

## Variational principle for the harmonic oscillator

$$\psi(x) = \frac{A}{x^2 + b^2} \quad \text{let} \quad \tilde{x} \equiv \frac{x}{b}$$

Normalization: [[Integral from Dwight 120.2.]]

$$\begin{aligned} 1 &= \int_{-\infty}^{+\infty} \psi^* \psi dx = \int_{-\infty}^{+\infty} \frac{|A|^2}{(x^2 + b^2)^2} dx = |A|^2 \int_{-\infty}^{+\infty} \frac{1}{(b^2 \tilde{x}^2 + b^2)^2} b d\tilde{x} = \frac{|A|^2}{b^3} \int_{-\infty}^{+\infty} \frac{d\tilde{x}}{(\tilde{x}^2 + 1)^2} \\ &= \frac{|A|^2}{b^3} \left[ \frac{\tilde{x}}{2(\tilde{x}^2 + 1)} + \frac{1}{2} \arctan \tilde{x} \right]_{-\infty}^{+\infty} = \frac{|A|^2}{b^3} \left[ \frac{1}{2} \left( \frac{\pi}{2} \right) - \frac{1}{2} \left( -\frac{\pi}{2} \right) \right] = \frac{|A|^2}{b^3} \frac{\pi}{2}. \end{aligned}$$

Kinetic energy:

$$\begin{aligned} \langle \text{KE} \rangle &= -\frac{\hbar^2}{2m} |A|^2 \int_{-\infty}^{+\infty} \frac{1}{x^2 + b^2} \frac{d^2}{dx^2} \left( \frac{1}{x^2 + b^2} \right) dx = -\frac{\hbar^2}{2m} |A|^2 \int_{-\infty}^{+\infty} \frac{1}{b^2 \tilde{x}^2 + b^2} \frac{1}{b^2} \frac{d^2}{d\tilde{x}^2} \left( \frac{1}{b^2 \tilde{x}^2 + b^2} \right) b d\tilde{x} \\ &= -\frac{\hbar^2}{2m} \frac{|A|^2}{b^5} \underbrace{\int_{-\infty}^{+\infty} \frac{1}{\tilde{x}^2 + 1} \frac{d^2}{d\tilde{x}^2} \left( \frac{1}{\tilde{x}^2 + 1} \right) d\tilde{x}}_{\equiv -C_K} = \frac{\hbar^2}{2m} \frac{2}{\pi b^2} C_K \end{aligned}$$

[This makes sense: a narrow wavefunction (small  $b$ ) will have large curvature and hence large kinetic energy.]

Potential energy:

$$\begin{aligned} \langle \text{PE} \rangle &= \frac{m\omega^2}{2} \langle x^2 \rangle = \frac{m\omega^2}{2} |A|^2 \int_{-\infty}^{+\infty} \frac{x^2}{(x^2 + b^2)^2} dx = \frac{m\omega^2}{2} |A|^2 \int_{-\infty}^{+\infty} \frac{b^2 \tilde{x}^2}{(b^2 \tilde{x}^2 + b^2)^2} b d\tilde{x} \\ &= \frac{m\omega^2}{2} \frac{|A|^2}{b} \underbrace{\int_{-\infty}^{+\infty} \frac{\tilde{x}^2}{(\tilde{x}^2 + 1)^2} d\tilde{x}}_{\equiv C_P} = \frac{m\omega^2}{2} \frac{2b^2}{\pi} C_P \end{aligned}$$

[This makes sense: a wide wavefunction (large  $b$ ) will extend into the region of high potential energy.]

Total energy:

$$\langle H \rangle = \frac{\hbar^2}{2m} \frac{2}{\pi b^2} C_K + \frac{m\omega^2}{2} \frac{2b^2}{\pi} C_P$$

To minimize  $\langle H \rangle$ , take the derivative with respect to  $b$  and set equal to zero:

$$\frac{\partial \langle H \rangle}{\partial b} = \frac{2}{\pi} \left[ -\frac{\hbar^2}{2m} \frac{2}{b^3} C_K + \frac{m\omega^2}{2} 2b C_P \right] = 0 \quad \implies \quad b^2 = \frac{\hbar}{m\omega} \sqrt{\frac{C_K}{C_P}}$$

This value of  $b^2$  results in

$$\langle H \rangle_{\min} = \frac{2}{\pi} \hbar\omega \sqrt{C_K C_P}.$$

Evaluate the integrals: [[For the  $C_K$  integral, use parts followed by Dwight 122.4.]]

$$\begin{aligned}C_K &= -\int_{-\infty}^{+\infty} \frac{1}{\tilde{x}^2+1} \frac{d^2}{d\tilde{x}^2} \left( \frac{1}{\tilde{x}^2+1} \right) d\tilde{x} = \int_{-\infty}^{+\infty} \frac{d}{d\tilde{x}} \left( \frac{1}{\tilde{x}^2+1} \right) \frac{d}{d\tilde{x}} \left( \frac{1}{\tilde{x}^2+1} \right) d\tilde{x} \\&= \int_{-\infty}^{+\infty} \left[ \frac{d}{d\tilde{x}} \left( \frac{1}{\tilde{x}^2+1} \right) \right]^2 d\tilde{x} = \int_{-\infty}^{+\infty} \left[ \frac{-2\tilde{x}}{(\tilde{x}^2+1)^2} \right]^2 d\tilde{x} = 4 \int_{-\infty}^{+\infty} \frac{\tilde{x}^2}{(\tilde{x}^2+1)^4} d\tilde{x} \\&= 4 \left[ \frac{1}{16} \arctan \tilde{x} \right]_{-\infty}^{+\infty} = \frac{1}{4} \left[ \frac{\pi}{2} - \left( -\frac{\pi}{2} \right) \right] = \frac{\pi}{4} \\C_P &= \int_{-\infty}^{+\infty} \frac{\tilde{x}^2}{(\tilde{x}^2+1)^2} d\tilde{x} = \left[ \frac{1}{2} \arctan \tilde{x} \right]_{-\infty}^{+\infty} = \frac{\pi}{2}\end{aligned}$$

So

$$\langle H \rangle_{\min} = \frac{1}{\sqrt{2}} \hbar \omega = 0.707 \hbar \omega > \frac{1}{2} \hbar \omega.$$

*Grading:* 2 points for each of sections “Normalization”, “Kinetic energy”, “Potential energy”, “Minimization”, and “Evaluate”.