The Heisenberg Uncertainty Principle can be written in an "extended" form as:

$$\sigma_A^2\sigma_B^2 \geq \left|\tfrac{1}{2}\left\langle\left\{\hat{A},\hat{B}\right\}\right\rangle - \left\langle\hat{A}\right\rangle\left\langle\hat{B}\right\rangle\right|^2 + \left|\tfrac{1}{2i}\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|^2 \tag{1.1}$$

implying that

$$\sigma_A^2\sigma_B^2 \geq \tfrac{1}{4}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|^2 \tag{1.2}$$

Special case: Position and momentum.

$$\sigma_x^2\sigma_p^2 \geq \tfrac{1}{4}\left|\left\langle\left[x,\hat{p}\right]\right\rangle\right|^2 \tag{1.3}$$

The right-hand-side can be simplified,

$$\begin{aligned}
\left\langle\left[\hat{x},\hat{p}\right]\right\rangle &= \int \Psi^*(x)\left(x\cdot -i\hbar\tfrac{d}{dx} - \left(-i\hbar\tfrac{d}{dx}x\right)\right)\Psi(x)\,dx \\
&= -i\hbar\int \Psi^*(x)\left(x\cdot\tfrac{d\Psi(x)}{dx} - \left(\tfrac{d}{dx}x\Psi(x)\right)\right)dx \\
&= -i\hbar\int \Psi^*(x)\left(x\cdot\tfrac{d\Psi(x)}{dx} - x\left(\tfrac{d\Psi(x)}{dx}\right) - \Psi(x)\right)dx \\
&= -i\hbar\int \Psi^*(x)\left(-\Psi(x)\right)dx \\
&= i\hbar
\end{aligned} \tag{1.4}$$

So

$$\begin{aligned}
\sigma_x^2\sigma_p^2 &\geq \tfrac{1}{4}\left|i\hbar\right|^2 = \tfrac{\hbar^2}{4} \\
\sigma_x\sigma_p &\geq \tfrac{1}{2}\hbar
\end{aligned} \tag{1.5}$$

Implication:

For a bound state,

$$\sigma_p^2 = \left\langle\hat{p}^2\right\rangle - \left\langle\hat{p}\right\rangle^2 = \left\langle\hat{p}^2\right\rangle = 2m\left\langle\hat{T}\right\rangle \tag{1.6}$$

So

$$\left\langle\hat{T}\right\rangle \geq \frac{\hbar}{2\sigma_x^2} = \frac{\hbar}{2\cdot\left(\int\Psi^*(x)x^2\Psi(x)\,dx - \left(\int\Psi^*(x)x\Psi(x)\,dx\right)^2\right)} \tag{1.7}$$

So the "smaller" the system is, the high its kinetic energy. Confining a system raises its kinetic energy.

Example:

For the particle in a box,

$$\begin{aligned}
\hat{T} &= E = \tfrac{h^2n^2}{8ma^2} \\
2m\hat{T} &= \sigma_p^2 = \frac{h^2n^2}{4a^2}
\end{aligned} \tag{1.8}$$

The average position is the middle of the box,

$$\int_0^a \Psi^*(x)x\Psi(x)\,dx = \tfrac{1}{2}a \tag{1.9}$$

and the expectation value of x^2 is

$$\int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)x^2\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)dx = \frac{2}{a}\int_0^a x^2\sin^2\left(\frac{n\pi x}{a}\right)dx$$
$$= \frac{2}{a}\left(\frac{a^2}{n^2\pi^2}\right)\int_0^a\left(\frac{n\pi x}{a}\right)^2\sin^2\left(\frac{n\pi x}{a}\right)dx$$
$$= \frac{2a}{n^2\pi^2}\int_0^{n\pi}u^2\sin^2 u\left(\tfrac{a}{n\pi}\right)dx \qquad u=\tfrac{n\pi x}{a} \quad du=\left(\tfrac{n\pi}{a}\right)dx \tag{1.10}$$
$$= \frac{2a^2}{n^3\pi^3}\left[\tfrac{1}{6}u^3-\tfrac{1}{4}\left(u^2\sin 2u+u\cos(2u)\right)+\tfrac{1}{8}\sin 2u\right]_0^{n\pi}$$
$$= \frac{2a^2}{n^3\pi^3}\left[\tfrac{1}{6}n^3\pi^3-\tfrac{1}{4}(0+n\pi)+0\right]_0^{n\pi}$$
$$= \left(\tfrac{1}{3}-\tfrac{1}{2n^2\pi^2}\right)a^2$$

I then have

$$\sigma_x^2 = \left(\left(\tfrac{1}{3}-\tfrac{1}{2n^2\pi^2}\right)-\tfrac{1}{4}\right)a^2 = \left(\tfrac{1}{12}-\tfrac{1}{2n^2\pi^2}\right)a^2$$
$$\sigma_p^2 = \frac{h^2n^2}{4a^2}$$
$$\sigma_x^2\sigma_p^2 = \frac{h^2n^2}{4a^2}\left(\frac{1}{12}-\frac{1}{2n^2\pi^2}\right)a^2 = h^2\left(\frac{n^2}{48}-\frac{1}{8\pi^2}\right) \ge h^2\left(\frac{1}{48}-\frac{1}{8\pi^2}\right) = h^2(0.008168) \tag{1.11}$$
$$\frac{\hbar^2}{4} = \frac{h^2}{(2\pi)^2\cdot 4} = \frac{h^2}{16\cdot\pi^2} = h^2(0.006333)$$

Derivation of Eq. (1.1)

It is helpful to introduce Dirac bra-ket notation,

$$\left\langle\Phi\middle|\hat{A}\middle|\Psi\right\rangle = \int\Phi^*(x)\hat{A}\Psi(x)dx = \left\langle\Phi\middle|\hat{A}\Psi\right\rangle$$
$$\left\langle A\Phi\middle|\Psi\right\rangle = \int\left(\hat{A}\Phi(x)\right)^*\Psi(x)dx \tag{1.12}$$

So I have:

$$\sigma_A^2\sigma_B^2 = \left\langle\Psi\middle|\left(\hat{A}-\langle\hat{A}\rangle\right)^2\middle|\Psi\right\rangle\left\langle\Psi\middle|\left(\hat{B}-\langle\hat{B}\rangle\right)^2\middle|\Psi\right\rangle$$
$$= \left\langle\Psi\middle|\left(\hat{A}-\langle\hat{A}\rangle\right)\left(\hat{A}-\langle\hat{A}\rangle\right)\middle|\Psi\right\rangle c$$
$$= \left\langle\left(\hat{A}-\langle\hat{A}\rangle\right)\Psi\middle|\left(\hat{A}-\langle\hat{A}\rangle\right)\Psi\right\rangle\left\langle\left(\hat{B}-\langle\hat{B}\rangle\right)\Psi\middle|\left(\hat{B}-\langle\hat{B}\rangle\right)\Psi\right\rangle \tag{1.13}$$
$$\ge \left\langle\left(\hat{A}-\langle\hat{A}\rangle\right)\Psi\middle|\left(\hat{B}-\langle\hat{B}\rangle\right)\Psi\right\rangle\left\langle\left(\hat{B}-\langle\hat{B}\rangle\right)\Psi\middle|\left(\hat{A}-\langle\hat{A}\rangle\right)\Psi\right\rangle$$
$$= \left|\left\langle\left(\hat{A}-\langle\hat{A}\rangle\right)\Psi\middle|\left(\hat{B}-\langle\hat{B}\rangle\right)\Psi\right\rangle\right|^2$$

This last line is the Cauchy-Schwarz inequality.

As a possible extra-credit problem, show that you can deduce the Cauchy-Schwarz inequality from:

$$0 \le \int \left| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi(x) - \frac{\left\langle \Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\left(\hat{B} - \langle \hat{B} \rangle\right) \middle| \Psi \right\rangle}{\left\langle \Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)^2 \middle| \Psi \right\rangle} \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi(x) \right|^2 dx \qquad \textit{(1.14)}$$

Intuitively, the inequality is true because

$$(\mathbf{u} \cdot \mathbf{v})^2 = \left(|\mathbf{u}||\mathbf{v}|\cos(\theta_{uv})\right)^2 \le |\mathbf{u}|^2 |\mathbf{v}|^2 \qquad (1.15)$$

Now, we rewrite the key equation in a strange way,

$$\begin{aligned}
\sigma_A^2 \sigma_B^2 &\ge \left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \right\rangle \left\langle \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \right\rangle \\
&= \left[\frac{1}{2} \left(\left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \right\rangle + \left\langle \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \right\rangle \right) \right]^2 \\
&\quad + \left[\frac{1}{2i} \left(\left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \right\rangle - \left\langle \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \right\rangle \right) \right]^2 \qquad (1.16) \\
&= \left(\tfrac{1}{4} - \tfrac{1}{4}\right) \left(\left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \right\rangle \right)^2 + \left(\tfrac{1}{4} - \tfrac{1}{4}\right) \left(\left\langle \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \right\rangle \right)^2 \\
&\quad + \left(\tfrac{1}{4} + \tfrac{1}{4}\right) \left(\begin{aligned} &\left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \right\rangle \left\langle \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \right\rangle \\ &+ \left\langle \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \right\rangle \left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \right\rangle \end{aligned} \right)
\end{aligned}$$

Now we have:

$$\begin{aligned}
&\left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \right\rangle + \left\langle \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \right\rangle \\
&\qquad = \left\langle \Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\left(\hat{B} - \langle \hat{B} \rangle\right) + \left(\hat{B} - \langle \hat{B} \rangle\right)\left(\hat{A} - \langle \hat{A} \rangle\right) \middle| \Psi \right\rangle \\
&\qquad = \left\langle \Psi \middle| \begin{aligned} &\hat{A}\hat{B} - \hat{A}\langle \hat{B} \rangle - \langle \hat{A} \rangle \hat{B} + \langle \hat{A} \rangle \langle \hat{B} \rangle \\ &+ \hat{B}\hat{A} - \langle \hat{B} \rangle \hat{A} - \hat{B}\langle \hat{A} \rangle + \langle \hat{A} \rangle \langle \hat{B} \rangle \end{aligned} \middle| \Psi \right\rangle \qquad (1.17) \\
&\qquad = \left\langle \Psi \middle| \hat{A}\hat{B} + \hat{B}\hat{A} - 2\langle \hat{A} \rangle \langle \hat{B} \rangle \middle| \Psi \right\rangle \\
&\qquad = \left\langle \Psi \middle| \left\{\hat{A}, \hat{B}\right\} - 2\langle \hat{A} \rangle \langle \hat{B} \rangle \middle| \Psi \right\rangle
\end{aligned}$$

$$\begin{aligned}
&\left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \middle| \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \right\rangle - \left\langle \left(\hat{B} - \langle \hat{B} \rangle\right)\Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\Psi \right\rangle \\
&\qquad = \left\langle \Psi \middle| \left(\hat{A} - \langle \hat{A} \rangle\right)\left(\hat{B} - \langle \hat{B} \rangle\right) - \left(\hat{B} - \langle \hat{B} \rangle\right)\left(\hat{A} - \langle \hat{A} \rangle\right) \middle| \Psi \right\rangle \\
&\qquad = \left\langle \Psi \middle| \begin{aligned} &\hat{A}\hat{B} - \hat{A}\langle \hat{B} \rangle - \langle \hat{A} \rangle \hat{B} + \langle \hat{A} \rangle \langle \hat{B} \rangle \\ &- \hat{B}\hat{A} + \langle \hat{B} \rangle \hat{A} + \hat{B}\langle \hat{A} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle \end{aligned} \middle| \Psi \right\rangle \qquad (1.18) \\
&\qquad = \left\langle \Psi \middle| \hat{A}\hat{B} - \hat{B}\hat{A} \middle| \Psi \right\rangle \\
&\qquad = \left\langle \Psi \middle| \left[\hat{A}, \hat{B}\right] \middle| \Psi \right\rangle
\end{aligned}$$

$$\sigma_A^2\sigma_B^2 \ge \left\langle \left(\hat{A}-\langle\hat{A}\rangle\right)\Psi \middle| \left(\hat{B}-\langle\hat{B}\rangle\right)\Psi\right\rangle \left\langle \left(\hat{B}-\langle\hat{B}\rangle\right)\Psi \middle| \left(\hat{A}-\langle\hat{A}\rangle\right)\Psi\right\rangle$$

$$= \left[\frac{1}{2}\left(\left\langle\left\{\hat{A},\hat{B}\right\}\right\rangle - 2\langle\hat{A}\rangle\langle\hat{B}\rangle\right)\right]^2 + \left[\frac{1}{2i}\left(\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right)\right]^2 \tag{1.19}$$

Example:

Show that the Heisenberg principle is true for *every state* of the harmonic oscillator using the ladder operators to evaluate the integrals explicitly as a possible extra credit problem.

Evaluate $\langle x^2\rangle$ using the Hellmann-Feynman theorem as an extra credit problem.

For the "unitless" coordinate y you can write, in the ground state, we can do this by mathematical trickery. First, the ground-state energy is

$$E = \tfrac{1}{2}\hbar\omega(2n+1) = \tfrac{1}{2}\hbar\sqrt{\tfrac{k}{\mu}}(2n+1) = \tfrac{1}{2}\hbar\sqrt{k}\sqrt{\mu^{-1}}(2n+1)$$

$$\frac{\partial E}{\partial\mu^{-1}} = \frac{\partial}{\partial\mu^{-1}}\left\langle\Psi\middle|\frac{-\hbar^2}{2\mu}\frac{d^2}{dx^2}+\tfrac{1}{2}kx^2\middle|\Psi\right\rangle = \left\langle\Psi\middle|\frac{-\hbar^2}{2}\frac{d^2}{dx^2}\middle|\Psi\right\rangle$$

$$\frac{\partial E}{\partial\mu^{-1}} = \mu\langle\hat{T}\rangle = \mu\left(\frac{\langle\hat{p}^2\rangle}{2\mu}\right) = \tfrac{1}{2}\langle\hat{p}^2\rangle$$

$$\frac{\partial E}{\partial\mu^{-1}} = \frac{\partial}{\partial\mu^{-1}}\tfrac{1}{2}\hbar\sqrt{k}\sqrt{\mu^{-1}}(2n+1) = \tfrac{1}{4}\hbar\sqrt{k}\left(\mu^{-1}\right)^{-1/2}(2n+1) = \tfrac{1}{4}\hbar\sqrt{k\mu}(2n+1)$$

$$\langle\hat{p}^2\rangle = \tfrac{1}{2}\hbar\sqrt{k\mu}(2n+1)$$

$$\langle\hat{p}\rangle = 0$$

$$\langle\hat{T}\rangle = \frac{1}{\mu}\frac{\partial E}{\partial\mu^{-1}} = \tfrac{1}{4}\hbar\sqrt{\frac{k}{\mu}}(2n+1) = \tfrac{1}{4}\hbar\omega(2n+1) = \tfrac{1}{2}E$$

$$\langle\hat{T}\rangle + \langle V\rangle = E$$

$$\tfrac{1}{2}E + \langle V\rangle = E$$

$$\langle V\rangle = \tfrac{1}{2}E$$

$$\left\langle\tfrac{1}{2}kx^2\right\rangle = \tfrac{1}{2}E$$

$$\langle x^2\rangle = \frac{2}{k}\left(\frac{1}{2}\right)\left(\tfrac{1}{2}\hbar\omega\right)(2n+1) = \tfrac{1}{2}\hbar\left(\tfrac{1}{k}\sqrt{\tfrac{k}{\mu}}\right)(2n+1) = \frac{\tfrac{1}{2}\hbar}{\sqrt{k\mu}}(2n+1) \tag{1.20}$$

$$\langle x\rangle = 0$$

and so

$$\sigma_p^2\sigma_x^2 = \left(\tfrac{1}{2}\hbar\sqrt{k\mu}(2n+1)\right)\frac{\tfrac{1}{2}\hbar}{\sqrt{k\mu}}(2n+1) = \tfrac{1}{4}\hbar^2(2n+1)^2 \ge \tfrac{1}{4}\hbar^2 \tag{1.21}$$