

## VARIATIONAL PRINCIPLE AND THE HARMONIC OSCILLATOR - 2

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.11.

Here's an estimate of the first two energy levels of the harmonic oscillator using the variational principle. Our trial function is

$$(1) \quad \psi = \begin{cases} A \cos \frac{\pi x}{a} & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ 0 & \text{otherwise} \end{cases}$$

First, we normalize the wave function:

$$(2) \quad 1 = |A|^2 \int_{-a/2}^{a/2} \cos^2 \frac{\pi x}{a} dx$$

$$(3) \quad A = \sqrt{\frac{2}{a}}$$

We can now calculate  $\langle H \rangle$ :

$$(4) \quad \langle H \rangle = \langle \psi | H | \psi \rangle = \langle \psi | T + V | \psi \rangle$$

The kinetic energy term  $T$  contains the second derivative of  $\psi$  which contains delta functions at  $x = \pm \frac{a}{2}$ . However, since  $\psi$  itself is zero at these two points, we don't need to worry about these points, so we can just ignore the delta functions in what follows.

For the kinetic energy operator  $T$  we have

$$(5) \quad T | \psi \rangle = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2}$$

$$(6) \quad = \frac{\hbar^2 \pi^2}{\sqrt{2} m a^{3/2}} \cos \frac{\pi x}{a}$$

The potential energy is

$$(7) \quad V|\psi\rangle = \frac{1}{2}m\omega^2x^2\psi$$

$$(8) \quad = \frac{m\omega^2x^2}{\sqrt{2a}} \cos \frac{\pi x}{a}$$

Combining them we get

$$(9) \quad \langle H \rangle = \sqrt{\frac{2}{a}} \int_{-a/2}^{a/2} \left( \frac{\hbar^2 \pi^2}{\sqrt{2ma^{3/2}}} \cos^2 \frac{\pi x}{a} + \frac{m\omega^2x^2}{\sqrt{2a}} \cos^2 \frac{\pi x}{a} \right) dx$$

$$(10) \quad = \frac{(\pi^2 - 6)m^2\omega^2a^4 + 12\pi^4\hbar^2}{24\pi^2ma^2}$$

To find the value of  $a$  that minimizes  $\langle H \rangle$  we take the derivative and set to zero as usual, and find that

$$(11) \quad a_{min} = \frac{3^{1/4}\pi}{(\pi^2 - 6)^{1/4}} \sqrt{\frac{2\hbar}{m\omega}}$$

with the corresponding energy of

$$(12) \quad \langle H \rangle_{min} = \frac{\sqrt{3(\pi^2 - 6)}}{6} \hbar\omega$$

$$(13) \quad \approx 0.569\hbar\omega$$

$$(14) \quad > \frac{1}{2}\hbar\omega$$

The estimate here is quite close to the exact value.

We can now use the corollary to the variational principle to get an estimate of the first excited state. To do this, we need to find a trial function that is orthogonal to the *true ground state* wave function. We know that this is

$$(15) \quad \psi_0 = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-m\omega x^2/2\hbar}$$

so, since it's an even function, any odd function is orthogonal to it. We can therefore use

$$(16) \quad \psi = B \sin \frac{\pi x}{a}$$

Following the same procedure as above, we first normalize  $\psi$ :

$$(17) \quad 1 = |B|^2 \int_{-a/2}^{a/2} \sin^2 \frac{\pi x}{a} dx$$

$$(18) \quad B = \frac{1}{\sqrt{a}}$$

For the kinetic energy operator  $T$  we have

$$(19) \quad T|\psi\rangle = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2}$$

$$(20) \quad = \frac{\hbar^2 \pi^2}{2ma^5/2} \sin \frac{\pi x}{a}$$

The potential energy is

$$(21) \quad V|\psi\rangle = \frac{1}{2} m \omega^2 x^2 \psi$$

$$(22) \quad = \frac{m \omega^2 x^2}{2\sqrt{a}} \sin \frac{\pi x}{a}$$

Combining them we get

$$(23) \quad \langle H \rangle = \frac{1}{\sqrt{a}} \int_{-a/2}^{a/2} \left( \frac{\hbar^2 \pi^2}{2ma^5/2} \sin^2 \frac{\pi x}{a} + \frac{m \omega^2 x^2}{2\sqrt{a}} \sin^2 \frac{\pi x}{a} \right) dx$$

$$(24) \quad = \frac{(2\pi^2 - 3) m^2 \omega^2 a^4 + 6\pi^4 \hbar^2}{12ma^2}$$

To find the value of  $a$  that minimizes  $\langle H \rangle$  we take the derivative and set to zero as usual, and find that

$$(25) \quad a_{min} = \frac{6^{1/4} \pi}{(2\pi^2 - 3)^{1/4}} \sqrt{\frac{\hbar}{m\omega}}$$

$$(26) \quad \langle H \rangle_{min} = \frac{\sqrt{6(2\pi^2 - 3)}}{6} \hbar \omega$$

$$(27) \quad \approx 1.67 \hbar \omega$$

$$(28) \quad > \frac{3}{2} \hbar \omega$$

Again, we get a reasonable upper bound on the energy.