Exact quantum dynamics : 1d Split Operator Fourier Trasform

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad , \quad \hat{H} = \frac{\hat{P}^2}{2M} + E(\hat{x})$$

Formal solution (time independent $\hat{H}$)

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t} |\psi(0)\rangle$$

In the coordinate representation

$$\langle x_t | \psi(t)\rangle = \langle x_t | e^{-\frac{i}{\hbar}\hat{H}t} |\psi(0)\rangle$$

$$= \int dx_0 \, \langle x_t | e^{-\frac{i}{\hbar}\hat{H}t} | x_0\rangle \langle x_0 | \psi(0)\rangle$$

$$= \int dx_0 \, K(x_t, x_0) \, \psi(x_0)$$

↳ propagator in the x repres. no analytic expression for generic $E(\hat{x})$

We can use the same strategy adopted in the classical case to obtain a controllably accurate approximation

Two steps : 1/ Use time composition property to write $K(x_t, x_0)$ as a sequence of short time propagators (this is exact) ; 2/ Use Trotter approximation to obtain a calculable expression of the short time propagator

1/ Let us consider

$$K(x_t, x_0) = \langle x_t | e^{-\frac{i}{\hbar}\hat{H}t} | x_0 \rangle \qquad (t \to N+1)$$

$$= \langle x_{N+1} | \underbrace{e^{-\frac{i}{\hbar}\hat{H}\frac{t}{N}} e^{-\frac{i}{\hbar}\hat{H}\frac{t}{N}} \cdots e^{-\frac{i}{\hbar}\hat{H}\frac{t}{N}}}_{N \text{ and } \cancel{t/N+1} = \varepsilon} | x_0 \rangle$$

Insert N resolution of the identity

$$= \int dx_N \ldots dx_1 \ \langle x_{N+1} | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_N \rangle \langle x_N | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_{N-1} \rangle$$

$$\ldots \langle x_1 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_0 \rangle$$

Then

$$\langle x_{N+1} | \psi(t) \rangle \equiv \psi(x_{N+1}, t) = \int dx_N \overbrace{}^{dx_{N-1} \ldots dx_1} \langle x_{N+1} | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_N \rangle$$

$$\langle x_N | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_{N-1} \rangle \ldots \langle x_1 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_0 \rangle \psi(x_0, 0)$$

Note that $\int dx_1 \langle x_1 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_0 \rangle \psi(x_0) \equiv \psi(x_1, \varepsilon)$

i.e. the wavefunction evolved for a time $\varepsilon = \frac{t}{N+1}$

→ This is a time stepping algorithm. E.g. for $N = 2$

$$\psi(x_3, t) = \int dx_2 \ \langle x_3 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_2 \rangle \int dx_1 \ \langle x_2 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_1 \rangle$$

$$\underbrace{\int dx_0 \ \langle x_1 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_0 \rangle \psi(x_0, 0)}_{\psi(x_1, \varepsilon)}$$

$$= \int dx_2 \ \langle x_3 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_2 \rangle \underbrace{\int dx_1 \ \langle x_2 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_1 \rangle \psi(x_1, \varepsilon)}_{\psi(x_2, 2\varepsilon)}$$

$$= \int dx_2 \ \langle x_3 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_2 \rangle \psi(x_2, 2\varepsilon)$$

2/ Let us then focus on the single step propagator

$$\langle x_1 | \psi(\varepsilon)\rangle = \psi(x_1, \varepsilon) = \int dx_0 \, \langle x_1 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_0\rangle \, \psi(x_0, 0)$$

We can use the Trotter approximation to write

$$\langle x_1 | e^{-\frac{i}{\hbar}\hat{H}\varepsilon} | x_0\rangle = \langle x_1 | e^{-\frac{i}{\hbar}\left(\frac{\hat{p}^2}{2m} + E(\hat{x})\right)\varepsilon} | x_0\rangle$$

$$\simeq \langle x_1 | e^{-\frac{i}{\hbar}E(\hat{x})\varepsilon/2} \, e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon} \, e^{-\frac{i}{\hbar}E(\hat{x})\frac{\varepsilon}{2}} | x_0\rangle$$

$$= e^{-\frac{i}{\hbar}E(x_1)\varepsilon/2} \langle x_1 | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon} | x_0\rangle \, e^{-\frac{i}{\hbar}E(x_0)\frac{\varepsilon}{2}}$$

$$= e^{-\frac{i}{\hbar}E(x_1)\frac{\varepsilon}{2}} \int dp \, \langle x_1 | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\varepsilon} | p\rangle \langle p | x_0\rangle$$

$$e^{-\frac{i}{\hbar}E(x_0)\varepsilon/2}$$

Remember $\boxed{\langle p | x_0\rangle = \frac{1}{\sqrt{2\pi\hbar}} \, e^{-\frac{i}{\hbar}p x_0}}$

$$= e^{-\frac{i}{\hbar}E(x_1)\varepsilon/2} \int \frac{dp}{2\pi\hbar} \, e^{\frac{i}{\hbar}p x_1} \, e^{-\frac{i}{\hbar}\frac{p^2}{2m}\varepsilon} \, e^{-\frac{i}{\hbar}p x_0}$$

So

$$\psi(x_1, \varepsilon) = e^{-\frac{i}{\hbar}E(x_1)\varepsilon/2} \int \frac{dp}{\sqrt{2\pi\hbar}} \, e^{\frac{i}{\hbar}p x_1} \, e^{-\frac{i}{\hbar}\frac{p^2}{2m}\varepsilon}$$

$$\underbrace{\int \frac{dx_0}{\sqrt{2\pi\hbar}} \, e^{-\frac{i}{\hbar}p x_0} \, \underbrace{e^{-\frac{i}{\hbar}E(x_0)\varepsilon/2} \, \psi(x_0, 0)}_{= \phi_{\varepsilon/2}(x_0)}}_{\tilde{\phi}_{\varepsilon/2}(p), \text{ Fourier transform of } \phi_{\varepsilon/2}(x_0)}$$

Then

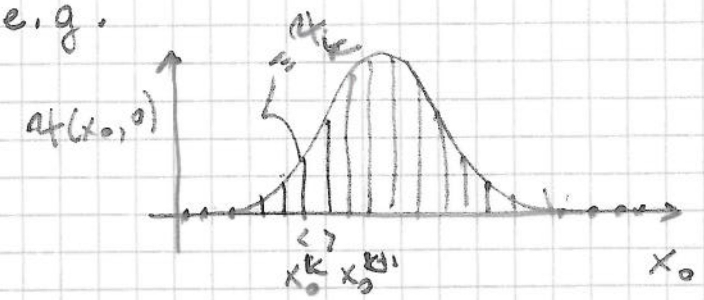
$$\psi(x_1,\varepsilon) = e^{-\frac{i}{\hbar}E(x_1)\varepsilon/2} \underbrace{\int \frac{dp}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px_1} \underbrace{e^{-\frac{i}{\hbar}\frac{p^2}{2m}\varepsilon} \tilde{\phi}_{\varepsilon/2}(p)}_{\tilde{\Phi}_\varepsilon(p)}}_{\Phi_\varepsilon(x_1),\ \text{anti Fourier transform of } \tilde{\Phi}_{\varepsilon/2}(p)}$$

$$= e^{-\frac{i}{\hbar}E(x_1)\frac{\varepsilon}{2}} \Phi_\varepsilon(x_1)$$

Then iterate N times to get $\psi(x_{N+1}, t=(N+1)\varepsilon)$

Numerically all this must be discretized on a grid

e.g.



Multiply at each discrete value of x_i by exponential to obtain

$$\phi_k = e^{-\frac{i}{\hbar}E_k\varepsilon/2}\psi_k$$

where $\phi_k = \phi_{\varepsilon/2}(x_0^k)$, $E_k = E(x_0^k)$ and $\psi_k = \psi(x_0^k, 0)$

Then discrete Fourier transform to obtain (on a p grid) $\tilde{\phi}_k = \tilde{\phi}(p_k)$

Then multiply at each point on the p grid by the exponential to obtain

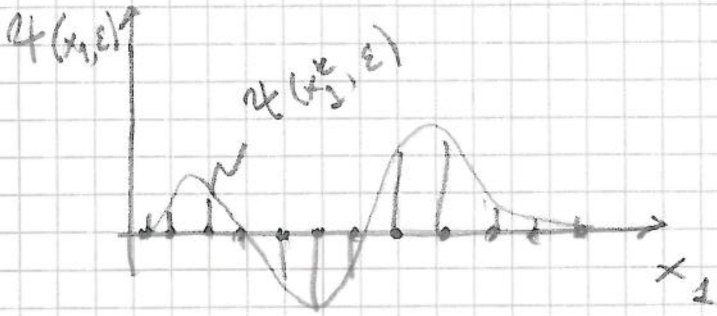
$$\tilde{\Phi}_\varepsilon(p_k^i) = e^{-\frac{i}{\hbar}\frac{p_k^2}{2m}\varepsilon}\,\tilde{\phi}_k^i$$

Then discrete anti-Fourier tranform to obtain (on a x grid) $\Phi_\varepsilon(x_1^k)$

Multiply at each point by the exponential to obtain

$$\psi(x_1^k, \varepsilon) = e^{-\frac{i}{\hbar}E(x_1^k)\frac{\varepsilon}{2}}\,\Phi_\varepsilon(x_1^k)$$

Note that, of course, this is a discrete representation of the wavefunction after one time step



- How do we test accuracy
- Numerical cost?