Numerical simulation of the time-dependent Schrödinger equation

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Outline:

- The physical problem: Conductance in an electron waveguide
- Computational units
- FDA approximation
- Implementation
- Results

Physical problem

Conductance in a 2D electron waveguide:

Landauer's formula:

$$G = \frac{e^2}{h} T$$

(derived from microscopic linear response theory)

Why interesting?

- Quantum devices
- Resonances in transmission

Resonances in 1D:

The Schrödinger equation with arbitrary metric

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m^*}g^{-1/2}\frac{\partial}{\partial u_i}\left(g^{1/2}g^{ij}\frac{\partial\psi}{\partial u_j}\right) + V\psi$$

$$g_{ij} = (w{+}h\xi(u_1))\begin{pmatrix} \frac{1+h^2u_2^2\dot{\xi}^2(u_1)}{w+h\xi(u_1)} & hu_2\dot{\xi}(u_1) \\ hu_2\xi(u_1) & w + h\xi(u_1) \end{pmatrix}$$

For example:

$$\xi(x) = e^{-\frac{x^{2p}}{2\sigma^2}}$$

Computational units

Schrödinger equation of a one particle system:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m^*}\nabla^2\psi + V\psi$$

Transformation:

$$\begin{aligned}
M: &\quad \frac{1}{m^*}m_{\text{phys}} \to m_{\text{comp}} = 1 \\
L: &\quad \frac{m^*c}{\hbar}x_{\text{phys}} \to x_{\text{comp}} \\
T: &\quad \frac{m^*c^2}{\hbar}t_{\text{phys}} \to x_{\text{comp}}
\end{aligned}$$

$$\Rightarrow \quad i\frac{\partial\psi}{\partial t_{\text{comp}}} = -\frac{1}{2}\nabla^2_{\text{comp}}\psi + \frac{V}{m^*c^2}\psi$$

FDA approximation of the Schrödinger equation

Formal solution of Schrödinger equation:

$$\psi(x,t) = e^{-iHt}\psi(x,0)$$

where $H = -\frac{1}{2}\nabla^2 + V$.

Cayley transform:
If A is a selfadjoint operator, then

$$V = (I + iA)\,(I - iA)^{-1}$$

is a unitary operator.

Try to write e^{-iHt} in this form and approximate it then:

$$\begin{aligned} & e^{\frac{1}{2}iHt}\psi(x,t) = e^{-\frac{1}{2}iHt}\psi(x,0) \\ \Rightarrow\ & (1 + \frac{1}{2}iHt)\psi(x,t) \approx (1 - \frac{1}{2}iHt)\psi(x,0) \\ \Rightarrow\ & e^{-iHt} \approx \frac{1 - \frac{1}{2}iHt}{1 + \frac{1}{2}iHt} \end{aligned}$$

Equivalent to Crank-Nicholson scheme: stable, second-order accurate in time and unitary!

FDA approximation of ∇^2:

$$\frac{\partial^2 \psi_{ij}}{\partial x^2} = \frac{1}{h_x^2}\left(\psi_{i-1,j} - 2\psi_{ij} + \psi_{i+1,j}\right)$$

$$\frac{\partial \psi_{ij}}{\partial x} = \frac{1}{2h_x}\left(\psi_{i+1,j} - \psi_{i-1,j}\right)$$

$$\begin{aligned}\frac{\partial^2 \psi_{ij}}{\partial x \partial y} &= \frac{1}{4h_x h_y}(\psi_{i+1,j+1} - \psi_{i+1,j-1} \\ &\quad -\psi_{i-1,j+1} + \psi_{i-1,j-1})\end{aligned}$$

Resulting stencil:

Implementation

Pseudo code:

```
Parse command-line input
Initialize wave function
Do requested number of timesteps:
    Apply Crank-Nicholson scheme:
        Calculate advanced ψ for Δt/2
        Calculate time propagator matrix
            for −Δt/2
        Solve linear equation
    Check norm
    Output solution
```

Results