1D-Simulation of Wave functions

Tutor: Edrick

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- Simulation of Wave Functions (1D)
- Fourier Transforms
- Summary

Time Evolution

- Time-Dependent Schrödinger Equation

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

Time Evolution

- Time-Dependent Schrödinger Equation

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

- Time-Evolution Operator

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

Time Evolution

- Time-Dependent Schrödinger Equation

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

- Time-Evolution Operator
  - Linear
  - Unitary
  - $U(t_n, t_1) = U(t_n, t_{n-1})\ldots U(t_3, t_2)U(t_2, t_1) \qquad t_1 < t_2 < t_3 < \cdots < t_n$

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

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

- 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 $U(t, t_0)$

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

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Time-Independent H

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

Simulation of Wave Functions (1D)

- Discretization of Derivatives

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

Simulation of Wave Functions (1D)

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

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- Split-Operator methods

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

Suzuki-Trotter Factorization

Simulation of Wave Functions (1D)

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

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

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

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

$$\mathcal{U}(\Delta t) = e^{-i\mathcal{H}\Delta t} = e^{-i[\hat{T}+\hat{V}]\Delta t}$$
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Fourier transforms

- Fourier Transform and inverse Fourier Transform

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x \, \mathrm{e}^{-\mathrm{i}kx} f(x)$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}k \, \mathrm{e}^{\mathrm{i}kx} \tilde{f}(k)$$

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$$\overline{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}px/\hbar} \psi(x)$$

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$$\langle p \,|\, x \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}$$

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

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

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

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Summary

- Eigenvalue of operators

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

- Evolution Operator

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle \qquad U(t, t_0) = \mathrm{e}^{-\mathrm{i}\, H(t-t_0)/\hbar} \qquad U(t_n, t_1) = U(t_n, t_{n-1}) \ldots U(t_3, t_2)U(t_2, t_1)$$

- Suzuki-Trotter Factorization

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

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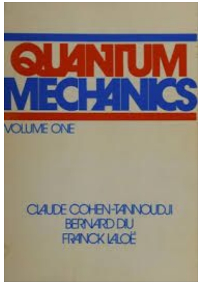
References

Complement F_{III}



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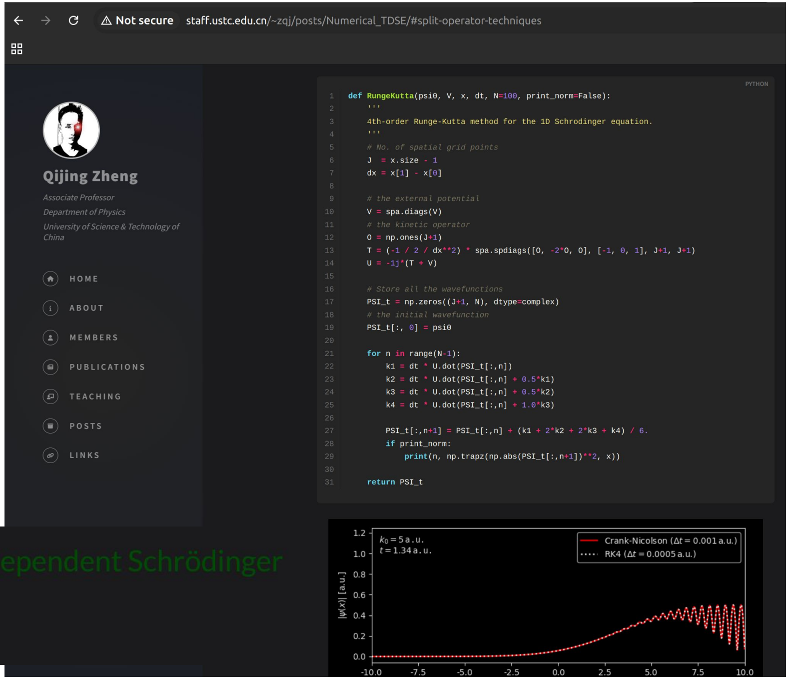

OSSCAR

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!