x''$$

↑ many
coupled Gaussian
integrals.

(see Tutorial 6).

$$= \lim_{N \rightarrow \infty} \int \left(\frac{m}{2\pi \hbar \epsilon} \right)^{N/2} \prod_{n=1}^{N-1} dx_n e^{-\frac{1}{\hbar} \sum_{k=1}^{N-1} \epsilon \left(\frac{dx_k}{dt} \right)^2}$$

$$= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi \hbar \epsilon} \right)^{N/2} \frac{1}{\sqrt{N}} \left(\frac{2\pi \epsilon \hbar}{m} \right)^{(N-1)/2}$$

$$e^{-\frac{1}{\hbar} \sum_{k=1}^N \frac{m}{2} \frac{(x_k - x_{k-1})^2}{\epsilon}}$$

$$x_0 = x'$$

$$x_N = x''$$

↑ many coupled Gaussian integrals.

(see Tutorial)

$$\left(\frac{2\pi\epsilon\hbar}{m} \right)^{(N-1)/2}$$

$$e^{-m(x'' - x')^2 / 2N\hbar\epsilon}$$

$$\left(\frac{m}{2\pi\hbar\epsilon} \right)^{N/2} \prod_{n=1}^N dx_n e^{-\frac{m}{2\hbar\epsilon} x_n^2} \quad \text{many coupled G}$$

$$\left(\frac{m}{2\pi\hbar\epsilon} \right)^{N/2} \frac{1}{\sqrt{N}} \left(\frac{2\pi\epsilon\hbar}{m} \right)^{(N-1)/2} e^{-\frac{m}{2N\hbar\epsilon} (x'' - x')^2}$$

$$\left(\frac{m}{2\pi\hbar(N\epsilon)} \right)^{1/2} e^{-\frac{m}{2(N\hbar\epsilon)} (x'' - x')^2} \quad T = N\epsilon = \tau'' - \tau'$$

For $V=0$,

$$K = \left(\frac{m}{2\pi\hbar T} \right)^{1/2} e^{-\frac{(x''-x')^2}{2\hbar T} m}$$

$\searrow \frac{1}{\hbar} \left(T \cdot \frac{1}{2} m \left(\frac{x''-x'}{T} \right)^2 \right)$

$\oplus$ undp: $\frac{1}{V}$ by dividing $P \pm \frac{1}{V}$

$$\text{For } V=0, \quad K = \left(\frac{m}{2\pi\hbar T} \right)^{1/2} e^{-\frac{(x''-x')^2}{2\hbar T} m}$$

$\rightarrow \frac{1}{\hbar} \left(T \cdot \frac{1}{2} m \left(\frac{x''-x'}{T} \right)^2 \right)$

$$= \left(\frac{m}{2\pi\hbar T} \right)^{1/2} e^{-\frac{(x''-x')^2}{2\hbar T} m}$$

$$\rightarrow \frac{1}{\hbar} \left(T \cdot \frac{1}{2} m \left(\frac{x''-x'}{T} \right)^2 \right)$$

$$K = \underbrace{\left(\frac{m}{2\pi\hbar T} \right)^{1/2}}_{\text{classical solution}} e^{-S_E(x_c)}$$

$$e^{-\frac{(x''-x')}{2\hbar T} m} \rightarrow \frac{1}{\hbar} \left(T \cdot \frac{1}{2} m \left(\frac{x''-x'}{T} \right)^2 \right) = S(x_c)$$

$e^{-S_E(x_c)}$
 $\uparrow$ classical solution
 $\hookrightarrow$ general feature

TODAY

• Propagator as path
integral on the
configuration space.

• Semi-classical expansion.

↓
→ Gaussian integral
→ Functional derivative.

$F[\varrho], \frac{\delta F}{\delta \varrho}$ defined

TODAY

by $\int \frac{\delta F}{\delta \varrho}(x) \phi(x) dx$

$$= \lim_{\varepsilon \rightarrow 0} \frac{F(\varrho + \varepsilon \phi) - F(\varrho)}{\varepsilon}$$

$$= \left. \frac{d}{d\varepsilon} F(\varrho + \varepsilon \phi) \right|_{\varepsilon=0}$$

• Propagator
integrals

• Semi-classical

→ G
→ F

classical expansion

$$S_E(x) = \int_{\tau'}^{\tau''} d\tau \left[\frac{m}{2} \dot{x}^2(\tau) + V(x(\tau)) \right]$$

classical solution: $x_c(\tau)$ such that $x_c(\tau'') = x''$, $x_c(\tau') = x'$

$$\rightarrow \frac{\delta S_E[x_c]}{\delta x(\tau)} = 0$$

partition

$$\int_{\tau_1}^{\tau_2} d\tau \left[\frac{m}{2} \dot{x}^2(\tau) + V(x(\tau)) \right]$$

classical solution: $x_c(\tau)$ such that $x_c(\tau_1) = x_1$, $x_c(\tau_2) = x_2$

$$\rightarrow \frac{\delta S_E[x_c]}{\delta x(\tau)} = 0$$

$$x(\tau) = x_c(\tau) + \sqrt{\hbar} u(\tau)$$

↳ fluctuation

$$u(\tau') = u(\tau'') = 0$$

$$\hbar^{-1} S_E[x] = \hbar^{-1} S_E[x_c] + \frac{1}{\sqrt{\hbar}} \int u(\tau) \left. \frac{\delta S}{\delta x(\tau)} \right|_{x=x_c} d\tau$$

$$\begin{array}{l}
 \delta x(c) |_{x=x_c} \\
 \\
 (\tau_2) \quad \frac{\delta^2 S}{\delta x(\tau_1) \delta x(\tau_2)} \Big|_{x=x_c} \\
 \\
 d\tau \quad u(\tau_1) u(\tau_2) u(\tau_3) \quad \frac{\delta^3 S}{\delta x(\tau_1) \delta x(\tau_2) \delta x(\tau_3)} \Big|_{x=x_c} + O(h)
 \end{array}$$

$$\sqrt{h} u(\tau)$$

↳ fluctuation

$$u(\tau') = u(\tau'') = 0.$$

$$\int u(\tau) \frac{\delta S}{\delta x(\tau)} \bigg|_{x=x_c} d\tau$$

$$\frac{\delta^2 S}{\delta x^2}$$

expansion:

$$K(z'', \tau''; z', \tau') = \mathcal{N} e^{-\frac{1}{\hbar} S_E(z_c)} \int_{u(z')=u(z'')=0} du[z].$$

$$= dP e^{-\frac{1}{\hbar} S_E(x_c)} \int_{u(z')=u(z'')=0} du[z] e^{-\frac{1}{2} \frac{\delta^2 S_E}{\delta x^2} u^2} [1 + O(\hbar)]$$

$$K(x'', \tau'', x', \tau') = \mathcal{D} e^{-\frac{1}{\hbar} S_E[x]} \int u(z') = u(z'') =$$

$$\frac{\delta^2 S_E}{\delta x(\tau_1) \delta x(\tau_2)} \Big|_{x=x_c}$$

$$\frac{\delta^3 S_E}{\delta x(\tau_1) \delta x(\tau_2) \delta x(\tau_3)} \Big|_{x=x_c}$$

$$u(z') = u(z'') = 0$$

in general?

case of HO?

$$e^{2\sqrt{\delta x^2}} [1 + O(\hbar)]$$

$$\frac{\delta}{\delta q(z)} \left(\frac{d q(z)}{d p} \right) = - \frac{2p}{(12-2)\delta}$$