VARIATIONAL PRINCIPLE AND THE HARMONIC OSCILLATOR (QUARTIC WAVE FUNCTION)

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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

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

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

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

$$=\frac{256}{315}a^9 \tag{3}$$

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

$$E=\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{4}$$

where the Hamiltonian contains the harmonic oscillator potential:

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

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

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

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

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

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

The expression to minimize is therefore

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

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

Taking the derivative, we need to solve

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

This gives an optimum value for a:

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

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

$$E_0 = \frac{\sqrt{33}}{11}\hbar\omega \simeq 0.522\hbar\omega \tag{14}$$

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

$$\frac{\sqrt{33}}{11} = \frac{1}{2}\frac{\sqrt{4\times33}}{11} = \frac{1}{2}\frac{\sqrt{12\times11}}{11} = \frac{1}{2}\sqrt{\frac{12}{11}} \tag{15}$$