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

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

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

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

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:

$$\boxed{\psi(x,0)} \xrightarrow{\text{FFT}} \boxed{\psi(k,0)} \xrightarrow{\times e^{-ik^2\Delta t/2}} \boxed{\psi(k,\Delta t)} \xrightarrow{\text{IFFT}} \boxed{\psi(x,\Delta t)}$$

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 complile 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

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

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

2 Harmonic Oscillator Potential (student exercise)

Now consider the harmonic oscillator,

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

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

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

   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

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

   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

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

   Modify the program to implement the split operator method.

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

   $$\langle x(t)\rangle = \int dx\; x|\psi(x)|^2 \qquad\qquad \langle p(t)\rangle = \int\; dk\; k|\psi(k)|^2 \tag{8}$$

   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 $t \to -it$. Since eigenstates satisfying $\hat{H}\phi_n = E_n\phi_n$ normally evolve as

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

   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:

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

   It follows that any intial 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:

   $$\psi(x) \to \frac{\psi(x)}{\left(\int|\psi(x')|^2 dx'\right)}, \tag{11}$$

   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.