

Computational Physics

PHYS 410 2014 W

Assignment # 2

Due: Friday, October 3, 2014 at 6PM

Consider a quantum mechanical treatment of a particle confined to a region $0 < x < L$. By solving the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) + V(x) \psi(x,t)$$

$$\text{for the potential } V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

it can be shown that the wavefunction for a particle with energy $E_n = \hbar \omega_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$ is $\psi_n(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-i\omega_n t}$ $0 < x < L$

In particular, the ground state has energy $\nearrow n=1$

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2} \quad \text{with} \quad \psi_1(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) e^{-i\omega_1 t}$$

Assignment # 2 cont.

If the potential is perturbed by a function $\delta V(x)$ then the first (leading) order correction to the energy of the state is

$$\delta E_n \equiv \langle \psi_n | \delta V | \psi_n \rangle$$

$$\delta E_n = \int_{-\infty}^{\infty} dx \psi_n^* \psi_n \delta V(x)$$

$$\delta E_n = \frac{2}{L} \int_0^L dx \sin^2\left(\frac{n\pi x}{L}\right) \delta V(x)$$

$$\delta E_1 = \frac{2}{L} \int_0^L dx \sin^2\left(\frac{\pi x}{L}\right) \delta V(x) \text{ etc...}$$

For I $\delta V(x) = \epsilon \frac{1}{1 + (\pi \tilde{x})^2}$ ϵ arbitrary small constant

II $\delta V(x) = \epsilon \frac{e^{-10\pi^2 \tilde{x}}}{10 + \tilde{x}}$

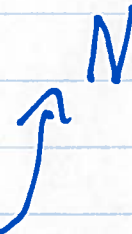
III A $\delta V(x)$ of your choice

$\tilde{x} = x/\lambda$ scale length $\lambda = \begin{cases} L \\ 10^{-2} L \\ 10^{-4} L \end{cases}$
try e.g.

Assignment #2 cont.

- a) Compute δE , and δE_{13} using the Trapezoidal, Simpson, and Gauss-Legendre methods.

Tabulate your results as a function of the number of points used, and make a plot of these for both δE , and δE_{13} to compare these methods. Compare and contrast how effective each method is for different functions. (Explain the relative efficiency of each method)



- b) Implement Romberg's method in a routine that takes a tolerance parameter K , and iterates until tolerance K in the fractional difference is achieved.

For I and II how many iterations are required to achieve tolerance K ? Explore this for different choices of K . Describe and explain your results.