Fourier transformations, Trotter expansion and algorithm

Settings

System:

A single particle of position x in one dimension, in a potential $V(x)$.

Hamiltonian:

$$H = H^{\text{free}} + V(x) \qquad \text{with} \qquad H^{\text{free}} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} \tag{1}$$

Schrödinger evolution of the wave function $\Psi(x,t)$:

$$i\frac{\partial}{\partial t}\Psi(x,t) = H\Psi(x,t) \qquad (\text{with } \hbar = 1) \tag{2}$$

Operator of evolution

$$\Psi(t) = e^{-iH}\Psi(0) \tag{3}$$

Fourier transformations

Relations between the position-space representation $\Psi(x,t)$ and momentum-space representation $\hat{\Psi}(p,t)$:

$$\hat{\Psi}(p,t) = \int_{-\infty}^{\infty} dx\, e^{-ipx}\Psi(x,t) \tag{4}$$

$$\Psi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dp\, e^{ipx}\hat{\Psi}(p,t) \tag{5}$$

Representation of the differentiation $\frac{\partial}{\partial x}$ in momentum space:

$$\frac{\partial}{\partial x}\Psi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dp\, e^{ipx} \times \underbrace{\left\{ip\hat{\Psi}(p,t)\right\}}_{\text{one writes: } \frac{\partial}{\partial x} \mapsto ip} \tag{6}$$

Using thus $\frac{\partial^2}{\partial x^2} \mapsto -p^2$, one has[1]:

$$e^{-iH^{\text{free}}} \mapsto e^{-ip^2/2} \tag{7}$$

Application to the Trotter expansion

Trotter expansion for the operator of evolution e^{-iH} of (3) with the Hamiltonian (1):

$$\exp\Big[-i\,\Delta t\, H^{\text{free}}\Big] \simeq \underbrace{\exp\Big[-iV(x)\,\Delta t/2\Big]\ \underbrace{\exp\Big[-i\,\Delta t H^{\text{free}}\Big]\ \underbrace{\exp\Big[-iV(x)\,\Delta t\,/2\Big]}_{\substack{\textbf{Step 1}\text{: multiply } \Psi(x,t)\\ \text{by } e^{-iV(x)\Delta t/2}}}}_{\substack{\textbf{Step 2}\text{: transform to momentum space using (4)}\\ \text{and multiply by } e^{-ip^2/2}}}}_{\substack{\textbf{Step 3}\text{: transform back to position space using (5)}\\ \text{and multiply by } e^{-iV(x)\,\Delta t/2}}} \tag{8}$$

Following these three steps allows you to obtain the evolution of the wave function along one time-step Δt

$$\Psi(t+\Delta t) = \exp\Big[-i\,\Delta t\, H^{\text{free}}\Big]\Psi(t) \tag{9}$$

[1] which, in details, means: $e^{-iH^{\text{free}}}\Psi(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dp\, e^{ipx} \times e^{-ip^2/2}\hat{\Psi}(p,t)$