Numerical resolution of the Schrödinger equation

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1 The Schrödinger equation

The Schrödinger equation is well known, and with a generic potential it is given by

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = \left\{\frac{1}{2m}\Big[\mathbf{p} - q\mathbf{A}(\mathbf{x},t)\Big]^2 + V(\mathbf{x},t) - g\frac{q}{2m}\mathbf{S}\cdot\mathbf{B}(\mathbf{x},t)\right\}\Psi(\mathbf{x},t)\,, \tag{1.1}$$

also written as

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = H(\mathbf{x},t)\,\Psi(\mathbf{x},t)\,, \tag{1.2}$$

where, in the $\mathbf{x}$ representation

$$\mathbf{p} = -i\hbar\boldsymbol{\nabla} \qquad\qquad \left(p_x = -i\hbar\frac{\partial}{\partial x},\ldots\right) \tag{1.3}$$

We can write the "formal" solution of the Schrödinger equation as

$$\Psi(\mathbf{x},t) = U(t,t_0)\,\Psi(\mathbf{x},t_0)\,, \tag{1.4}$$

$$U(t,t_0) = T\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,H(t')\right)\right], \tag{1.5}$$

where T is the time-ordered-product operator. We dropped the $\mathbf{x}$ dependence in the Hamiltonian and in the evolution operator U, for ease of notation.

In the following, we will neglect the potential $\mathbf{A}$ and the interaction with the electron spin. We can then write the Hamiltonian as

$$H(\mathbf{x},\mathbf{p},t) = V(\mathbf{x}) + T(\mathbf{p})\,, \tag{1.6}$$

$$T(\mathbf{p}) = -\frac{\hbar^2}{2m}\nabla^2\,. \tag{1.7}$$

What makes things more complicated is the fact that V and T do **not** commute. In fact, it can be shown that (Lie–Trotter formula) if A and B are non-commutative operators, we have

$$\exp(A+B) = \lim_{n\to\infty}\left[\exp\left(\frac{A}{n}\right)\exp\left(\frac{B}{n}\right)\right]^n. \tag{1.8}$$

We can then start with the time-evolution operator in its "infinitesimal" form, and apply it to the wave function

$$U(t+\delta t,t) = \exp\left[-\frac{i}{\hbar}\delta t\,(V+T)\right]. \tag{1.9}$$

It is then easy to prove that

$$\exp\left[\tau(A+B)\right] = \exp\left(\tau A\right)\exp\left(\tau B\right) + \mathcal{O}\left(\tau^2\right) \tag{1.10}$$

or, even better,

$$\exp\left[\tau(A+B)\right] = \exp\left(\frac{1}{2}\tau A\right)\exp\left(\tau B\right)\exp\left(\frac{1}{2}\tau A\right) + \mathcal{O}\left(\tau^3\right) \tag{1.11}$$

Problem: *Demonstrate the previous two identities.*

Problem: *Generalize the previous cases using as starting point*

$$\exp\left[\tau(A+B)\right] = \prod_{i=1}^{k}\exp\left(c_i\tau A\right)\exp\left(d_i\tau B\right) + \mathcal{O}\left(\tau^{n+1}\right) \tag{1.12}$$

The goal is to determine k and the coefficients c_i and d_i.

Note that U is unitary at each step ($UU^\dagger = 1$) so that the evolution of the wave function preserves the normalization.

For small Δt, we can then write the evolution of the wave function as

$$\Psi\left(\mathbf{x}, t+\Delta t\right) = \exp\left(-\frac{i}{\hbar}\frac{V\left(\mathbf{x},t\right)}{2}\Delta t\right)\exp\left(-\frac{i}{\hbar}\frac{\mathbf{p^2}}{2m}\Delta t\right)\exp\left(-\frac{i}{\hbar}\frac{V\left(\mathbf{x},t\right)}{2}\Delta t\right)\Psi\left(\mathbf{x},t\right) \tag{1.13}$$

On a computer simulation, we can discretize the $\mathbf{x}$ space $\{\mathbf{x}_i\}$, and, given an initial wave funtion $\Psi_0\left(\mathbf{x}_i, t_0\right)$, we can evolve it with eq. (1.13).

2 One spatial dimension

For ease of notation, we write the following formulae in one spatial dimension. They can be easily generalized to three dimensions

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{ipx}{\hbar}\right) \tag{2.1}$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(-\frac{ipx}{\hbar}\right) \tag{2.2}$$

$$\Psi(x) \equiv \langle x|\Psi\rangle \tag{2.3}$$

$$\tilde{\Psi}(p) \equiv \langle p|\Psi\rangle \tag{2.4}$$

Inserting a completion

$$\Psi(x) \equiv \langle x|\Psi\rangle = \int dp\,\langle x|p\rangle\langle p|\Psi\rangle = \int dp\,\frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{ipx}{\hbar}\right)\tilde{\Psi}(p) \tag{2.5}$$

$$\tilde{\Psi}(p) \equiv \langle p|\Psi\rangle = \int dx\,\langle p|x\rangle\langle x|\Psi\rangle = \int dx\,\frac{1}{\sqrt{2\pi\hbar}}\exp\left(-\frac{ipx}{\hbar}\right)\Psi(x) \tag{2.6}$$

As you know this is just the **Fourier transform** $\mathcal{F}$

$$\tilde{\Psi}(p) = \mathcal{F}\left\{\Psi(x)\right\} \tag{2.7}$$

and

$$\Psi(x) = \mathcal{F}^{-1}\left\{\tilde{\Psi}(p)\right\}. \tag{2.8}$$

Since

$$\mathcal{F}\left\{\frac{d\Psi(x)}{dx}\right\} = \frac{i}{\hbar}\, p\, \tilde{\Psi}(p)\,, \tag{2.9}$$

we get

$$\mathcal{F}\left\{\exp\left[-\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\Delta t\right]\Psi(x)\right\} = \exp\left[-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t\right]\tilde{\Psi}(p) \tag{2.10}$$

3 Summary

The steps to perform in order to implement eq. (1.13) are then the following:

1. Given the state function at a time t, in $\mathbf{x}$ space, compute

$$\Psi^{(1)}(\mathbf{x}) = \exp\left(-\frac{i}{\hbar}\frac{V(\mathbf{x},t)}{2}\Delta t\right)\Psi(\mathbf{x},t) \tag{3.1}$$

   with a simple multiplication in $\mathbf{x}$ space

2. Compute the Fourier transform of $\Psi^{(1)}(\mathbf{x})$ to go to the momentum space

$$\tilde{\Psi}^{(1)}(\mathbf{p}) = \mathcal{F}\left\{\Psi^{(1)}(\mathbf{x})\right\} \tag{3.2}$$

3. Multiply $\tilde{\Psi}^{(1)}(\mathbf{p})$ by the kinetic part of the evolution equation

$$\tilde{\Psi}^{(2)}(\mathbf{p}) = \exp\left[-\frac{i}{\hbar}\frac{\mathbf{p}^2}{2m}\Delta t\right]\tilde{\Psi}^{(1)}(\mathbf{p}) \tag{3.3}$$

4. Go back to $\mathbf{x}$ space with the inverse Fourier transform

$$\Psi^{(2)}(\mathbf{x}) = \mathcal{F}^{-1}\left\{\tilde{\Psi}^{(2)}(\mathbf{p})\right\} \tag{3.4}$$

5. And finally

$$\Psi(\mathbf{x}, t+\Delta t) = \exp\left(-\frac{i}{\hbar}\frac{V(\mathbf{x},t)}{2}\Delta t\right)\Psi^{(2)}(\mathbf{x}) \tag{3.5}$$

With a few more "tricks" the entire procedure can be performed when a potential $\mathbf{A}(\mathbf{x},t)$ is present. If interested, ask me. Same if the particle has spin $\mathbf{S}$.

4 The Discrete Fourier Transform

Everything in this section is done in one dimension, but can be generalized, in a straightforward way, to three dimensions. We start with a finite x space

$$0 \leq x \leq L \tag{4.1}$$

Divide this interval with N equally-spaced points

$$x_i = \frac{L}{N}\, i\,, \qquad\qquad i = 0, \ldots, N-1 \tag{4.2}$$

$$\tilde{\Psi}(p) \approx \frac{1}{\sqrt{2\pi\hbar}} \frac{L}{N} \sum_{j=0}^{N-1} \exp\left(-i \frac{p}{\hbar} \frac{L}{N}\, j\right) \Psi\left(\frac{L}{N}\, j\right) \tag{4.3}$$

The finite range in x induces a periodicity in p. In fact

$$\tilde{\Psi}(p) = \tilde{\Psi}(p + \bar{p}) \tag{4.4}$$

if

$$\exp\left(-\frac{i\bar{p}}{\hbar} \frac{L}{N}\, j\right) = 1\,, \qquad \forall\, j \tag{4.5}$$

that is satisfied by

$$\bar{p} = \frac{2\pi\hbar}{L}\, N \tag{4.6}$$

so

$$0 \leq p < \frac{2\pi\hbar}{L}\, N \tag{4.7}$$

and we can discretize the p space too, by dividing the allowed interval with N points

$$p_k = \frac{2\pi\hbar}{L}\, k\,, \qquad\qquad k = 0, \ldots, N-1 \tag{4.8}$$

The wave function in p space of eq. (4.3) is then discretized as

$$\tilde{\Psi}_k = \frac{1}{\sqrt{2\pi\hbar}} \frac{L}{N} \sum_{j=0}^{N-1} \exp\left(-i \frac{2\pi}{N}\, j\, k\right) \Psi_j \tag{4.9}$$

where we have defined

$$\Psi_j \equiv \Psi\left(\frac{L}{N}\, j\right) \tag{4.10}$$

The inverse discrete Fourier transform is then given by (see eq. (2.6))

$$\Psi_j = \frac{\sqrt{2\pi\hbar}}{L} \sum_{k=0}^{N-1} \exp\left(+i \frac{2\pi}{N}\, j\, k\right) \tilde{\Psi}_k \tag{4.11}$$

Problem: *Check that, by inserting eq. (4.9) into (4.11), you obtain and identity.*

Notice that the order of normal modes in p space is **not** the most natural one. The lower k values correspond to positive small momenta. The central values of k correspond to ultraviolet modes, with the change of sign at $k = N/2$ (from positive to negative large momenta). Then back to smaller negative momenta. A shift in momentum space needs to be performed, in order to get a physical picture of $\tilde{\Psi}(p)$.

5 Work to do

1. Compute the Fourier transform of

$$\Psi(x) = \frac{1}{\left(\frac{\pi}{2}\right)^{1/4}\sqrt{\sigma}} \underbrace{\exp\left[-i\frac{p_0}{\hbar}(x-x_0)\right]}_{\text{boost}} \exp\left[-\frac{(x-x_0)^2}{\sigma^2}\right] \tag{5.1}$$

   Comment on the role of x_0 and p_0.

2. Check that $|\Psi(x)|^2 = 1$

3. Compute the exact free propagation of a gaussian wave packet and compare it with your numerical solution.

   In particular, compute the expectation value of the position and the width of the wave packet as a funtion of time.

4. Implement the semi-infinite-width barrier

5. Implement the finite-width barrier

6. Implement the infinite-height barrier. How can it be implemented?

7. Implement the harmonic osciallator.

8. Implement the anharmonic osciallator.

9. ...

6 Validation and internal consistency checks

You have to address two major points:

1. how you have **validated** your code: the checks you have performed to be sure that the code does what is supposed to do. Checks on the Fourier transform, on its inverse, on the evolution procedure...

2. the **internal consistency checks**: the code itself checks that the parameters chosen by the user are self compatible and that the run is going to produce physically-sound results (time interval is "appropriate" for the potential chosen, initial momentum and kinetic energy are always within the validity limits...