week13: Kapitel 4: Herleitung der Lagrange-Funktion aus der Quantenmechanik

(dieses Material ist nicht mehr 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

$$i\hbar \tfrac{\partial}{\partial t}\psi_t \;=\; H\,\psi_t \tag{1}$$

with Hamilton operator

$$H \;=\; \tfrac{p^2}{2m} \,+\, V(x) \;=\; -\tfrac{\hbar^2}{2m}\tfrac{\partial^2}{\partial x^2} \,+\, V(x) \tag{2}$$

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

$$\psi_t \;=\; e^{-\frac{i}{\hbar}tH}\,\psi_0 \tag{3}$$

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

$$\begin{aligned} \psi_{kdt} \;&=\; e^{-\frac{i}{\hbar}\,kdt\,H}\,\psi_0 \;=\; e^{-\frac{i}{\hbar}\,kdt\,(H_0+V)}\,\psi_0 \\ &=\; \left(e^{-\frac{i}{\hbar}\,dt\,(H_0+V)}\right)^k \psi_0 \\ &\overset{dt\to 0}{=}\; \left(e^{-\frac{i}{\hbar}\,dt\,H_0}\,e^{-\frac{i}{\hbar}\,dt\,V}\right)^k \psi_0 \end{aligned} \tag{4}$$

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

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

Let's temporarily abbreviate

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

Using the Fourier representation

$$f(x) \;=\; \int_{\mathbb{R}} \tfrac{dq}{2\pi}\,e^{ixq}\,\hat{f}(q) \tag{7}$$

with Fourier transform

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

we can write

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

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

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

Let's temporarily abbreviate

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

Then we can write

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

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

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

we obtain

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

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

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

and we arrive at

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

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

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

Then,

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

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

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

with Fresnel kernels

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

The Fresnel kernels have the following basic properties

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

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

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

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

Thus we obtain the representation

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

This representation (27) is the Feynman path integral representation. And the quantity in the exponent (with $t = t_k = kdt$ fixed),

$$\sum_{j=0}^{k-1} \Big[\, \tfrac{m}{2}\left(\tfrac{x_{j+1}-x_j}{dt}\right)^2 - V(x_j)\Big]\, dt \;\;\overset{dt\to 0}{\rightarrow}\;\; \textstyle\int_0^t \big[\, \frac{m}{2}\,(\dot{x}_s)^2 - V(x_s)\,\big]\, ds \;=\; \int_0^t L(x_s,\dot{x}_s)\, ds$$

can be considered as an integral over the classical Langangian.