

Homework week 7 (Part B) Due Tuesday Chemistry 455A

These are problems from Engel and Reid (or Engel in parentheses)

P18.11, P18.4, P18.5, P18.8, P 18.10, P18 .13.

(or: P7.11 (see also 7.1, same problem), P18.4, P7.5, P7.8, P7 .10, P 7.13)

P7.11 Calculate the force constant for the effective spring about which HCl atoms vibrate. (See 18.1, as it gives you an idea of what the spring force constant should be). The second part is a bit different. Here you use the same spring force constant to balance the pull of gravity. Set the two potential energies, that of a stretched spring and that of a mass at a different distance from the earth, equal to find the mass.

The following are problems for the Harmonic Oscillator. To gear up for them we need to take advantage of the things we know about average quantities. The following problems ask you to compute the mean and mean square positions and momenta for various eigenstates.

From the virial Theorem we know:

$$\langle T \rangle = \langle V \rangle = \frac{1}{2} E = \frac{1}{2} \hbar \omega_{os} \left(n + \frac{1}{2} \right)$$
$$\frac{1}{2} \hbar \omega_{os} \left(n + \frac{1}{2} \right) = \frac{1}{2m} \langle p^2 \rangle = \frac{k_s}{2} \langle x^2 \rangle$$

And From the ladder operators:

$$\hat{a} \phi_n = \left(i \sqrt{\frac{1}{2m}} \hat{p} + \sqrt{\frac{k_s}{2}} \hat{x} \right) \phi_n = \sqrt{\hbar \omega_{os} n} \phi_{n-1}$$
$$\langle a \rangle = \int \phi_n^* \hat{a} \phi_n dx = \left(i \sqrt{\frac{1}{2m}} \langle p \rangle + \sqrt{\frac{k_s}{2}} \langle x \rangle \right) = \sqrt{\hbar \omega_{os} n} \int \phi_n^* \phi_{n-1} dx = 0$$

So from these rules we have all the mean observables and the mean squared observables. Now use can use these forms or do the integrations directly using the rules we developed in class:

$$I = \int e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$$
$$I_2 = \int x^2 e^{-\alpha x^2} dx = -\frac{d}{d\alpha} \int e^{-\alpha x^2} dx = -\frac{d}{d\alpha} \sqrt{\frac{\pi}{\alpha}}$$

P18.4

P18.5

P18.8 (Rely on previous results).

P18.10. Please use the virial theorem results, quoted above. Do not work out all the integrals needed by hand, although you can.

P18.13 This is useful to have a feel for how much the bond length changes. This calculation was done from the information in Zumdahl and is on the set of power point slides from the first lecture.

https://courses.washington.edu/bhrchem/c455/qm_review.pdf, slide 33.