PHY 115L
Shooting Method

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January 27, 2024

Chapter 1

Time-Independent Schrödinger Equation

We will numerically integrate the Time-Independent Schrödinger Equation (TISE):

$$-\frac{\hbar^2}{2m}\,\frac{d^2\psi}{dx^2} + V(x)\,\psi(x) = E\,\psi(x) \tag{1.1}$$

For numerical work, it is a good habit to introduce a system of units that keeps quantities near "1". We'll introduce a characteristic length a to be determined by the particular problem we are solving. Multiplying both sides by a^2 and rearranging we have:

$$a^2\,\frac{d^2\psi}{dx^2} = -\frac{2ma^2}{\hbar^2}\,\left(E - V(x)\right)\,\psi(x) \tag{1.2}$$

Defining:

$$E_0 \equiv \frac{\hbar^2}{2ma^2} \tag{1.3}$$

We have:

$$a^2\,\frac{d^2\psi}{dx^2} = -\frac{E - V(x)}{E_0}\,\psi(x) \tag{1.4}$$

We will integrate this equation using the Runge-Kutta technique for a first order differential equation, so we define a new variable ϕ by:

$$a\,\frac{d\psi}{dx} \equiv \phi \tag{1.5}$$

and so:

$$a\,\frac{d\phi}{dx} = -\frac{E - V(x)}{E_0}\,\psi(x) \tag{1.6}$$

In our computer programs, we'll measure x in units of a and E in units of E_0. In these units $a = 1$ and $E_0 = 1$, so our equations will read:

$$\frac{d\psi}{dx} \equiv \phi \tag{1.7}$$

and so:

$$\frac{d\phi}{dx} = \left(V(x) - E\right)\,\psi(x) \tag{1.8}$$

1.1 Euler's Method

We can write our system of first order differential equations by defining:

$$Y \equiv \begin{pmatrix} \psi \\ \phi \end{pmatrix} \tag{1.9}$$

and

$$\frac{dY}{dx} = \begin{pmatrix} \frac{d\psi}{dx} \\ \frac{d\phi}{dx} \end{pmatrix} = F(Y, x, E) \tag{1.10}$$

where:

$$F(Y, x, E) \equiv \begin{pmatrix} \phi \\ (V(x) - E)\ \psi \end{pmatrix} \tag{1.11}$$

for Euler's method, we approximate the change to Y during a step in x of size h as:

$$K_1 = h\frac{dY}{dx} = hF(Y, x, E)$$

and at each step we have:

$$Y \rightarrow Y + K_1$$

which have global error of h.

1.2 Fourth-Order Runge-Kutta Method

The Euler method is actually a 1st-order Runge-Kutta Method. The fourth order method samples the derivative column matrix F in more places:

$$\begin{aligned}
K_1 &= h\ \ F(Y, x, E) \\
K_2 &= h\ \ F\left(Y + \frac{K_1}{2}, x + \frac{h}{2}, E\right) \\
K_3 &= h\ \ F\left(Y + \frac{K_2}{2}, x + \frac{h}{2}, E\right) \\
K_4 &= h\ \ F(Y + K_3, x + h, E)
\end{aligned}$$

where:

$$Y \equiv \begin{pmatrix} \psi \\ \phi \end{pmatrix} \tag{1.12}$$

and

$$F(Y, x, E) \equiv \begin{pmatrix} \phi \\ (V(x) - E)\ \psi \end{pmatrix} \tag{1.13}$$

At each step we have:

$$Y \rightarrow Y + \frac{K_1 + 2\,K_2 + 2\,K_3 + K_4}{6}$$

1.3 The Infinite Square Well

An example python code for numerically integrating the TISE for the infinite square well using Euler's method is provide:

```
# System of Units:
# Position:  a = 1
# Energy:   E0 = hbar^2 / (2 m a^2)

# Potential V(x) in units of E0
def V(x):
    return 0

# TISE as two first order diff eqs:
# Y = (psi, phi)
# F = dY/dx = (dpsi/dx, dphi/dx)
# dpsi/dx = phi
# dphi/dx = (V-E) psi
def F(Y,x,E):
    psi = Y[0]
    phi = Y[1]
    dpsi_dx = phi
    dphi_dx = (V(x)-E)*psi
    F = np.array([dpsi_dx, dphi_dx], float)
    return F

# Numerical integration (using Runge-Kutta Order 1)
def tise_rk1(E,psi0,phi0,a,b,h):
    Y = np.array([psi0, phi0], float)
    X   = np.arange(a,b,h, float)
    PSI = np.array([psi0], float)
    for x in X:
        # 1st order Runge-Kutta:
        K1 = h*F(Y,x,E)
        Y += K1
        PSI = append(PSI,Y[0])
    X = np.append(X,b)
    return X,PSI

X,PSI = tise_rk1(E=20,psi0=1,phi0=0,a=0,b=0.5,h=0.01)
print("psi(b) = ", PSI[-1])

plt.plot(X,PSI,"b")
plt.axhline(c="k")
plt.axvline(x=0.5, c="k")
plt.ylim(-1.5,1.5)
plt.xlabel("x")
plt.ylabel("psi(x)")
```

1.4 The Harmonic Oscillator

For the harmonic oscillator with

$$\omega = \sqrt{\frac{k}{m}}$$

we take our characteristic length scale as:

$$a \equiv \sqrt{\frac{\hbar}{m\omega}}$$

and so:

$$E_0 = \frac{\hbar^2}{2ma^2} = \frac{\hbar\omega}{2}$$

1.5 Homework Problems

Problem 1: For an infinite potential well of width a, the allowed energies are

$$E = \frac{\pi^2 \hbar^2 n^2}{2\,m\,a^2}$$

Determine the allowed energies in units of

$$E_0 = \frac{\hbar^2}{2\,m\,a^2}$$

(A) Use your own code or modify the example code to numerically integrate the TISE for $n = 1$ which should meet boundary condition $\psi(1/2) = 0$. Make a plot that shows $n = 1$ meets the boundary conditions but $n = 0.7$ and $n = 1.3$ do not.

(B) Create plots of for $n = 1, 3, 5$ with $h = 0.01$ You should notice that Euler's method is not stable: the amplitude of the wave function is changing!

(C) Make a copy of the function `tise_rk1` called `tise_rk4` and modify it to implement the 4th order Runge-Kutta method. You should not need to change much! Just the calculation of the K_i and the weighted average! Make a plot comparing the output of RK-1 and RK-4 for the same step size that illustrates the instability of Euler's method.

(D) As written, the software will only integrate an even solution. Modify your code so that it can handle odd solutions as well. In the same plot, show the *properly normalized wave functions* for $n = 1, 2, 3, 4, 5, 6$ from $x = -1/2$ to $x = 1/2$. Be clever about how you deduce the wave function in $[-1/2, 0]$.

Problem 2-4: (There will be a few more problems that will explore the tool you have just created, but I wanted to post this ASAP so you can get started...)