Unitary Time-Propagators

Both space-splitting method (SSM) and spectral method (SM) are split-operator methods based on Trotter expansion. They perform *exact exponentiation* of an approximate time-propagation operator, by keeping infinite sum of Taylor expansion.

Q. Why exact exponentiation?

A. To conserve the probability.

Time-Propagation Operator

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

where $|\psi(t)\rangle$ is wave function at time *t* and *H* is Hamiltonian operator.

Norm Conservation

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|\underbrace{\left(e^{-iHt}\right)^{\dagger}}_{e^{iH^{\dagger}t}=e^{iHt}} e^{-iHt}|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle = 1$$

Here, we have used Hermiticity of the Hamiltonian, *i.e.*, its Hermitian conjugate is itself.

Euler Method

$$e^{-iH\Delta} = 1 - iH\Delta + O(\Delta^2)$$

$$\langle\psi(\Delta)|\psi(\Delta)\rangle = \langle\psi(0)|(1 + iH\Delta)(1 - iH\Delta)|\psi(0)\rangle = 1 + \Delta^2\langle\psi(0)|H^2|\psi(0)\rangle > 1$$

Bad to truncate the Taylor expansion — probability not conserved!

Crank-Nicholson Method (CNM)

$$e^{-iH\Delta} = \frac{1-iH\Delta/2}{1+iH\Delta/2} + O(\Delta^2)$$

$$\langle\psi(\Delta)|\psi(\Delta)\rangle = \langle\psi(0)|\frac{1+iH\Delta/2}{1-iH\Delta/2}\frac{1-iH\Delta/2}{1+iH\Delta/2}|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle = 1$$ // It's unitary!

In addition to SSM and SM, CNM is a unitary time propagator.

Application of rational operator

$$|\psi(t)\rangle = \frac{1-iH\Delta/2}{1+iH\Delta/2}|\psi(0)\rangle \quad \Rightarrow \quad \underbrace{(1 + iH\Delta/2)}_{A\text{:tridigonal matrix}} \underbrace{|\psi(t)\rangle}_{x\text{:unknown vector}} = \underbrace{(1 - iH\Delta/2)|\psi(0)\rangle}_{b\text{:known vector}}$$

Linear system of equations: $Ax = b$