

## VARIATIONAL PRINCIPLE AND THE HARMONIC OSCILLATOR (QUARTIC WAVE FUNCTION)

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.4.

Here we'll apply the variational principle again to the harmonic oscillator, this time with potential

$$\psi(x) = \begin{cases} (x-a)^2(x+a)^2 & x \leq |a| \\ 0 & |x| > a \end{cases} \quad (1)$$

Here  $a$  is the parameter to be varied, and we can see that it controls the width of the trial wave function as well as its height. We first find the normalization constant

$$N \equiv \langle \psi | \psi \rangle = \int_{-a}^a (x-a)^4 (x+a)^4 dx \quad (2)$$

$$= \frac{256}{315} a^9 \quad (3)$$

where I used Maple to do and simplify the integral. If you want to do it by hand, it's probably easiest to use the substitution  $u = x - a$  before multiplying out the factors in the integrand.

The energy estimate is then obtained by minimizing

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad (4)$$

where the Hamiltonian contains the harmonic oscillator potential:

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \quad (5)$$

To calculate  $\langle \psi | H | \psi \rangle$  requires integrating a sixth-degree polynomial which is straightforward but very tedious to do by hand if you like (which is probably why the exercise is marked as 'optional' in Shankar), but again I used Maple to get

$$\frac{d^2\psi}{dx^2} = 12x^2 - 4a^2 \quad (6)$$

$$\langle \psi | H | \psi \rangle = \int_{-a}^a (x-a)^2 (x+a)^2 \left[ -\frac{\hbar^2}{2m} (12x^2 - 4a^2) + \right. \quad (7)$$

$$\left. \frac{1}{2} m \omega^2 x^2 (x-a)^2 (x+a)^2 \right] dx \quad (8)$$

$$= \frac{128}{3465} \left( a^{11} m \omega^2 + 33 \frac{\hbar^2 a^7}{m} \right) \quad (9)$$

The expression to minimize is therefore

$$E = \frac{128}{3465} \left( a^{11} m \omega^2 + 33 \frac{\hbar^2 a^7}{m} \right) \times \frac{315}{256 a^9} \quad (10)$$

$$= \frac{1}{22} \left( a^2 m \omega^2 + \frac{33 \hbar^2}{m} a^{-2} \right) \quad (11)$$

Taking the derivative, we need to solve

$$\frac{dE}{da} = \frac{1}{11} \left( 2 a m \omega^2 - \frac{33 \hbar^2}{m} a^{-3} \right) = 0 \quad (12)$$

This gives an optimum value for  $a$ :

$$a_0 = 33^{1/4} \sqrt{\frac{\hbar}{m \omega}} \quad (13)$$

Substituting into 11 we get the estimate of the ground state energy

$$E_0 = \frac{\sqrt{33}}{11} \hbar \omega \simeq 0.522 \hbar \omega \quad (14)$$

The exact ground state energy for the harmonic oscillator is  $\frac{1}{2} \hbar \omega$  so this estimate is reasonably good.

This answer agrees with the back-of-the-book answer in Shankar, since

$$\frac{\sqrt{33}}{11} = \frac{1}{2} \frac{\sqrt{4 \times 33}}{11} = \frac{1}{2} \frac{\sqrt{12 \times 11}}{11} = \frac{1}{2} \sqrt{\frac{12}{11}} \quad (15)$$