

Workshop #: IVPs with PDEs and Spectral Methods

The Schrodinger Equation

Reading: Numerical Recipes, Ch. 20.7 (& Sec. 20.2.1)

In quantum physics, a particle is described by a (complex) wavefunction $\psi(x, t)$. The evolution of the wavefunction is given by the Schrodinger equation

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

where \hbar is Planck's constant and m is the particle mass. The Hamiltonian operator \hat{H} consists of the kinetic energy operator \hat{T} and the external potential $V(x)$. Aside from quantum physics, Schrodinger-type equations (including nonlinear versions) also arise in areas such as optics and hydrodynamics. This worksheet covers some key techniques for solving them numerically using spectral methods.

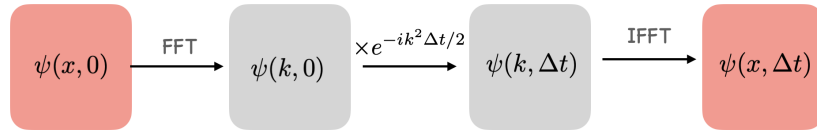
1 Particle in a Ring (walkthrough / demonstration)

First consider the dynamics of a particle in a ring-shaped trap of radius R . This can be modelled using the 1D Schrodinger equation with $V(x) = 0$ and periodic boundary conditions.

1. **Nondimensionalization:** By defining appropriate dimensionless variables (denoted by tildes) we can show that the Schrodinger equation becomes

$$i \frac{\partial \tilde{\psi}}{\partial \tilde{t}} = -\frac{1}{2} \frac{\partial^2 \tilde{\psi}}{\partial \tilde{x}^2}. \quad (2)$$

2. **Dynamics:** The Fourier transform gives us a simple procedure for finding the wavefunction at any time t by simply hopping between position space and wavenumber space:



3. **Compile and Run:** Code to solve the free space dynamics is provided in the file `schrodinger.cpp`. Familiarize yourself with the code, and the corresponding `makefile`. To compile the program, simply type `make` into the command line.
4. **Analyse:** Simulate the dynamics of a gaussian wavepacket $\psi(x, 0) = 1/(\pi\sigma^2)^{1/4} \exp(-x^2/2\sigma^2)$ with $\sigma \ll R$. Make a plot of the probability amplitude $|\psi(x, t)|^2$ for several time instances t . Modify the code to calculate and save the variance of the particles position

$$\langle x^2(t) \rangle = \int dx \, x^2 |\psi(x, t)|^2 \quad (3)$$

Plot $\langle x^2 \rangle$ vs t and comment on the result.

2 Harmonic Oscillator Potential (student exercise)

Now consider the harmonic oscillator,

$$V(x) = \frac{1}{2}m\omega^2 x^2. \quad (4)$$

1. **Dimensionless variables:** As above, we can work with dimensionless variables by writing $\tilde{x} = x/\ell$, $\tilde{t} = t/\tau$, $\tilde{\psi} = \psi/\sqrt{\ell}$. Show that the Schrodinger equation can be written (dropping the tildes) in the dimensionless form

$$i\frac{\partial\psi(x,t)}{\partial t} = \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2\right]\psi(x,t) \quad (5)$$

Find expressions for τ and ℓ . What (physically) do these parameters correspond to?

2. **Algorithm:** To extend our program to deal with the potential, we will make use of the *Split Operator Method*. As before, the wavefunction at any time $t + \Delta t$ is given exactly by

$$\psi(x, t + \Delta t) = \exp\left[-i(\hat{T} + \hat{V})\Delta t\right]\psi(x, t). \quad (6)$$

To perform the evolution purely in either x - or k -space, we would have to evaluate one of the operators as a (costly) matrix exponential. However, for a small step δt , then we may write

$$\exp\left[-i(\hat{T} + \hat{V})\delta t\right] \approx \exp\left[-i\hat{T}\delta t\right]\exp\left[-i\hat{V}\delta t\right] + \mathcal{O}(\delta t)^2. \quad (7)$$

Modify the program to implement the split operator method.

3. **Dynamics:** Suppose a particle is initially in the ground state of the well, with $\psi(x) = (1/\pi)^{1/4} \exp[-x^2/2]$, and the trap is then suddenly displaced by a distance $a = 1$. Simulate the dynamics and calculate

$$\langle x(t) \rangle = \int dx x |\psi(x)|^2 \quad \langle p(t) \rangle = \int dk k |\psi(k)|^2 \quad (8)$$

Do the same for a case where instead the trap frequency is suddenly changed to $\omega' = 0.5\omega$ and calculate $\langle x^2(t) \rangle$ and $\langle p^2(t) \rangle$.

4. **Groundstate using imaginary time:** The same techniques for dynamics can be used to find the groundstate of any potential. The trick is to make the replacement $t \rightarrow -it$. Since eigenstates satisfying $\hat{H}\phi_n = E_n\phi_n$ normally evolve as

$$\phi_n(x, t) = e^{-iE_n t}\phi_n(x), \quad (9)$$

each state will decay at a rate proportional to its energy under imaginary time evolution. Any wavefunction can be decomposed into the eigenstates, since they form a complete basis:

$$\psi(x, t) = \sum_n c_n(0) e^{-iE_n t} \phi_n(x). \quad (10)$$

It follows that any initial guess (as long as it doesn't have *zero* overlap with ϕ_0) will eventually be dominated by groundstate, since it decays at the slowest rate. If we renormalize the wavefunction after each timestep:

$$\psi(x) \rightarrow \frac{\psi(x)}{(\int |\psi(x')|^2 dx')^{1/2}}, \quad (11)$$

we maintain the condition $\int |\psi(x)|^2 dx = 1$, and will obtain the correctly normalized groundstate. Modify your code to solve for the groundstate of the potential.