2/21/2013

The same Hamiltonian is used in both CM and QM. Only difference in QM is that the Hamiltonian is converted to an operator.

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(t=0)\rangle$$

For a very short time (infinitesimal) period Δt, the exponential term can be expressed;

$$|\psi(\Delta t)\rangle = \left(\mathbb{1} - \frac{iH\Delta t}{\hbar}\right)|\psi(t=0)\rangle$$

Or

$$|\psi(t)\rangle = \left(\mathbb{1} - \frac{iHt}{\hbar n}\right)^n |\psi(t=0)\rangle$$

$$\Delta t = \frac{t}{n} \ , \quad n \to \infty$$

In this expression Hamiltonian looks like a constant. It works if $H(t_1) = H(t_2)$. However Hamiltonian can be dependent on the time. When H depends on time:

$$\left(\mathbb{1} - \frac{iHt}{\hbar n}\right)^n \to \cdots \left(\mathbb{1} - \frac{iH(2\Delta t)\Delta t}{\hbar}\right)\left(\mathbb{1} - \frac{iH(\Delta t)\Delta t}{\hbar}\right)\left(\mathbb{1} - \frac{iH(0)\Delta t}{\hbar}\right)$$

If

$$[H(t_1), H(t_2)] = 0 \quad \to \quad e^{-\frac{i}{\hbar}\int H dt}$$

Assume this is true. Then,

$$|\psi(t)\rangle = e^{-i\int Hdt/\hbar}|\psi(t=0)\rangle$$

$$\langle x|\psi(t)\rangle = \left\langle x\middle|e^{-i\int Hdt/\hbar}\middle|\psi(0)\right\rangle = \int dx' \left\langle x\middle|e^{-i\int Hdt/\hbar}\middle|x'\right\rangle\langle x'|\psi(0)\rangle$$

where $\left\langle x\middle|e^{-i\int Hdt/\hbar}\middle|x'\right\rangle = U(x,t;x',t=0)$

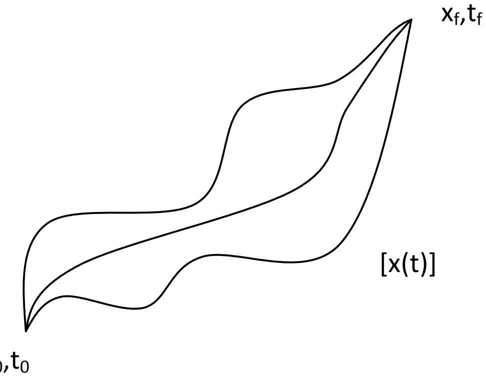
For

$$H = H_0 = \frac{p^2}{2m}$$

$$U = \sqrt{\frac{m}{2\pi\hbar i(t-t_0)}} \ e^{-(x-x')^2/2\left(\sqrt{i\hbar(t-t_0)/m}\right)^2}$$

We will try to find a different way to calculate the propagator U. Try Lagrangian instead of Hamiltonian. Lagrangian accommodates infinite coordinate system better than Hamiltonian.

Reformulating QM from Hamiltonian to Lagrangian



$L(x(t),\dot{x}(t),t) = L(t)$ is defined for every path [$x(t)$] that connects x_0 at time t_0 with x_f at time t_f.

$$\int_{t_0}^{t_f} \mathcal{L}(t)dt = S = S([x(t)])$$

The classical path will be make $S([x(t)])$ an extremum ("least action"). Note: *S* is not an operator even in quantum mechanics – it's just a functional that gives a number for each possible path. Now:

$$U = A\int_{\substack{all\\possible\\paths}} e^{\frac{i}{\hbar}S[x(t)]}d(path)$$

Check a couple of examples to see if it can be true or feasible.

<u>Example 1)</u> Free particle. CLAIM: In this case, the integral over all possible paths gives the same result as if we simply calculate the integrand for only ONE path, namely the classical one. In that case:

$$\mathcal{L} = \frac{m}{2}\dot{x}^2$$

$$U = Ae^{\frac{i}{\hbar}S[x_{classical}(t)]}$$

$$t = t_f - t_0$$

$$\dot{x} = \frac{x_f - x_0}{t}$$

$$\mathcal{L} = \frac{m}{2}\frac{(x_f - x_0)^2}{t^2}$$

$$S = \frac{m}{2}\frac{\left(x_f - x_0\right)^2}{\left(t_f - t_0\right)^2}\left(t_f - t_0\right) = \frac{m}{2}\frac{\left(x_f - x_0\right)^2}{\left(t_f - t_0\right)}$$

$$e^{i\frac{S}{\hbar}} = e^{\frac{im\left(x_f - x_0\right)^2}{2\hbar\ \left(t_f - t_0\right)}}$$

This is exactly what we already know is the right answer, if we assume that the normalization constant in this case is $A = \sqrt{\frac{m}{2\pi\hbar i(t-t_0)}}$.

Example 2)

$$\psi = e^{\frac{i}{\hbar}S[x(t)]}$$

$$\frac{\partial s}{\partial x} = p \qquad \rightarrow \qquad \frac{\partial s}{\partial x_f} = \frac{m}{2}\cdot 2\frac{\left(x_f - x_0\right)}{\left(t_f - t_0\right)} = mv$$

which agrees with the WKB method and our definition of the momentum as the derivative of the phase angle.

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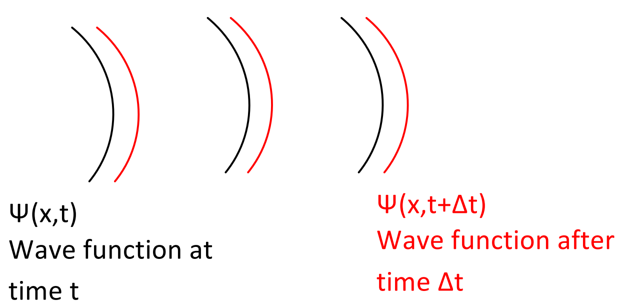


$$H = \frac{P^2}{2m} \quad , \quad x_{cl}(t) = v\Delta t$$

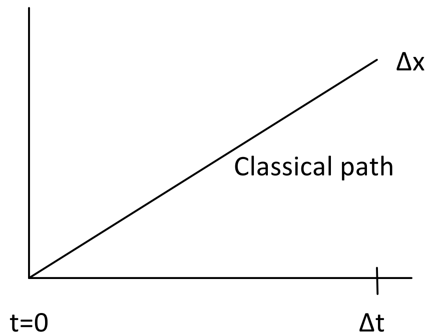
$$\mathcal{L}_{cl} = m\frac{v^2}{2} = \frac{m\Delta x^2}{2\Delta t^2}$$

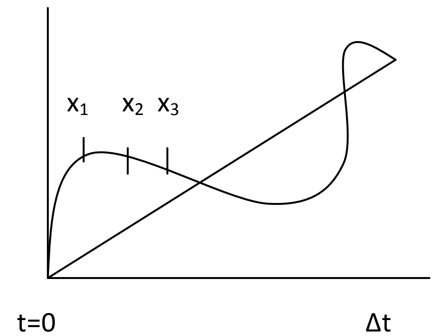
$$S_{cl} = \int_0^{\Delta t}\mathcal{L}\,dt' = \frac{m\Delta x^2}{2\Delta t}$$

Propagator;

$$A\int d[x(t)]\, e^{\frac{i}{\hbar}S[x(t)]} = \sqrt{\frac{m}{2\pi\hbar i\Delta t}}\, e^{\frac{i}{\hbar}\frac{m\Delta x^2}{2\Delta t}}$$

Integral of all paths turns out to be the same as the classical path. The phase factor gets larger as the deviation from the classical path becomes larger. These are cancelled out leaving the classical path alone.





x1, x2, and x3 are approximation, i.e., straight segment and Lagrangian is constant at each segment.

$$A\int dx_1\int dx_2\int dx_3 \cdots \int dx_{N-1}\; e^{\frac{im}{\hbar}\left[\frac{(x_1-x_0)^2}{\frac{2\Delta t}{N}}+\frac{(x_2-x_1)^2}{\frac{2\Delta t}{N}}+\frac{(x_3-x_2)^2}{\frac{2\Delta t}{N}}+\cdots+\frac{(x_N-x_{N-1})^2}{\frac{2\Delta t}{N}}\right]}$$

$$= A\int dx_1\int dx_2\, e^{\frac{im}{\hbar}\left[\frac{(x_1-x_0)^2}{\frac{2\Delta t}{N}}+\frac{(x_2-x_1)^2}{\frac{2\Delta t}{N}}\right]}\int dx_3 \cdots$$

$$= A\int dx_2\int dx_1\, e^{\frac{im}{2\hbar\Delta t/N}\left[{x_1}^2-2x_1x_0+{x_0}^2+{x_2}^2-2x_2x_1+{x_1}^2\right]}\int dx_3 \cdots$$

The exponent can be simplified;

$$\begin{aligned}
{x_1}^2-2x_1x_0+{x_0}^2+{x_2}^2-2x_2x_1+{x_1}^2 &= 2{x_1}^2-2x_1(x_0+x_2)+{x_0}^2+{x_2}^2 \\
&= 2\left({x_1}^2-x_1(x_0+x_2)+\frac{{x_0}^2}{2}+\frac{{x_2}^2}{2}\right) \\
&= 2\left({x_1}^2-2x_1\frac{(x_0+x_2)}{2}+\frac{(x_0+x_2)^2}{4}+\frac{{x_0}^2}{4}+\frac{{x_2}^2}{4}-\frac{2x_0x_2}{4}\right) \\
&= 2\left(x_1-\frac{(x_0+x_2)}{2}\right)^2+\frac{1}{2}(x_2-x_0)^2
\end{aligned}$$

$$A\int dx_2\int dx_1\, e^{\frac{im}{2\hbar\Delta t/N}[x_1{}^2-2x_1x_0+x_0{}^2+x_2{}^2-2x_2x_1+x_1{}^2]}\int dx_3\cdots$$

$$= A\int dx_2\int dx_1\, e^{-\frac{m}{\frac{\hbar i\Delta t}{N}}\left(x_1-\frac{(x_0+x_2)}{2}\right)^2} e^{-\frac{m}{\frac{4\hbar i\Delta t}{N}}(x_2-x_0)^2}\int dx_3\cdots$$

$$= A\sqrt{\frac{\frac{2\pi\hbar i\Delta t}{N}}{m}}\sqrt{\frac{1}{2}}\int dx_2\int dx_3\, e^{-\frac{m}{\frac{4\hbar i\Delta t}{N}}(x_2-x_0)^2} e^{\frac{im}{\frac{2\hbar\Delta t}{N}}(x_3-x_2)^2}\int dx_4\cdots$$

$$= A\sqrt{\frac{\frac{2\pi\hbar i\Delta t}{N}}{m}}\sqrt{\frac{1}{2}}\int dx_3\int dx_2\, e^{-\frac{m}{\frac{2\hbar i\Delta t}{N}}\left(\frac{(x_2-x_0)^2}{2}+(x_3-x_2)^2\right)}\int dx_4\cdots\int dx_{N-1}\, e^{\cdots}$$

$$= A\left(\sqrt{\frac{\frac{2\pi\hbar i\Delta t}{N}}{m}}\right)^{N-1}\sqrt{\frac{1}{2}}\sqrt{\frac{2}{3}}\sqrt{\frac{3}{4}}\cdots\sqrt{\frac{N-1}{N}}\, e^{\frac{im}{\frac{2\hbar\Delta t}{N}}\frac{(x_N-x_0)^2}{N}}$$

$$= A\left(\sqrt{\frac{\frac{2\pi\hbar i\Delta t}{N}}{m}}\right)^{N}\underbrace{\sqrt{\frac{m}{2\pi\hbar i\Delta t/N}}\sqrt{\frac{1}{N}}\, e^{\frac{im}{2\hbar\Delta t}(x_N-x_0)^2}}_{\text{Identical to the classical results}}$$

Now when we set $A=\left(\sqrt{\frac{m}{2\pi\hbar i\Delta t/N}}\right)^N$ the results is identical to the classical case.

Integral over $dx_1,\cdots,dx_{N-1}$ must be replaced by "measure" in "path space "$d_{path}[x(t)]$

By comparison

$$d_{path}[x(t)]\ \rightarrow\ \prod_i dx_i\sqrt{\frac{m}{2\pi\hbar i\Delta t/N}}$$

and an overall constant $\sqrt{\frac{m}{2\pi\hbar i\Delta t/N}}$ "for the whole path".

Connection to Huygen's principle for a plane wave:

$$\psi(x,t=0)=\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

What does it look like after a short time Δt? Of course we know the answer (plane wave with momentum p and Energy $E = p^2/2m$):

$$\psi(x,t=\Delta t)=\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\cdot e^{-i\frac{p^2}{2m}\Delta t/\hbar}$$

Using our knowledge of path integral formalism:

$$\psi(x, t = \Delta t) = \sqrt{\frac{m}{2\pi\hbar i\Delta t}} \int d\delta x \, \psi(x - \delta x, t = 0) \; e^{\frac{i}{\hbar}\frac{m\delta x^2}{2\Delta t}}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{m}{2\pi\hbar i\Delta t}} \int d\delta x \;\; e^{ip(x-\delta x)/\hbar} \, e^{\frac{i}{\hbar}\frac{m\delta x^2}{2\Delta t}} \approx \frac{1}{\sqrt{2\pi\hbar}} \, e^{\frac{ipx}{\hbar}} \, e^{-i\frac{p^2}{2m}\Delta t/\hbar}$$

where we used the Gaussian Integral $\sqrt{\frac{m}{2\pi\hbar i\Delta t}} \int d\delta x \;\; e^{-ip\delta x/\hbar} \, e^{\frac{i}{\hbar}\frac{m\delta x^2}{2\Delta t}} = e^{-i\frac{p^2}{2m}\Delta t/\hbar}$

The integral is in principle over all δx but the significant contribution comes from a specific range where the phase is approximately stationary (coherent interference):

$$phase = -i\frac{p}{\hbar}\delta x + \frac{i}{\hbar}\frac{m\delta x^2}{2\Delta t}$$

$$Stationary\ phase \;\rightarrow\; \frac{\partial\, phase}{\partial\, \delta x} = 0 \;\rightarrow\; -i\frac{p}{\hbar} + \frac{i}{\hbar}\frac{m\delta x}{\Delta t} = 0$$

$$\therefore \;\; \delta x = \frac{p}{m}\,\Delta t$$

This means that the value of the wave function at $(x, t = \Delta t)$ propagates mostly from the wave function $\psi(x - \delta x, t = 0)$ at a point $x - \delta x$ from which the "Huygens' spherical wavelet" propagates with the SAME wavelength as the incoming wave, $\lambda = 2\pi(\frac{p}{\hbar})^{-1}$.