Time–Dependent Schödinger Equation

PDE Waves: Complex, Quantum Wave Packets

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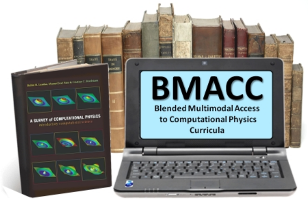
Based on *A Survey of Computational Physics* by Landau, Páez, & Bordeianu

with Support from the National Science Foundation

Course: **Computational Physics II**



Problem: Describe e Given p & x_{atomic}

Theory: T-Dependent Schrödinger Equation

Applet

- Atom-sized confinement $\Rightarrow$ QM
- Definite p and x $\Rightarrow$ wave packet $\Rightarrow$ real SE

$$i\,\frac{\partial\psi(x,t)}{\partial t} = H\psi = -\frac{1}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \qquad (1)$$

- $\neq$ definite E $\Rightarrow$ eigenstate $\psi(x,t) = \psi(x)\exp(-i\omega t)$
- Model: e localized at $t=0$, momentum k_0

$$\psi(x,t=0) = \exp\left[-\frac{1}{2}\left(\frac{x-5}{\sigma_0}\right)^2\right] e^{ik_0 x} \qquad (2)$$

- NB $\tilde{H}\psi$ [RHS of (1)] $\neq E\psi \Rightarrow \psi(x,t)$

$\psi(x, t)$: Finite-Difference Staggered Time Algorithm

Real ψ + Imag ψ Coupled Via $i\partial_t\psi$

$$\psi(x,t) = R(x,t) + i\, I(x,t) \quad (1)$$

$$\text{SE} \Rightarrow \quad \frac{\partial R(x,t)}{\partial t} = -\frac{1}{2m}\frac{\partial^2 I(x,t)}{\partial x^2} + V(x) I(x,t), \quad (2)$$

$$\frac{\partial I(x,t)}{\partial t} = +\frac{1}{2m}\frac{\partial^2 R(x,t)}{\partial x^2} - V(x) R(x,t) \quad (3)$$

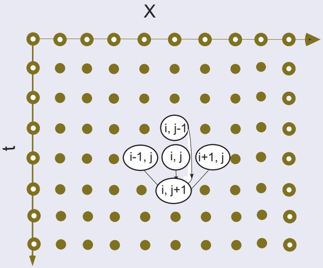
- Numerical challenge $\int dx\ \rho(x,t) \simeq$ constant
- $\Rightarrow$ Solve at staggered times: low O errors cancel

$$\mathrm{Re}\psi: \ 0,\ \ \Delta t,\ \ 2\Delta t,\ \ \ldots \quad (4)$$

$$\mathrm{Im}\psi: \ \frac{1}{2}\Delta t,\ \ \frac{3}{2}\Delta t,\ \ \frac{5}{2}\Delta t,\ \ \ldots \quad (5)$$

$\psi(x, t)$: Finite-Difference Staggered Time Algorithm

- R & I Taylor expansions, $\alpha = \Delta t/(2\Delta x^2)$
- $\rho = \sqrt{R^2 + I^2} \uparrow \mathcal{O}(\Delta^2)$
- Probability density ρ 3 t's
- $\Delta t \to 0$, $\to$ usual $(x \leftrightarrow i)$

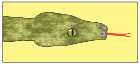


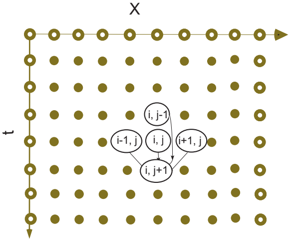
$$R_i^{n+1} = R_i^n - 2\left\{\alpha\left[I_{i+1}^n + I_{i-1}^n\right] - 2\left[\alpha + V_i\,\Delta t\right] I_i^n\right\} \quad (1)$$

$$I_i^{n+1} = I_i^n + 2\left\{\alpha\left[R_{i+1}^n + R_{i-1}^n\right] - 2\left[\alpha + V_i\,\Delta t\right] R_i^n\right\} \quad (2)$$

$$\rho(t) = \begin{cases} R^2(t) + I(t + \frac{\Delta t}{2})\,I(t - \frac{\Delta t}{2}), & \text{for integer } t, \\ I^2(t) + R(t + \frac{\Delta t}{2})\,R(t - \frac{\Delta t}{2}), & \text{for half-integer } t \end{cases} \quad (3)$$

Implementation





1. `psr[751][2],psi[751][2]`
2. IC: `psr[j][1]` $\leftrightarrow t = 0$; `psi[j][1]` $\leftrightarrow t = \frac{1}{2}\Delta t$
3. BC: `Rho[1] = Rho[751] = 0.0`
4. Time increment = $\frac{1}{2}\Delta t$
5. $\sim$5000 time steps

Animation

loading 2slits.mpg

Exercise

1. Output `Rho` ea 200 Δt
2. Surface plot $\rho(x, t)$
3. Animation $\psi(x, t)$

1. $\int_{-\infty}^{+\infty} dx\, \rho(x)$ = constant?
2. Why wall collisions
   $\Rightarrow$ break up?

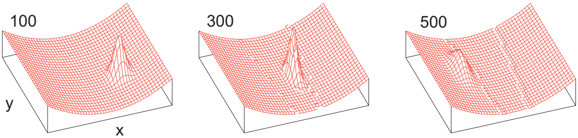
Exploration: Other Wells Applet Square Well

- 1-D Harmonic oscillator potential:

$$V(x) = \frac{1}{2}x^2$$

- 2-D parabolic tube (2-D SE):

$$V(x, y) = 0.9x^2, \quad -9.0 \leq x \leq 9.0, \quad 0 \leq y \leq 18.0 \qquad (4)$$



Extension*: 2 Particle Wave Packets Collide

$$i\,\frac{\partial\psi(x_1,x_2,t)}{\partial t} = -\frac{1}{2m_1}\frac{\partial^2\psi(x_1,t)}{\partial x_1^2} - \frac{1}{2m_2}\frac{\partial^2\psi(x_2,t)}{\partial x_2^2} + V(x_1-x_2)\psi(x_1,x_2,t)$$

$$\rho(x_1,t) \stackrel{\text{def}}{=} \int_{-\infty}^{+\infty} dt\,\rho(x_1,x_2,t)$$

- Movie
- $\rho(x_1,x_2,t)$: