

## Homework H11 Solution

### 1. Problem 4.2 (Page 66/67)

Solution: For HCl, the reduced mass is  $\mu = \frac{m_H m_{Cl}}{m_H + m_{Cl}} = \frac{35}{36} * \frac{10^{-3} kg}{mol} = 1.615 * \frac{10^{-27} kg}{molecule}$

$$\text{Therefore } \omega = \sqrt{\frac{k}{\mu}} = 5.65 * 10^{14} s^{-1}$$

$$\text{and } E_0 = \frac{1}{2} \hbar \omega = 2.98 * 10^{-20} J (molecule)^{-1} = 17.94 kJ mol^{-1}$$

$$\text{For DCl, } \mu = \frac{70}{37} * \frac{10^{-3} kg}{mole} = 3.14 * \frac{10^{-27} kg}{molecule}$$

$$\text{Therefore } \omega = \sqrt{\frac{k}{\mu}} = 4.05 * 10^{14} s^{-1}$$

$$\text{and } E_0 = \frac{1}{2} \hbar \omega = 2.136 * 10^{-20} J (molecule)^{-1} = 12.86 kJ mol^{-1}$$

### 2. Problem 4.3 (Page 67)

Solution: For transition from  $n=0$  to  $n=1$  (or  $v=0$  to  $v=1$ ), the energy separation is  $\hbar\omega$ .

$$\hbar\omega = \frac{hc}{\lambda}$$

$$\omega = 3.54 * 10^{14} s^{-1}$$

For NO, the reduced mass is  $\mu = \frac{14*16}{14+16} * 10^{-3} kg/mole$

$$= 1.24 * 10^{-26} kg/mole$$

$$\text{Therefore } k = \mu\omega^2 = 1554.31 N/m$$

**Turn in 3.** In class we discussed that we can expand ANY wavefunction  $\Psi(x)$  as a sum of harmonic oscillator eigenstates  $\Psi_n(x)$ , and ANY time-dependent wavefunction  $\Psi(x,t)$  as a sum of harmonic oscillator stationary states  $\Psi_n(x)e^{-\frac{i}{\hbar}E_n t}$ . It's a similar idea as expanding any function  $y(x)$  in a Taylor series of 1,  $x$ ,  $x^2$  and so on.

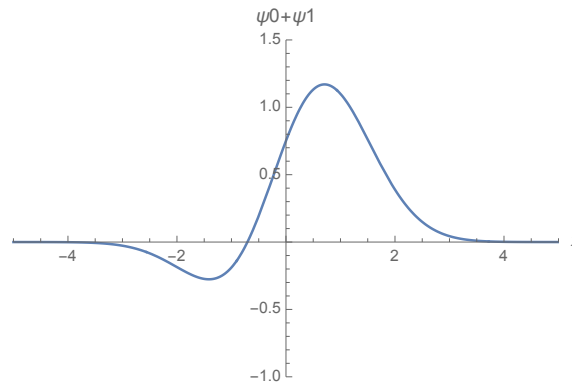
Show that the function  $L = \Psi_0(x) + \Psi_1(x)$  is a wavefunction peaked on one side of  $x=0$ , and the function  $R = \Psi_0(x) - \Psi_1(x)$  is a wavefunction peaked on the other side of  $x=0$ . First write down the formula for  $L$  and  $R$ , then make a plot or sketch. (You can use a graphing calculator or other software for plotting that you like.) You can see how combinations of

$\Psi_0(x)$  and  $\Psi_1(x)$  that change in time could give a wavefunction that wiggles back and forth, just like a classical particle on a spring would swing back and forth.

**Solution:**

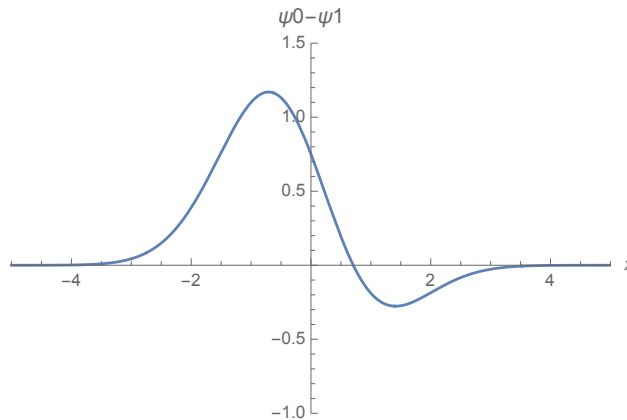
For L we have

$$L = \varphi_0(x) + \varphi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} + \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \sqrt{2} \sqrt{\frac{m\omega}{\hbar}} x e^{-\frac{m\omega x^2}{2\hbar}}$$



And for R we have

$$R = \varphi_0(x) + \varphi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} - \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \sqrt{2} \sqrt{\frac{m\omega}{\hbar}} x e^{-\frac{m\omega x^2}{2\hbar}}$$



Where we have achieved the desired results for L and R (L is peaked on the right side of the y-axis and R is peaked on the left side). If we took the square modulus of L or R and propagated it in time, we would see the probability distribution moving back and forth periodically, just like the quantum simulation program you have used online!