15.4 Lower Bounds for Ground State Energies

We have used the variational principle to find upper bounds on ground state energies. The uncertainty principle can be used to find *lower* bounds for the ground state energy of certain systems. These two approaches work together nicely in some cases. Below we use the uncertainty principle in the form $\Delta x \Delta p \geq \hbar/2$ to find rigorous lower bounds for the ground state energy of one-dimensional Hamiltonians.

This is best illustrated by example. Consider the Hamiltonian $\hat{H}$ for a particle in a one-dimensional quartic potential:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \alpha\,\hat{x}^4, \quad \alpha > 0. \tag{15.4.1}$$

You did a variational analysis of this potential in problem 7.17, and the relevant energy scales were discussed in section 7.6. Our goal is to find a *lower bound* for the ground state energy $\langle \hat{H} \rangle_{\text{gs}}$. Taking the ground state expectation value of the Hamiltonian, we find that

$$\langle \hat{H} \rangle_{\text{gs}} = \frac{\langle \hat{p}^2 \rangle_{\text{gs}}}{2m} + \alpha\,\langle \hat{x}^4 \rangle_{\text{gs}}. \tag{15.4.2}$$

For the ground state, or in fact any bound state, the expectation value of $\hat{p}$ vanishes. Therefore, $\langle \hat{p} \rangle_{\text{gs}} = 0$, and

$$\langle \hat{p}^2 \rangle_{\text{gs}} = (\Delta p)^2_{\text{gs}}. \tag{15.4.3}$$

From the inequality $\langle \hat{Q}^2 \rangle \geq \langle \hat{Q} \rangle^2$, we find that

$$\langle \hat{x}^4 \rangle \geq \langle \hat{x}^2 \rangle^2. \tag{15.4.4}$$

Moreover, $(\Delta x)^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$ leads to $\langle \hat{x}^2 \rangle \geq (\Delta x)^2$ so that, on arbitrary states,

$$\langle \hat{x}^4 \rangle \geq (\Delta x)^4. \tag{15.4.5}$$

Therefore,

$$\langle \hat{H} \rangle_{gs} = \frac{\langle \hat{p}^2 \rangle_{gs}}{2m} + \alpha \langle \hat{x}^4 \rangle_{gs} \geq \frac{(\Delta p_{gs})^2}{2m} + \alpha (\Delta x_{gs})^4. \tag{15.4.6}$$

From the uncertainty principle,

$$\Delta x_{gs} \, \Delta p_{gs} \geq \tfrac{\hbar}{2} \quad \Rightarrow \quad \Delta p_{gs} \geq \frac{\hbar}{2 \Delta x_{gs}}. \tag{15.4.7}$$

Back to the value of $\langle \hat{H} \rangle_{gs}$, we get

$$\langle \hat{H} \rangle_{gs} \geq \frac{\hbar^2}{8m(\Delta x_{gs})^2} + \alpha (\Delta x_{gs})^4 \equiv f(\Delta x_{gs}). \tag{15.4.8}$$

The quantity to the right of the inequality defines the function $f(\Delta x_{gs})$. Figure 15.2 shows a plot of $f(\Delta x)$.

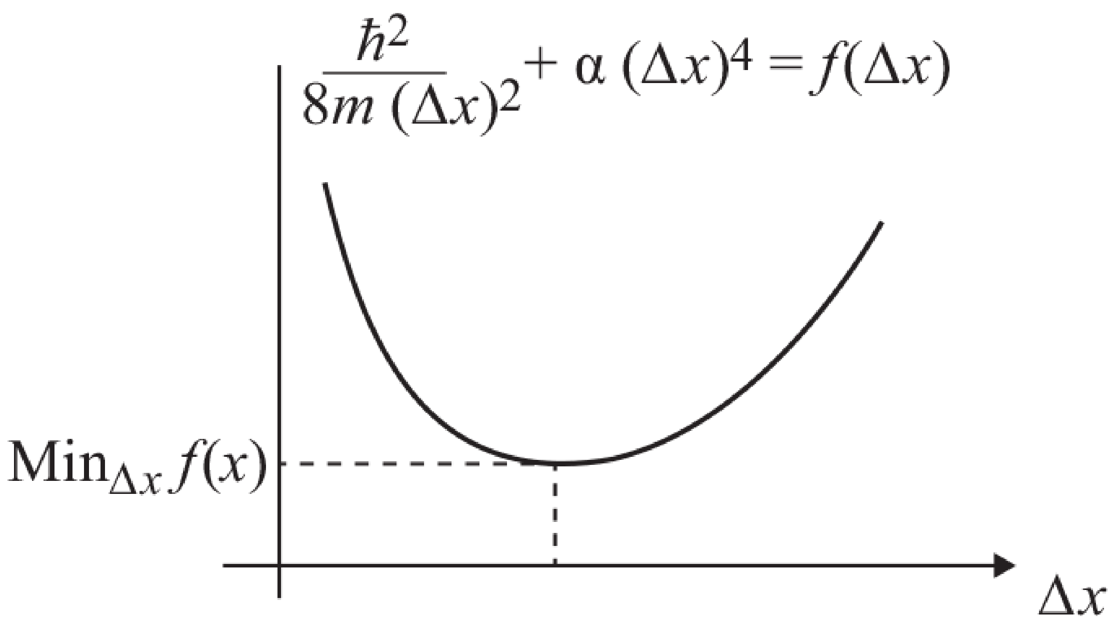

Figure 15.2
We know that $\langle \hat{H}_{gs} \rangle \geq f(\Delta x_{gs})$, but we don't know the value of Δx_{gs}. As a result, we can only be certain that $\langle \hat{H}_{gs} \rangle$ is greater than or equal to the *minimum* value the function $f(\Delta x_{gs})$ can take.

If we knew the value of Δx_{gs}, we could immediately use $\langle \hat{H} \rangle_{gs} \geq f(\Delta x_{gs})$. Since we don't know the value of Δx_{gs}, however, the only thing we can say for sure is that $\langle \hat{H} \rangle_{gs}$ is bigger than the *minimum* value that can be taken by $f(\Delta x_{gs})$ as we vary Δx_{gs}:

$$\langle \hat{H} \rangle_{\rm gs} \;\geq\; \text{Min}_{\Delta x}\Big(\frac{\hbar^2}{8m(\Delta x)^2} + \alpha\,(\Delta x)^4 \Big). \tag{15.4.9}$$

The minimization problem is straightforward. In fact, you can check that

$$\text{Min}_x\Big(\frac{A}{x^2} + Bx^4\Big) = 2^{\frac{1}{3}}\,\tfrac{3}{2}\,(A^2B)^{\frac{1}{3}}. \tag{15.4.10}$$

Applied to (15.4.9), we obtain

$$\langle \hat{H} \rangle_{\rm gs} \;\geq\; 2^{\frac{1}{3}}\,\frac{3}{8}\Big(\frac{\hbar^2\sqrt{\alpha}}{m}\Big)^{\frac{2}{3}} \;\simeq\; 0.4724\,\Big(\frac{\hbar^2\sqrt{\alpha}}{m}\Big)^{\frac{2}{3}}. \tag{15.4.11}$$

This is the final lower bound for the ground state energy. It is actually not too bad: for the exact ground state, instead of 0.4724 we would have 0.668 (obtained numerically by the shooting method in problem 7.7).