Quantum Mechanics 2

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Variational Method

Harmonic Oscillator

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Harmonic Oscillator

Let us use the variational method to make an approximation of the ground state energy of a harmonic oscillator

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

The important thing to remember in selecting a trial function is that it must satisfy the boundary conditions of the system. In this case, the boundary condition is that the wave function must vanish at $\pm\infty$. One such function is

$$\tilde{\psi} = e^{-\alpha|x|}$$

With this,

$$\langle\tilde{\psi}|\tilde{\psi}\rangle = \int_{-\infty}^{\infty} e^{-2\alpha|x|}\,dx = 2\int_{0}^{\infty} e^{-2\alpha x}\,dx = -2\left.\frac{e^{-2\alpha x}}{2\alpha}\right|_0^{\infty} = \frac{2}{2\alpha}$$

Harmonic Oscillator

For $x < 0$, $x = -|x|$

$$H\tilde{\psi} = -\frac{\hbar^2}{2m}\frac{d^2 e^{\alpha x}}{dx^2} + \frac{1}{2}m\omega^2 x^2 e^{\alpha x} = \left[-\frac{\hbar^2\alpha^2}{2m} + \frac{1}{2}m\omega^2 x^2\right] e^{-\alpha|x|}$$

For $x > 0$, $x = |x|$

$$H\tilde{\psi} = -\frac{\hbar^2}{2m}\frac{d^2 e^{-\alpha x}}{dx^2} + \frac{1}{2}m\omega^2 x^2 e^{-\alpha x} = \left[-\frac{\hbar^2\alpha^2}{2m} + \frac{1}{2}m\omega^2 x^2\right] e^{-\alpha|x|}$$

Thus,

$$\langle\tilde{\psi}|H|\tilde{\psi}\rangle = \int_{-\infty}^{\infty}\left[-\frac{\hbar^2\alpha^2}{2m} + \frac{1}{2}m\omega^2 x^2\right] e^{-2\alpha|x|}\, dx$$

$$= 2\int_{0}^{\infty}\left[-\frac{\hbar^2\alpha^2}{2m} + \frac{1}{2}m\omega^2 x^2\right] e^{-2\alpha x}\, dx$$

Harmonic Oscillator

The first term is

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

The second term may be evaluated using Gamma functions

$$\Gamma(z) = \int_0^\infty t^{z-1}\,e^{-t}dt$$

So

$$m\omega^2\int_0^\infty x^2 e^{-2\alpha x}\,dx = \frac{m\omega^2}{(2\alpha)^3}\Gamma(3) = \frac{m\omega^2}{(2\alpha)^3}2!$$

and

$$\bar{H} = \frac{\langle\tilde{\psi}|H|\tilde{\psi}\rangle}{\langle\tilde{\psi}|\tilde{\psi}\rangle} = -\frac{\hbar^2\alpha^2}{2m} + \frac{m\omega^2}{4\alpha^2}$$

Harmonic Oscillator

To optimize, we set

$$\frac{\partial \bar{H}}{\partial \alpha} = 0$$

This yields

$$-\frac{\hbar^2 \alpha}{m} - \frac{m\omega^2}{2\alpha^3} = 0$$

$$\alpha^4 = -\frac{m^2\omega^2}{2\hbar^2}$$

$$\alpha^2 = \pm i \frac{m\omega}{\sqrt{2}\hbar}$$

This however gives

$$\bar{H} = -\frac{\hbar^2\alpha^2}{2m} + \frac{m\omega^2}{4\alpha^2} = -i\frac{\hbar\omega}{2\sqrt{2}} + \frac{\sqrt{2}\hbar\omega}{4i} = -\frac{i}{\sqrt{2}}\hbar\omega$$

This shows that $\tilde{\psi} = e^{-\alpha|x|}$ is not a tenable trial function.