

**week12: Kapitel 4: Herleitung der Lagrange-Funktion
aus der Quantenmechanik**
(nicht klausurrelevant)

We consider the motion of a quantum mechanical particle in 1 dimension under the influence of some potential $V(x)$. If the time zero initial state of the particle is given by the wavefunction $\psi_0 = \psi_0(x) \in L^2(\mathbb{R})$, then, according to the laws of quantum physics, the time evolved state at time t is given by the solution of the time dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi_t = H \psi_t \quad (1)$$

with Hamilton operator

$$H = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (2)$$

The solution of the time dependent Schrödinger equation (1) can be written as

$$\psi_t = e^{-\frac{i}{\hbar} t H} \psi_0 \quad (3)$$

If we discretize time with $t = t_k = kdt$ and use the notation $H = H_0 + V$, we can write in the limit $dt \rightarrow 0$:

$$\begin{aligned} \psi_{kdt} &= e^{-\frac{i}{\hbar} kdt H} \psi_0 = e^{-\frac{i}{\hbar} kdt (H_0 + V)} \psi_0 \\ &= \left(e^{-\frac{i}{\hbar} dt (H_0 + V)} \right)^k \psi_0 \\ &\stackrel{dt \rightarrow 0}{\equiv} \left(e^{-\frac{i}{\hbar} dt H_0} e^{-\frac{i}{\hbar} dt V} \right)^k \psi_0 \end{aligned} \quad (4)$$

Let's first consider the time evolution for a single time step dt . We have

$$\psi_{dt}(x) = \left(e^{-\frac{i}{\hbar} dt H_0} e^{-\frac{i}{\hbar} dt V} \psi_0 \right)(x) \quad (5)$$

Let's temporarily abbreviate

$$f(x) := \left(e^{-\frac{i}{\hbar} dt V} \psi_0 \right)(x) = e^{-\frac{i}{\hbar} dt V(x)} \psi_0(x) \quad (6)$$

Using the Fourier representation

$$f(x) = \int_{\mathbb{R}} \frac{dq}{2\pi} e^{ixq} \hat{f}(q) \quad (7)$$

with Fourier transform

$$\hat{f}(q) = \int_{\mathbb{R}} dx e^{-iqx} f(x) \quad (8)$$

we can write

$$\begin{aligned}
(e^{-\frac{i}{\hbar} dt H_0} f)(x) &= e^{-\frac{i}{\hbar} dt H_0} \int_{\mathbb{R}} \frac{dq}{2\pi} e^{ixq} \hat{f}(q) \\
&= \int_{\mathbb{R}} \frac{dq}{2\pi} e^{-\frac{i}{\hbar} dt \frac{\hbar^2 q^2}{2m}} e^{ixq} \hat{f}(q) \\
&= \int_{\mathbb{R}} \frac{dq}{2\pi} e^{-i \frac{\hbar}{m} dt \frac{q^2}{2}} e^{ixq} \hat{f}(q)
\end{aligned} \tag{9}$$

since

$$H_0 e^{ixq} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} e^{ixq} = \frac{\hbar^2 q^2}{2m} e^{ixq} \tag{10}$$

Thus we obtain

$$\begin{aligned}
(e^{-\frac{i}{\hbar} dt H_0} f)(x) &= \int_{\mathbb{R}} \frac{dq}{2\pi} e^{-i \frac{\hbar}{m} dt \frac{q^2}{2}} e^{ixq} \hat{f}(q) \\
&= \int_{\mathbb{R}} \frac{dq}{2\pi} e^{-i \frac{\hbar}{m} dt \frac{q^2}{2}} e^{ixq} \int_{\mathbb{R}} dy e^{-iqy} f(y) \\
&= \int_{\mathbb{R}} dy \int_{\mathbb{R}} \frac{dq}{2\pi} e^{-i \frac{\hbar}{m} dt \frac{q^2}{2}} e^{i(x-y)q} f(y)
\end{aligned} \tag{11}$$

Let's temporarily abbreviate

$$\alpha := \frac{\hbar}{m} dt \tag{12}$$

Then we can write

$$\begin{aligned}
\int_{\mathbb{R}} \frac{dq}{2\pi} e^{-i \frac{\hbar}{m} dt \frac{q^2}{2}} e^{i(x-y)q} &= \int_{\mathbb{R}} \frac{dq}{2\pi} e^{-i\alpha \frac{q^2}{2}} e^{i(x-y)q} \\
&= \int_{\mathbb{R}} \frac{dp}{2\pi\sqrt{\alpha}} e^{-i \frac{p^2}{2}} e^{i \frac{x-y}{\sqrt{\alpha}} p}
\end{aligned} \tag{13}$$

Now recall the Fresnel integral

$$\int_{\mathbb{R}} e^{-i\lambda\phi} e^{i\frac{\phi^2}{2}} \frac{d\phi}{\sqrt{2\pi i}} = e^{-i\frac{\lambda^2}{2}} \tag{14}$$

or

$$\int_{\mathbb{R}} e^{+i\lambda\phi} e^{-i\frac{\phi^2}{2}} \frac{d\phi}{\sqrt{2\pi(-i)}} = e^{+i\frac{\lambda^2}{2}} \tag{15}$$

with

$$\begin{aligned}
\sqrt{i} &:= e^{i\frac{\pi}{4}} \\
\sqrt{-i} &:= e^{-i\frac{\pi}{4}}
\end{aligned}$$

With

$$\lambda = \frac{x-y}{\sqrt{\alpha}} \tag{16}$$

we obtain

$$\begin{aligned}
\int_{\mathbb{R}} \frac{dq}{2\pi} e^{-i\frac{\hbar}{m} dt \frac{q^2}{2}} e^{i(x-y)q} &= \int_{\mathbb{R}} \frac{dp}{2\pi\sqrt{\alpha}} e^{-i\frac{p^2}{2}} e^{i\frac{x-y}{\sqrt{\alpha}} p} \\
&= \frac{1}{2\pi\sqrt{\alpha}} \sqrt{2\pi(-i)} e^{+i\frac{(x-y)^2}{2\alpha}} \\
&= \frac{1}{\sqrt{2\pi\alpha i}} e^{+i\frac{(x-y)^2}{2\alpha}} \\
&=: p_{\alpha}(x, y) = p_{\frac{\hbar}{m} dt}(x, y)
\end{aligned} \tag{17}$$

with Fresnel kernel $p_{\alpha}(x, y)$. Thus, with (11) and (17) we get

$$\begin{aligned}
(e^{-\frac{i}{\hbar} dt H_0} f)(x) &= \int_{\mathbb{R}} dy \int_{\mathbb{R}} \frac{dq}{2\pi} e^{-i\frac{\hbar}{m} dt \frac{q^2}{2}} e^{i(x-y)q} f(y) \\
&= \int_{\mathbb{R}} dy p_{\frac{\hbar}{m} dt}(x, y) f(y)
\end{aligned} \tag{18}$$

and we arrive at

$$\begin{aligned}
\psi_{dt}(x) &= (e^{-\frac{i}{\hbar} dt H_0} e^{-\frac{i}{\hbar} dt V} \psi_0)(x) \\
&= \int_{\mathbb{R}} dy p_{\frac{\hbar}{m} dt}(x, y) e^{-\frac{i}{\hbar} dt V(y)} \psi_0(y)
\end{aligned} \tag{19}$$

or, since we want to iterate this, we can use the notation

$$\psi_{dt}(x_1) = \int_{\mathbb{R}} dx_0 p_{\frac{\hbar}{m} dt}(x_1, x_0) e^{-\frac{i}{\hbar} dt V(x_0)} \psi_0(x_0) \tag{20}$$

Then,

$$\begin{aligned}
\psi_{2dt}(x_2) &= \left[(e^{-\frac{i}{\hbar} dt H_0} e^{-\frac{i}{\hbar} dt V})^2 \psi_0 \right](x_2) \\
&= \left[(e^{-\frac{i}{\hbar} dt H_0} e^{-\frac{i}{\hbar} dt V}) \psi_{dt} \right](x_2) \\
&= \int_{\mathbb{R}} dx_1 p_{\frac{\hbar}{m} dt}(x_2, x_1) e^{-\frac{i}{\hbar} dt V(x_1)} \psi_{dt}(x_1) \\
&= \int_{\mathbb{R}} dx_1 p_{\frac{\hbar}{m} dt}(x_2, x_1) e^{-\frac{i}{\hbar} dt V(x_1)} \int_{\mathbb{R}} dx_0 p_{\frac{\hbar}{m} dt}(x_1, x_0) e^{-\frac{i}{\hbar} dt V(x_0)} \psi_0(x_0) \\
&= \int_{\mathbb{R}^2} dx_1 dx_0 p_{\frac{\hbar}{m} dt}(x_2, x_1) p_{\frac{\hbar}{m} dt}(x_1, x_0) e^{-\frac{i}{\hbar} dt [V(x_1)+V(x_0)]} \psi_0(x_0)
\end{aligned} \tag{21}$$

and by induction on k , we arrive at the following representation

$$\begin{aligned}
\psi_{kdt}(x_k) &= \int_{\mathbb{R}^k} dx_{k-1} \cdots dx_0 p_{\frac{\hbar}{m} dt}(x_k, x_{k-1}) \cdots p_{\frac{\hbar}{m} dt}(x_1, x_0) e^{-\frac{i}{\hbar} dt [V(x_{k-1})+\cdots+V(x_0)]} \psi_0(x_0) \\
&= \int_{\mathbb{R}^k} \prod_{j=0}^{k-1} dx_j p_{\frac{\hbar}{m} dt}(x_{j+1}, x_j) e^{-\frac{i}{\hbar} dt \sum_{j=0}^{k-1} V(x_j)} \psi_0(x_0)
\end{aligned} \tag{22}$$

with Fresnel kernels

$$p_t(x, y) = \frac{1}{\sqrt{2\pi it}} e^{+i\frac{(x-y)^2}{2t}} \quad (23)$$

The Fresnel kernels have the following basic properties

$$\int_{\mathbb{R}} p_t(x, y) p_s(y, z) dy = p_{t+s}(x, z) \quad (24)$$

$$\int_{\mathbb{R}} p_t(x, y) dy = 1 \quad (25)$$

In particular because of the latter property, it is natural to leave the normalization factors $1/\sqrt{2\pi it}$ at the exponentials. To see how the Lagrange function emerges from the above representation, we separate the normalization factors and write

$$\begin{aligned} p_{\frac{\hbar}{m}dt}(x_k, x_{k-1}) \cdots p_{\frac{\hbar}{m}dt}(x_1, x_0) &= \prod_{j=0}^{k-1} p_{\frac{\hbar}{m}dt}(x_{j+1}, x_j) \\ &= \frac{1}{\left\{ 2\pi i \frac{\hbar}{m} dt \right\}^{\frac{k}{2}}} \exp \left\{ i \sum_{j=0}^{k-1} \frac{(x_{j+1} - x_j)^2}{2 \frac{\hbar}{m} dt} \right\} \\ &= \frac{1}{\left\{ 2\pi i \frac{\hbar}{m} dt \right\}^{\frac{k}{2}}} \exp \left\{ \frac{i}{\hbar} \sum_{j=0}^{k-1} \frac{m}{2} \left(\frac{x_{j+1} - x_j}{dt} \right)^2 dt \right\} \end{aligned} \quad (26)$$

Thus we obtain the representation

$$\begin{aligned} \psi_{kdt}(x_k) &= \int_{\mathbb{R}^k} dx_{k-1} \cdots dx_0 p_{\frac{\hbar}{m}dt}(x_k, x_{k-1}) \cdots p_{\frac{\hbar}{m}dt}(x_1, x_0) e^{-\frac{i}{\hbar} dt [V(x_{k-1}) + \cdots + V(x_0)]} \psi_0(x_0) \\ &= \int_{\mathbb{R}^k} \prod_{j=0}^{k-1} \frac{dx_j}{\left\{ 2\pi i \frac{\hbar}{m} dt \right\}^{\frac{1}{2}}} \exp \left\{ \frac{i}{\hbar} \sum_{j=0}^{k-1} \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{dt} \right)^2 - V(x_j) \right] dt \right\} \psi_0(x_0) \end{aligned} \quad (27)$$

This representation (27) is the Feynman path integral representation.