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 boundary condition in this case is that the wave function must vanish at $\pm\infty$. One such function is

$$\tilde{\psi} = e^{-\alpha x^2}$$

With this,

$$\langle\tilde{\psi}|\tilde{\psi}\rangle = \int_{-\infty}^{\infty} e^{-2\alpha x^2}\,dx = \sqrt{\frac{\pi}{2\alpha}}$$

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Now

$$\frac{d^2 e^{-\alpha x^2}}{dx^2} = \frac{d}{dx}\left(-2\alpha x e^{-\alpha x^2}\right) = -2\alpha e^{-\alpha x^2} + (-2\alpha x)^2 e^{-\alpha x^2}$$

Hence

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

Thus,

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

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

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The first term is

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

The second term may be evaluated using Gamma functions

$$\Gamma(z) = 2\int_0^\infty u^{2z-1}\, e^{-u^2}\,du$$

So

$$2\int_0^\infty x^2 e^{-2\alpha x^2}\,dx = \frac{\Gamma(3/2)}{(2\alpha)^{3/2}} = \frac{1}{(2\alpha)^{3/2}}\frac{\Gamma(1/2)}{2} = \frac{1}{4\alpha}\sqrt{\frac{\pi}{2\alpha}}$$

and

$$\bar{H} = \frac{\langle\tilde{\psi}|H|\tilde{\psi}\rangle}{\langle\tilde{\psi}|\tilde{\psi}\rangle} = \frac{\hbar^2\alpha}{m} + \left(\frac{1}{2}m\omega^2 - \frac{2\hbar^2\alpha^2}{m}\right)\frac{1}{4\alpha} = \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha}$$

Harmonic Oscillator

To optimize, we set

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

This yields

$$\frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha^2} = 0$$

or

$$\alpha = \frac{m\omega}{2\hbar}$$

This gives

$$\bar{H} = \frac{\hbar^2 \alpha}{2m} + \frac{m\omega^2}{8\alpha} = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

which is the exact value of the ground state.