

1D-Simulation of Wave functions

Tutor: Edrick

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Time Evolution

- Time-Dependent Schrödinger Equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

Time Evolution

- Time-Dependent Schrödinger Equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

- Time-Evolution Operator

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle$$

Time Evolution

- Time-Dependent Schrödinger Equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

- Time-Evolution Operator

- Linear
- Unitary

- $U(t_n, t_1) = U(t_n, t_{n-1}) \dots U(t_3, t_2) U(t_2, t_1) \quad t_1 < t_2 < t_3 < \dots < t_n$

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- Equation & Solution for $U(t, t_0)$

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- Equation & Solution for $U(t, t_0)$

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) |\psi(t_0)\rangle = H(t) U(t, t_0) |\psi(t_0)\rangle$$

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- Equation & Solution for $U(t, t_0)$

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) |\psi(t_0)\rangle = H(t) U(t, t_0) |\psi(t_0)\rangle \Leftrightarrow i\hbar \frac{\partial}{\partial t} U(t, t_0) = H(t) U(t, t_0)$$

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- Equation & Solution for $U(t, t_0)$

Time-Independent H

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) |\psi(t_0)\rangle = H(t) U(t, t_0) |\psi(t_0)\rangle \Rightarrow i\hbar \frac{\partial}{\partial t} U(t, t_0) = H(t) U(t, t_0) \Rightarrow U(t, t_0) = e^{-iH(t-t_0)/\hbar}$$

Simulation of Wave Functions (1D)

- Discretization of Derivatives

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

Simulation of Wave Functions (1D)

$$\nabla^2 \psi(\mathbf{r}_j, t^n) \approx \frac{\psi_{j+1}^n + \psi_{j-1}^n - 2 \cdot \psi_j^n}{(\Delta r)^2}$$

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- Split-Operator methods

$$U(\Delta t) = e^{-i\mathcal{H}\Delta t} = e^{-i[\hat{T}+\hat{V}]\Delta t} \\ \approx e^{-i\hat{V}\Delta t/2} e^{-i\hat{T}\Delta t} e^{-i\hat{V}\Delta t/2} + \mathcal{O}(\Delta t^3)$$

Suzuki-Trotter
Factorization

Simulation of Wave Functions (1D)

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- Discretization of Derivatives

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

$$\frac{dy}{dx} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

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$$U(\Delta t) = e^{-i\mathcal{H}\Delta t} \approx \sum_n a_n P_n(\mathcal{H})$$

$$e^{-i(A+B)t} = \lim_{n \rightarrow \infty} \left[e^{-\frac{i}{2}A \frac{t}{n}} e^{-iB \frac{t}{n}} e^{-\frac{i}{2}A \frac{t}{n}} \right]^n$$

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Fourier transforms

- Fourier Transform and inverse Fourier Transform

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx e^{-ikx} f(x)$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk e^{ikx} \tilde{f}(k)$$

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$$\begin{aligned} \langle u_i | \psi \rangle &= \langle u_i | \mathbb{1} | \psi \rangle = \langle u_i | P_{\{t_k\}} | \psi \rangle \\ &= \sum_k \langle u_i | t_k \rangle \langle t_k | \psi \rangle \\ &= \sum_k S_{ik} \langle t_k | \psi \rangle \end{aligned}$$

Summary

- Eigenvalue of operators

$$\hat{A} | \psi \rangle = a | \psi \rangle$$

$$F(\hat{A}) | \psi \rangle = F(a) | \psi \rangle$$

- Evolution Operator

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$$

$$U(t, t_0) = e^{-iH(t-t_0)/\hbar}$$

$$U(t_n, t_1) = U(t_n, t_{n-1}) \dots U(t_3, t_2)U(t_2, t_1)$$

- Suzuki-Trotter Factorization

$$e^{-i[\hat{T}+\hat{V}]\Delta t} \approx e^{-i\hat{V}\Delta t/2} e^{-i\hat{T}\Delta t} e^{-i\hat{V}\Delta t/2} + \mathcal{O}(\Delta t^3)$$

- Fourier Transforms

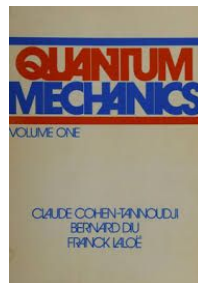
$$\bar{\psi}(p) = \int_{-\infty}^{+\infty} dx \langle p|x \rangle \psi(x)$$

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References

- Evolution Operator
- 1D-Simulations of WFs: Blog
- SOFT: OSSCAR

Complement F_{III}



- Trotter-Decomposition

Suzuki-Trotter Decomposition

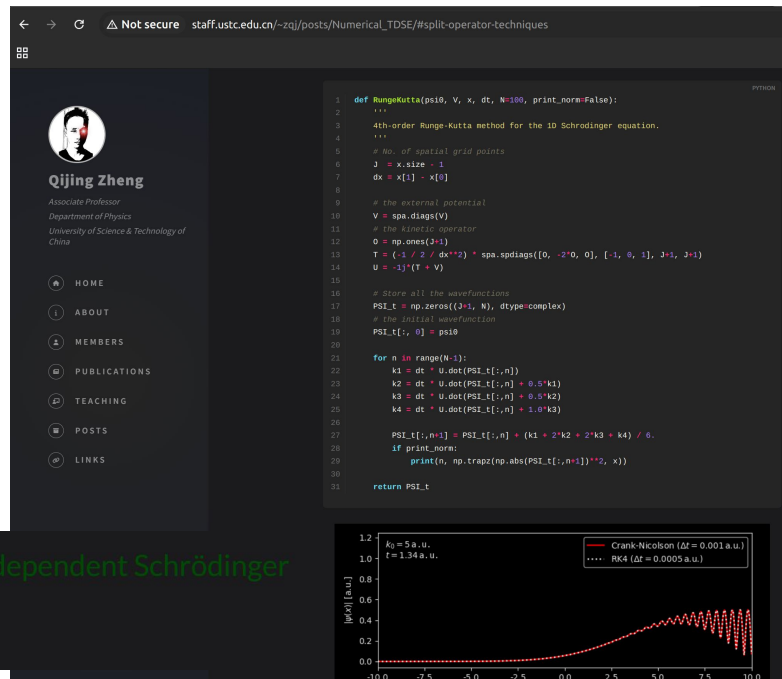
Tilock Sadhukhan
C-DAC Bangalore
January, 2025

Application of S-T factorization:

Reversible multiple time scale molecular dynamics

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```
def RungeKutta(psi0, V, x, dt, N=100, print_norm=False):  
    ...  
    # 4th-order Runge-Kutta method for the 1D Schrödinger equation.  
    ...  
    # No. of spatial grid points  
    J = x.size - 1  
    dx = x[1] - x[0]  
    ...  
    # The external potential  
    V = spa.diags(V)  
    # The kinetic operator  
    O = np.ones(J+1)  
    T = (-1 / 2 / dx**2) * spa.spdia([0, -2*O, 0], [-1, 0, 1], J+1, J+1)  
    U = -1j * (T + V)  
    ...  
    # Store all the wavefunctions  
    PSI_t = np.zeros((J+1, N), dtype=complex)  
    # The initial wavefunction  
    PSI_t[:, 0] = psi0  
    ...  
    for n in range(N-1):  
        k1 = dt * U.dot(PSI_t[:,n])  
        k2 = dt * U.dot(PSI_t[:,n] + 0.5*k1)  
        k3 = dt * U.dot(PSI_t[:,n] + 0.5*k2)  
        k4 = dt * U.dot(PSI_t[:,n] + k3)  
        ...  
        PSI_t[:,n+1] = PSI_t[:,n] + (k1 + 2*k2 + 2*k3 + k4) / 6.  
        if print_norm:  
            print(n, np.trapz(np.abs(PSI_t[:,n+1])**2, x))  
    ...  
    return PSI_t
```

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OSSCAR

Numerical Solution of 1D Time Dependent Schrödinger Equation by Split Operator Fourier Transform (SOFT) Method

Authors: Dou Du, Taylor James Baird and Sara Bonella

Thanks for your attention!