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

$$\tilde{\psi} = \frac{1}{x^2 + a^2}$$

With this,

$$\langle\tilde{\psi}|\tilde{\psi}\rangle = \int_{-\infty}^{\infty}\left(\frac{1}{x^2 + a^2}\right)^2 dx$$

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If we let

$$x = a\tan\theta$$

$$dx = a\sec^2\theta\, d\theta$$

$$\left(\frac{1}{x^2+a^2}\right)^2 dx = \frac{a\sec^2\theta\, d\theta}{(a^2\tan^2\theta + a^2)^2} = \frac{\sec^2\theta\, d\theta}{a^3\sec^4\theta} = \frac{1}{a^3}\cos^2\theta\, d\theta$$

then

$$\langle\tilde{\psi}|\tilde{\psi}\rangle = \int_{-\infty}^{\infty}\left(\frac{1}{x^2+a^2}\right)^2 dx = \frac{1}{a^3}\int_{-\pi/2}^{\pi/2}\cos^2\theta\, d\theta = \frac{1}{a^3}\left[\frac{\theta}{2} - \frac{1}{4}\sin 2\theta\right]_{-\pi/2}^{\pi/2} = \frac{\pi}{2a^3}$$

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Now

$$\frac{d^2}{dx^2}\left(\frac{1}{x^2+a^2}\right)=\frac{d}{dx}\left(\frac{-2x}{(x^2+a^2)^2}\right)=\frac{8x^2}{(x^2+a^2)^3}-\frac{2}{(x^2+a^2)^2}$$

Hence

$$H\tilde{\psi}=-\frac{\hbar^2}{2m}\left[\frac{8x^2}{(x^2+a^2)^3}-\frac{2}{(x^2+2)^2}\right]+\frac{m\omega^2x^2}{2(x^2+a^2)}$$

and

$$\langle\tilde{\psi}|H|\tilde{\psi}\rangle=\int_{-\infty}^{\infty}\left[-\frac{\hbar^2}{2m}\left[\frac{8x^2}{(x^2+a^2)^4}-\frac{2}{(x^2+a^2)^3}\right]+\frac{m\omega^2x^2}{2(x^2+a^2)^2}\right]dx$$

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With

$$x = a\tan\theta$$
$$dx = a\sec^2\theta\, d\theta$$

We have

$$\frac{8x^2dx}{(x^2+a^2)^4} = \frac{8a^3\tan^2\theta\sec^2\theta\, d\theta}{a^8\sec^8\theta} = \frac{8\sin^2\theta d\theta}{a^5\sec^4\theta} = \frac{8}{a^5}\sin^2\theta\cos^4\theta d\theta$$

$$\frac{2dx}{(x^2+a^2)^3} = \frac{2a\sec^2\theta\, d\theta}{a^6\sec^6\theta} = \frac{2}{a^5}\cos^4\theta d\theta$$

$$\frac{x^2dx}{(x^2+a^2)^2} = \frac{a^3\tan^2\theta\sec^2\theta\, d\theta}{a^4\sec^4\theta} = \frac{1}{a}\sin^2\theta\, d\theta$$

and

$$\langle\tilde{\psi}|H|\tilde{\psi}\rangle = \int_{-\pi/2}^{\pi/2}\left[-\frac{\hbar^2}{2m}\left[\frac{8}{a^5}\sin^2\theta\cos^4\theta - \frac{2}{a^5}\cos^4\theta\right] + \frac{m\omega^2}{2a}\sin^2\theta\right]d\theta$$

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Now

$$\frac{8}{a^5}\sin^2\theta\cos^4\theta - \frac{2}{a^5}\cos^4\theta = \left[\frac{8}{a^5}(1-\cos^2\theta) - \frac{2}{a^5}\right]\cos^4\theta = \frac{6}{a^5}\cos^4\theta - \frac{8}{a^5}\cos^6\theta$$

Using the general formula

$$\cos^{2\mathrm{n}}\theta = \frac{1}{2^{2n}}\binom{2n}{n} + \frac{1}{2^{2n-1}}\left\{\cos 2n\theta + \binom{2n}{1}\cos(2n-2)\theta + \cdots + \binom{2n}{n-1}\cos 2\theta\right\}$$

We have

$$\cos^4\theta = \frac{3}{8} + \frac{1}{2}\cos 2\theta + \frac{1}{8}\cos 4\theta$$

$$\cos^6\theta = \frac{5}{16} + \frac{15}{32}\cos 2\theta + \frac{3}{16}\cos 4\theta + \frac{1}{32}\cos 6\theta$$

We also have

$$\sin^2\theta = \frac{1}{2} - \frac{1}{2}\cos 2\theta$$

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Hence

$$\frac{8}{a^5}\sin^2\theta\cos^4\theta-\frac{2}{a^5}\cos^4\theta$$
$$=\frac{1}{a^5}\left[\frac{9}{4}+3\cos 2\theta+\frac{3}{4}\cos 4\theta-\frac{5}{2}-\frac{15}{4}\cos 2\theta-\frac{3}{2}\cos 4\theta-\frac{1}{4}\cos 6\theta\right]$$
$$=\frac{1}{a^5}\left[-\frac{1}{4}-\frac{3}{4}\cos 2\theta-\frac{3}{4}\cos 4\theta-\frac{1}{4}\cos 6\theta\right]$$

and

$$\langle\tilde{\psi}|H|\tilde{\psi}\rangle=\int_{-\pi/2}^{\pi/2}\left[\frac{\hbar^2}{8ma^5}(1+3\cos 2\theta+3\cos 4\theta+\cos 6\theta)+\frac{m\omega^2}{4a}(1-\cos 2\theta)\right]d\theta$$
$$=\left[\frac{\hbar^2}{8ma^5}\left(\theta+\frac{3}{2}\sin 2\theta+\frac{3}{4}\sin 4\theta+\frac{1}{6}\sin 6\theta\right)+\frac{m\omega^2}{4a}\left(\theta-\frac{1}{2}\sin 2\theta\right)\right]_{-\pi/2}^{\pi/2}$$
$$=\frac{\hbar^2\pi}{8ma^5}+\frac{m\omega^2\pi}{4a}$$

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We thus have

$$\bar{H} = \frac{\langle\tilde{\psi}|H|\tilde{\psi}\rangle}{\langle\tilde{\psi}|\tilde{\psi}\rangle} = \frac{\hbar^2}{4ma^2} + \frac{1}{2}m\omega^2 a^2$$

To optimize, we set

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

This translates to

$$-\frac{\hbar^2}{2ma^3} + m\omega^2 a = 0$$

which gives

$$a^2 = \frac{\hbar}{\sqrt{2}m\omega}$$

Harmonic Oscillator

Our best estimate for the oscillator ground state energy using the trial function

$$\tilde{\psi} = \frac{1}{x^2 + a^2}$$

is therefore

$$\bar{H} = \frac{\sqrt{2}\hbar\omega}{4} + \frac{\hbar\omega}{2\sqrt{2}} = \frac{\hbar\omega}{\sqrt{2}}$$

Note that this is higher than the actual ground state energy $\frac{\hbar\omega}{2}$. The error of our estimate is

$$\frac{\frac{\hbar\omega}{\sqrt{2}} - \frac{\hbar\omega}{2}}{\frac{\hbar\omega}{2}} = \sqrt{2} - 1 = 41.4\%$$

This just goes to show that the choice of trial function matters a lot.