Lab Assignment 4

Wednesday, April 7, 2021

Question:

A particle in the infinite square well has the initial wavefunction

$$\Psi(x,0) = \sqrt{\frac{30}{a^5}}x(a-x) \tag{1}$$

where 'a' is the width of the well. Outside the well $\Psi = 0$. $\Psi(x,0)$ can be expressed as a linear combination of stationary states of infinite square well by appropriate choice of the co-efficients c_n :

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} sin\Big(\frac{n\pi x}{a}\Big) \tag{2}$$

The nth co-efficient, c_n is,

$$c_n = \begin{cases} 0, \text{ if n is even }, \\ 8\sqrt{15}/(n\pi)^3, \text{ if n is odd.} \end{cases}$$

The expectation value of energy can be determined by:

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n^2| E_n = \frac{480\hbar^2}{\pi^4 m a^2} \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n^4} \tag{3}$$

where $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$. Take the values, $\hbar = 1$, a=1 and $m = 1$.

Write a program in single precision to calculate the summation in eq.(3).

1. For n=10,000, by computing the same from i = 1 to 10,000.
2. Repeat the calculation in the reverse order from i=10,000 to 1.
3. In each case, compute the percentage of relative error. Tabulate your results as follows.

n	Forward Sum	Rel. Error (%)	Backward Sum	Rel. Error (%)
1 3 5 7 . . 9999				

4. Calculate and print the expectation value of energy from the forward and backward summations and also print the absolute error and percentage of relative error in each case.

Note: You can use the following series for evaluating the analytical solution

$$\frac{1}{1^6} + \frac{1}{3^6} + \frac{1}{5^6} + ... = \frac{\pi^6}{960}$$

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$$\frac{1}{1^4} + \frac{1}{3^4} + \frac{1}{5^4} + ... = \frac{\pi^4}{96}$$

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