

4?

Problem 2: Variational Method (10 Points)

The Hamiltonian of a one-dimensional harmonic oscillator is

$$H = \frac{P^2}{2m} + \frac{m\omega^2 X^2}{2}.$$

The ground state energy is $E_0 = \hbar\omega/2$.

Let us employ the variational method with the following trial function as the ground-state wave function

$$\langle x|\psi\rangle = \psi(x) = Ne^{-\beta|x|}.$$

- a. Determine the constant N by applying the normalization condition. (2 points)
- b. Find the value of β that minimizes $\langle\psi|H|\psi\rangle$. (2 points)
- c. What is the ground-state energy calculated with the variational method? (5 points)
N.B. *The derivative of the trial function has a discontinuity.*
- d. How close do you get to the true ground-state energy? (1 points)

Jan 2017

Quantum #2

a) The normalization condition is: $1 = \int_{-\infty}^{\infty} |\psi|^2 dx$

$$\Rightarrow 1 = N^2 \int_{-\infty}^{\infty} e^{-2\beta|x|} dx$$

$$1 = N^2 \left[\int_{-\infty}^0 e^{2\beta x} dx + \int_0^{\infty} e^{-2\beta x} dx \right]$$

$$1 = N^2 \left[\frac{1}{2\beta} e^{2\beta x} \Big|_{-\infty}^0 + \frac{1}{2\beta} e^{-2\beta x} \Big|_0^{\infty} \right]$$

$$1 = N^2 \left[\frac{1}{2\beta} (e^{2\beta(0)} - e^{2\beta(-\infty)}) - e^{-2\beta(0)} + e^{-2\beta(\infty)} \right]$$

$$1 = N^2 \frac{1}{2\beta} (2)$$

$$1 = \frac{N^2}{\beta} \Rightarrow N = \sqrt{\beta}$$

b) $\langle \psi | H | \psi \rangle = \langle \psi | x' \rangle \langle x' | H | x \rangle \langle x | \psi \rangle$

$$= \int dx' \int dx \psi^*(x') H \psi(x)$$

$$= \int dx' \int dx \psi^*(x') \left[\frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \right] \psi(x)$$

$$= \int dx' \int dx \psi^*(x') \left[\frac{1}{2m} (-i\hbar \frac{\partial}{\partial x})^2 + \frac{m\omega^2}{2} x^2 \delta(x-x') \right] \psi(x)$$

$$= \int_{-\infty}^{\infty} dx \psi^*(x) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2} x^2 \right] \psi(x)$$

* minimum occurs when $\frac{d}{d\beta} \langle \psi | H | \psi \rangle = 0$

$$0 = \frac{d}{d\beta} \int_{-\infty}^{\infty} \frac{1}{\sqrt{\beta}} e^{-\beta|x|} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2} x^2 \right] \frac{1}{\sqrt{\beta}} e^{-\beta|x|} dx$$

$$= \frac{d}{d\beta} \int_{-\infty}^{\infty} \frac{1}{\beta} e^{\beta x} \left[-\frac{\hbar^2 \beta^2}{2m} e^{\beta x} + \frac{m\omega^2}{2} x^2 \right] e^{\beta x} dx + \int_0^{\infty} \frac{1}{\beta} e^{-\beta x} \left[-\frac{\hbar^2 \beta^2}{2m} e^{-\beta x} + \frac{m\omega^2}{2} x^2 e^{-\beta x} \right] dx$$

$$= \frac{d}{d\beta} \int_{-\infty}^0 \frac{-\hbar^2 \beta}{2m} e^{2\beta x} + \frac{m\omega^2 x^2}{2\beta} e^{2\beta x} dx + \int_0^{\infty} \frac{-\hbar^2 \beta}{2m} e^{-2\beta x} + \frac{m\omega^2 x^2}{2\beta} e^{-2\beta x} dx$$

$$= \frac{d}{d\beta} \left[\frac{-\hbar^2}{4m} e^{2\beta x} \Big|_{-\infty}^0 + \frac{m\omega^2}{2} \frac{1}{4\beta^4} + \frac{\hbar^2}{2m} \cdot \frac{1}{2} e^{-2\beta x} \Big|_0^{\infty} + \frac{m\omega^2}{2} \frac{1}{4\beta^4} \right]$$

$$= \frac{d}{d\beta} \left[\frac{-\hbar^2}{4m} + \frac{m\omega^2}{8\beta^4} - \frac{\hbar^2}{4m} + \frac{m\omega^2}{8\beta^4} \right]$$

$$= \frac{d}{d\beta} \left[\frac{-\hbar^2}{2m} + \frac{m\omega^2}{4\beta^4} \right]$$

#2 (cont.)

$$b) \quad 0 = -\frac{m\omega^2}{\beta^5}$$