PROBLEM 6: Variational approach

A particle with mass, m, moving in one dimension finds itself in a potential given by,

$$V = \infty \quad \text{for} \quad x < 0$$

and

$$V = \beta x^3 \quad \text{for} \quad x > 0$$

where β is a positive constant.

a) Find an approximation to the ground state energy, using the trial wavefunction

$$\Psi = 0 \quad \text{for} \quad x < 0$$

and

$$\Psi = Cxe^{-\alpha x} \quad \text{for} \quad x > 0.$$

where C and α are positive constants. (5 Points)

b) Would you expect the exact ground state energy to be less than your answer to part (a), or greater than it? Justify. (3 Points)

c) How would you go about finding an excited state in this system using the same approach? (2 Points)

Hint: $\int_0^\infty x^2 \mathrm{e}^{-ax} = 2a^{-3}$, for $a > 0$.

Aug 2014

Quantum #6

a) The Variational principle states that $E_{gs} \le \langle \psi | H | \psi \rangle = \langle H \rangle$ where $|\psi\rangle$ is a normalized trial wave function

$$\hookrightarrow H = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \beta x^3 = E\psi$$

$$V = \begin{cases} 0 & x < 0 \\ \beta x^3 & x \ge 0 \end{cases}$$

$$\psi = \begin{cases} Cxe^{-\alpha x} & x \ge 0 \\ 0 & x < 0 \end{cases}$$

* We first normalize our trial wave function, domain of interest is $[0, \infty)$

$$1 = C^2 \int_0^\infty x^2 e^{-2\alpha x}\, dx$$

* we know $\int_0^\infty x^2 e^{-ax} = 2a^{-3}$, $a > 0$

$$\hookrightarrow a = 2\alpha$$

$$1 = C^2 \cdot 2(2\alpha)^{-3}$$

$$1 = C^2 \cdot \frac{1}{4\alpha^3}$$

$$\hookrightarrow C = 2\alpha^{3/2}$$

$$\Rightarrow \psi(x) = \begin{cases} 2\alpha^{3/2} x e^{-\alpha x} & x \ge 0 \\ 0 & x < 0 \end{cases}$$

$$\langle H \rangle = \langle \psi | H | \psi \rangle$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \beta x^3\right) 2\alpha^{3/2} x e^{-\alpha x}\, dx$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left[-\frac{\hbar^2 \alpha^{3/2}}{m}\frac{d^2(xe^{-\alpha x})}{dx^2} + 2\alpha^{3/2}\beta x^4 e^{-\alpha x}\right] dx$$

$$= \int_0^\infty 2\alpha^{3/2} x e^{-\alpha x}\left[-\frac{\hbar^2 \alpha^{3/2}}{m}(\alpha^2 x - 2\alpha) e^{-\alpha x} + 2\alpha^{3/2}\beta x^4 e^{-\alpha x}\right] dx$$

$$= \int_0^\infty -\frac{2\alpha^3 x \hbar^2}{m}(\alpha^2 x - 2\alpha) e^{-2\alpha x} + 4\alpha^3 \beta x^5 e^{-2\alpha x}\, dx$$

#6 (cont.)

a) $$\langle H \rangle = \frac{-2\alpha^5\hbar^2}{m}\int_0^\infty x^2 e^{-2\alpha x}\,dx + \frac{4\alpha^4\hbar^2}{m}\int_0^\infty x e^{-2\alpha x}\,dx + 4\alpha^3\beta\int_0^\infty x^5 e^{-2\alpha x}\,dx$$

* in general, $\int_0^\infty x^n e^{-bx} = \frac{n!}{b^{n+1}}$

$$= -\frac{2\alpha^5\hbar^2}{m}\left[\frac{2!}{(2\alpha)^3}\right] + \frac{4\alpha^4\hbar^2}{m}\left[\frac{1!}{(2\alpha)^2}\right] + 4\alpha^3\beta\left[\frac{5!}{(2\alpha)^6}\right]$$

$$= \frac{-4\alpha^5\hbar^2}{8\alpha^3 m} + \frac{4\alpha^4\hbar^2}{4\alpha^2 m} + \frac{4\alpha^3\beta\cdot 120}{64\alpha^6}$$

$$= \frac{-\alpha^2\hbar^2}{2m} + \frac{\alpha^2\hbar^2}{m} + \frac{30\beta}{4\alpha^3}$$

$$= \frac{\alpha^2\hbar^2}{2m} + \frac{15\beta}{2\alpha^3}$$

b) By definition, our $E_{gs} \leq \langle H \rangle$. To prove this, we write our trial function as an expansion in eigenfunctions of H

$$|\psi\rangle = \sum_n c_n |\psi_n\rangle \quad \text{where} \quad H|\psi_n\rangle = E_n|\psi_n\rangle$$
$$|c_n|^2 = 1$$

$$\Rightarrow \langle H \rangle = \langle \psi | H | \psi \rangle$$
$$= \sum_{nm} \langle \psi_m | c_m^* H c_n | \psi_n \rangle$$
$$= \sum_{nm} c_m^* c_n \langle \psi_m | H | \psi_n \rangle$$
$$= \sum_{nm} c_m^* c_n E_n \langle \psi_m | \psi_n \rangle$$
$$= \sum_{nm} c_m^* c_n E_n \delta_{mn}$$
$$= \sum_n |c_n|^2 E_n$$

$\Rightarrow$ $E_{gs} = \sum_n |c_n|^2 E_n$ if n is ground state, otherwise

$$E_{gs} < \sum_n |c_n|^2 E_n$$

#6 (cont.)

c) To get an upper bound on the first excited state, we need a wavefunction that is orthogonal to the ground state wave function ψ_{gs}. However, since this is difficult to know, an equivalent option is to use a trial wave function with a parity opposite to that of the potential. Then we proceed as before.