Anharmonic Oscillator

a. Using the results from the problem "Ladder Operators for the Simple Harmonic Oscillator",

$$\begin{split} &\langle m|\hat{x}^{3}|n\rangle \\ &= \sum_{\ell} \langle m|\hat{x}|\ell\rangle \langle \ell|\hat{x}^{2}|n\rangle \\ &= \left(\frac{\hbar}{2m\omega}\right)^{3/2} \sum_{\ell} \left[\sqrt{\ell}\,\delta_{m,\ell-1} + \sqrt{\ell+1}\,\delta_{m,\ell+1}\right] \\ &\times \left[\sqrt{n(n-1)}\,\delta_{\ell,n-2} + (2n+1)\delta_{\ell,n} + \sqrt{(n+1)(n+2)}\,\delta_{\ell,n+2}\right] \\ &= \left(\frac{\hbar}{2m\omega}\right)^{3/2} \left\{\sum_{\ell} \sqrt{\ell}\,\delta_{m,\ell-1}\left[\sqrt{n(n-1)}\,\delta_{\ell,n-2} + (2n+1)\delta_{\ell,n} + \sqrt{(n+1)(n+2)}\,\delta_{\ell,n+2}\right]\right\} \\ &+ \sum_{\ell} \sqrt{\ell+1}\,\delta_{m,\ell+1}\left[\sqrt{n(n-1)}\,\delta_{\ell,n-2} + (2n+1)\delta_{\ell,n} + \sqrt{(n+1)(n+2)}\,\delta_{\ell,n+2}\right]\right\} \\ &= \left(\frac{\hbar}{2m\omega}\right)^{3/2} \left\{\sqrt{m+1}\left[\sqrt{n(n-1)}\,\delta_{m+1,n-2} + (2n+1)\delta_{m+1,n} + \sqrt{(n+1)(n+2)}\,\delta_{m+1,n+2}\right] \\ &+ \sqrt{m}\left[\sqrt{n(n-1)}\,\delta_{m-1,n-2} + (2n+1)\delta_{m-1,n} + \sqrt{(n+1)(n+2)}\,\delta_{m-1,n+2}\right]\right\} \\ &= \left(\frac{\hbar}{2m\omega}\right)^{3/2}\left[\sqrt{n-2}\sqrt{n(n-1)}\,\delta_{m,n-3} + \sqrt{n}\,(2n+1)\delta_{m,n-1} + \sqrt{n+2}\,\sqrt{(n+1)(n+2)}\,\delta_{m,n+1} \\ &+ \sqrt{n-1}\,\sqrt{n(n-1)}\,\delta_{m,n-1} + \sqrt{n+1}\,(2n+1)\delta_{m,n+1} + \sqrt{n+3}\,\sqrt{(n+1)(n+2)}\,\delta_{m,n+3}\right] \\ &= \left(\frac{\hbar}{2m\omega}\right)^{3/2}\left[\sqrt{n(n-1)(n-2)}\,\delta_{m,n-3} + 3n\sqrt{n}\,\delta_{m,n-1} \\ &+ 3(n+1)\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{(n+1)(n+2)(n+3)}\,\delta_{m,n+3}\right]. \end{split}$$

b. The perturbation is $\hat{H}' = b\hat{x}^3$, so to first order

$$E_n^{(1)} = b\langle n | \hat{x}^3 | n \rangle = 0.$$

To second order (which, in this case, is the leading non-vanishing correction)

$$E_n^{(2)} = \sum_{m \neq n} \frac{H'_{n,m} H'_{m,n}}{E_n^{(0)} - E_m^{(0)}}.$$

In this case $E_n^{(0)} - E_m^{(0)} = \hbar \omega (n-m)$ and $H'_{n,m} = H'_{m,n}$, so

$$E_n^{(2)} = \sum_{m=0}^{\infty} \frac{b^2 \langle n | \hat{x}^3 | n \rangle^2}{\hbar \omega (n-m)}$$
$$= \frac{b^2}{\hbar \omega} \left(\frac{\hbar}{2m\omega}\right)^3 \sum_{m=0}^{\infty} \sum_{m \neq n}^{\infty} \frac{\text{stuff from part a}}{n-m}.$$

The sum is

$$\frac{n(n-1)(n-2)}{3} + \frac{9n^3}{1} + \frac{9(n+1)^3}{-1} + \frac{(n+1)(n+2)(n+3)}{-3} = -(30n^2 + 30n + 11)$$

whence

$$E_n^{(2)} = -\frac{b^2}{\hbar\omega} \left(\frac{\hbar}{2m\omega}\right)^3 (30n^2 + 30n + 11).$$

For large *n*, the ratio $E_n^{(2)}/E_n^{(0)}$ increases linearly with n — the energy shifts are not small. This makes sense: the SHO approximation $V(x) = \frac{1}{2}kx^2$ is valid only near the origin. Far from the origin, the "correction" term bx^3 dominates $\frac{1}{2}kx^2$. High energy states are spread out far (remember from "Ladder Operators for the Simple Harmonic Oscillator" that $\Delta x = \sqrt{\hbar/m\omega}\sqrt{n+\frac{1}{2}}$) so they sample regions where bx^3 is large.

[[Grading: 5 points for part (a); 5 points for part (b).]]