Oblig 9

Oskar Idland

Problem 9.2 H

We know that for any state the upper bound for the ground state energy is given by

$$E_{\mathrm{gs}} \leq \frac{\langle\psi| H |\psi\rangle}{\langle\psi|\psi\rangle}$$

I guess a state of the form:

$$|\psi(x)\rangle\, Ae^{-bx^2}$$

As the potential would trap the particle around the origin. First we must normalize the state:

$$\int_{-\infty}^{\infty} \psi^* \psi \; dx = A^2 \int_{-\infty}^{\infty} e^{-2bx^2} \; \mathrm{d}x = 1$$

Using Rottman we get:

$$A^2 = \sqrt{\frac{\pi}{2b}} \rightarrow A = \sqrt[4]{\frac{\pi}{2b}}$$

With this normalized state we can calculate the upper bound for the ground state energy using:

$$E_{\mathrm{gs}} \leq \langle\psi| \hat{H} |\psi\rangle$$

Next we must find the Hamiltonian given by:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

Then let it act on our state:

$$\hat{H}\,|\psi(x)\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,|\psi(x)\rangle + V(x)\,|\psi(x)\rangle$$

$$\hat{H}\,|\psi(x)\rangle = -\frac{\hbar^2}{2m}\left(-2bAe^{-bx^2} + 4bx^2e^{-bx^2}\right) + \alpha\,|x|\,Ae^{-bx^2}$$

$$\hat{H}\,|\psi(x)\rangle = \frac{\hbar^2}{m}bAe^{-bx^2} - \frac{\hbar^2}{m}2bAx^2e^{-bx^2} + \alpha\,|x|\,Ae^{-bx^2}$$

The expectation value of the Hamiltonian is then given by:

$$\langle\psi(x)|\,\hat{H}\,|\psi(x)\rangle = \frac{\hbar^2}{m}bA^2 \underbrace{\int_{-\infty}^{\infty} e^{-2bx^2} \; dx}_{\text{Term 1}} - \frac{\hbar^2}{m}2bA^2 \underbrace{\int_{-\infty}^{\infty} x^2 e^{-2bx^2} \; dx}_{\text{Term 2}} + \alpha A^2 \underbrace{\int_{-\infty}^{\infty} |x|\, e^{-2bx^2} \; dx}_{\text{Term 3}}$$

Term 1

We have already normalized this term previously and therefore get:

$$\underline{\frac{\hbar^2}{m}bA}$$

Term 2

Using Rottman we find that this integral is evaluated to the following:

$$\int_{-\infty}^{\infty} x^2 e^{-2bx^2} \, \mathrm{d}x = \frac{1}{2}\sqrt{\frac{\pi}{8b^3}}$$

This gives the final:

$$\underline{-\frac{\hbar^2}{m} A \sqrt{\frac{\pi}{8b^3}}}$$

Term 3

Splitting up the integral into two parts we get:

$$\int_{-\infty}^{\infty} |x| \, e^{-2bx^2} \, \mathrm{d}x = \int_{-\infty}^{0} -xe^{-2bx^2} \, \mathrm{d}x + \int_{0}^{\infty} xe^{-2bx^2} \, \mathrm{d}x$$

Which can be rewritten as:

$$2\int_{0}^{\infty} xe^{-2bx^2} \, \mathrm{d}x$$

Again using Rottman we find this to be:

$$\frac{1}{2b}$$

Adding the constants we get:

$$\underline{\alpha A^2 \frac{1}{2b}}$$

Final result

$$\left\langle \hat{H} \right\rangle = \frac{\hbar^2}{m} bA - \frac{\hbar^2}{m} A \sqrt{\frac{\pi}{8b^3}} + \alpha A^2 \frac{1}{2b}$$

Problem 9.3 (H)

Using the given Hamiltonian, we find its expectation value.

$$\langle \psi | \, \hat{H} \, | \psi \rangle = \int_{-\infty}^{\infty} \langle \psi | \left(\frac{p^2}{2m} - \alpha \delta^3(\vec{r}) \right) | \psi \rangle \, \mathrm{d}x$$

The dirac-delta picks out the value of the wavefunction at the origin and for the other integral we use Rottman:

$$\langle \psi | \, \hat{H} \, | \psi \rangle = A\sqrt{2L^2\pi} \frac{\vec{p}^2}{2m} - \alpha A$$

Problem 9.4 (H)

We try the same state as in the previous exercise:

$$|\psi(x,y,z)\rangle = Ae^{-r^2/2L} = Ae^{-(x^2+y^2+z^2)/2L}$$

Again we must normalize:

$$\int_{-\infty}^{\infty} |\psi|^2 \ \mathrm{d}r = A^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-(x^2+y^2+z^2)} \ \mathrm{d}x \ \mathrm{d}y \ \mathrm{d}z = 1$$

This is just the same integral repeated. Using Rottmann we find that this is equal to:

$$A^2 \left(\sqrt{\pi L^2}\right)^3 = 1 \rightarrow A = \frac{1}{(\pi L^2)^{3/4}} = \left(\pi L^2\right)^{-3/4}$$

For simplicity, we divide the Hamiltonian into a kinetic and potential part:

$$\hat{H} = \hat{T} + \hat{V} \rightarrow \left\langle \hat{H} \right\rangle = \left\langle \hat{T} \right\rangle + \left\langle \hat{V} \right\rangle$$

$$\left\langle \hat{T} \right\rangle = -\frac{\hbar^2}{2m} |A|^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle\psi| \nabla^2 |\psi\rangle \ \mathrm{d}x \ \mathrm{d}y \ \mathrm{d}z$$