DOING PHYSICS WITH PYTHON

QUANTUM MECHANICS

TIME DEPENDENT SCHRODINGER EQUATION FINITE DIFFERENCE TIME DEVELOPMENT METHOD

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Example codes for wavepacket propagation: **qm002.py qm005.py**

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The Schrodinger equation is the basis of quantum mechanics. The state of a particle is described by its wavefunction $\Psi(\vec{r},t)$ which is a function of position $\vec{r}$ and time t. The wavefunction is a complex variable and one cannot attribute any distinct physical meaning to it.

We will consider solving the **[1D] time dependent Schrodinger Equation** using the **Finite Difference Time Development Method** (**FDTD**).

The one-dimensional time dependent Schrodinger equation for a particle of mass m is given by

(1) $$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+U(x,t)\Psi(x,t)$$

where $U(x,t)$ is the potential energy function for the system.

The wavefunction is best expressed in terms of its real and imaginary parts

(2)

$$\Psi(x,t)=\Psi_R(x,t)+i\Psi_I(x,t) \qquad \Psi^*(x,t)=\Psi_R(x,t)-i\Psi_I(x,t)$$

Inserting equation 2 into equation 1 and separating real and imaginary parts results in the following pair of coupled equations

(3a) $$\frac{\partial\Psi_R(x,t)}{\partial t}=-\frac{\hbar}{2m}\frac{\partial^2\Psi_I(x,t)}{\partial x^2}+\frac{1}{\hbar}U(x,t)\Psi_I(x,t)$$

(3b) $$\frac{\partial \Psi_I(x,t)}{\partial t} = \frac{\hbar}{2m}\frac{\partial^2 \Psi_R(x,t)}{\partial x^2} - \frac{1}{\hbar}U(x,t)\Psi_R(x,t)$$

We can now apply the finite difference approximations for the first derivative in time and the second derivative in space. The time step is Δt and the spatial grid spacing is Δx. Time, position and the wavefunction are expressed in terms of the time index n_t and the spatial index n_x

Time $$t \to (n_t - 1)\Delta t \qquad n_t = 1,2,3,\ldots,N_t$$

Grid positions $$x \to (n_x - 1)\Delta x \qquad n_x = 1,2,3,\ldots,N_x$$

Wavefunction is calculated at each time step n_t

$$\Psi_R(x,t) \to y_R(n_x) \qquad \Psi_I(x,t) \to y_I(n_x)$$

(4) $$\frac{\partial \Psi(x,t)}{\partial t} = \frac{\Psi(x,t+\Delta t) - \Psi(x,t)}{\Delta t}$$

(5) $$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{\Psi(x+\Delta x,t) - 2\Psi(x,t) + \Psi(x-\Delta x,t)}{\Delta x^2}$$

The second derivative of the wavefunction given by equation 5 is not defined at the boundaries. The simplest approach to solve this problem is to set the wavefunction at the boundaries to be zero. This can cause problems because of reflections at both boundaries. Usually, a simulation is terminated before the reflections dominate.

Substituting equations 4 and 5 into equations 3a and 3b and applying the discrete times and spatial grid gives the latest value of the wavefunction expressed in terms of earlier values of the wavefunction as given by equations 6a and 6b

(6a)

$$y_R\left(n_x\right) = y_R\left(n_x\right) - C_1\left(y_I\left(n_x+1\right) - 2\,y_I\left(n_x\right) + y_I\left(n_x-1\right)\right) + C_2\left(U(n_x)\; y_I\left(n_x\right)\right)$$

(6b)

$$y_I\left(n_x\right) = y_I\left(n_x\right) + C_1\left(y_R\left(n_x+1\right) - 2\,y_R\left(n_x\right) + y_r\left(n_x-1\right)\right) - C_2\left(U(n_x)\; y_R\left(n_x\right)\right)$$

where the y is the wavefunction, and C_1 and C_2 are

(7) $\quad C_1 = \dfrac{\Delta t\,\hbar}{2\,m\,\Delta x^2}$ and $\quad C_2 = \dfrac{e\,\Delta t}{\hbar}$

The potential U is given in electron-volts (eV) and to convert to joules, the charge of the electron e is included in the equation for the constant C_2.

In equations 6a and 6b, the y variables on the RHS gives the values of the wavefunction at time $t + \Delta t$ and the y variables on the LHS are the values of the wavefunction at time t. Hence, given the initial values of the wavefunction, equations 6a and 6b explicitly determine the evolution of the system. The FDTD method can "blow-up" if appropriate time increments or grid spacings are not used. For a given grid spacing Δx we will set $C_1 = 1/10$ which means the time increment Δt is determined by

$$\Delta t = \left(\frac{2m\Delta x^2}{\hbar} \right) C_1 \qquad (8)$$

It is a relatively easy task to model an electron in a system with a potential energy function $U(x)$ in the region $x = 0$ to $x = L$. The potential energy function will be considered to be time independent. However, you can easily input a potential energy function that does depend upon time.