Computational Physics

PHYS 410 2014W

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

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

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 $\psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-i\omega_n t}$ $\quad 0<x<L$

$n=1$

In particular, the ground state has energy

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

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

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

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

$$\boxed{\begin{aligned} \delta E_n &= \frac{2}{L} \int_0^{L} dx \, \sin^2\left(\frac{n\pi x}{L}\right) \delta V(x) \\ \delta E_1 &= \frac{2}{L} \int_0^{L} dx \, \sin^2\left(\frac{\pi x}{L}\right) \delta V(x) \text{ etc...} \end{aligned}}$$

For

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

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

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

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

Assignment #2 cont.

a) Compute δE_1 and δE_{13} using the Trapazoidal, Simpson, and Gauss-Legendre methods.

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Tabulate your results as a function of the number of points used, and make a plot of these for both δE_1 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.