PHY-851: QUANTUM MECHANICS I
Quiz 4
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NAME..

PROBLEM. Consider a particle of mass m in a potential box of width a with infinitely high walls. Using a second order polynomial as a trial wave function, find the approximate value for the ground state energy and compare with the exact solution.

SOLUTION

It is obvious that the best trial function has to satisfy the boundary conditions $\psi(0) = \psi(a) = 0$. Therefore we make our choice in the form

$$\psi(x) = \begin{cases} Cx(a-x), & 0 \le x \le a, \\ 0, & x < 0,\ x > a. \end{cases} \tag{1}$$

The normalization

$$\int dx\, \psi^2(x) = 1 \tag{2}$$

determines

$$C^2 = \frac{30}{a^5}. \tag{3}$$

The expectation value of potential energy vanishes since inside the well $U = 0$, while outside the wave function is identically zero (the product $U\psi^2$ goes to zero when the potential infinitely grows because $\psi \to 0$ as $\exp(-\kappa|x|)$, $\kappa = \sqrt{2mU/\hbar^2}$). We need to calculate the expectation value of kinetic energy only,

$$\langle H \rangle = \langle K \rangle = -\frac{\hbar^2}{2m} \int_0^a dx\, \psi\psi'' = \frac{\hbar^2}{2m} \int_0^a dx\, |\psi'|^2 = 5\,\frac{\hbar^2}{ma^2}. \tag{4}$$

The exact value of the ground state energy is

$$E_{g.s.} = \frac{\pi^2}{2}\,\frac{\hbar^2}{ma^2}. \tag{5}$$

Our trial function is rather good, the variational value of energy (4) is only slightly higher than the exact one,

$$\frac{\langle H \rangle}{E_{g.s.}} = 1.013. \tag{6}$$