HW #8

1. Coupled Harmonic Oscillators

The Hamiltonian is

$H = \frac{p_1{}^2}{2M} + \frac{p_2{}^2}{2M} + \frac{p_3{}^2}{2m} + \frac{1}{2} k(x_3 - x_1 - d)^2 + \frac{1}{2} k(x_2 - x_3 - d)^2$

For the sake of simplicity, we redefine $x_1 \to x_1 - d$, $x_2 \to x_2 + d$ and the Hamiltonian is

$H = \frac{p_1{}^2}{2M} + \frac{p_2{}^2}{2M} + \frac{p_3{}^2}{2m} + \frac{1}{2} k(x_3 - x_1)^2 + \frac{1}{2} k(x_2 - x_3)^2$

(a) Born-Oppenheimer Approximation

Assume x_1 and x_2 are fixed. Then the potential energy for x_3 is

$\frac{1}{2} k(x_3{}^2 - 2\,x_3\,x_1 + x_1{}^2 + x_2{}^2 - 2\,x_2\,x_3 + x_3{}^2) = \frac{1}{2} k(2\,x_3{}^2 - 2\,(x_1 + x_2)\,x_3 + x_1{}^2 + x_2{}^2)$

$= \frac{1}{2}\,2\,k(x_3 - \frac{x_1 + x_2}{2})^2 - k\,\frac{(x_1 + x_2)^2}{4} + \frac{1}{2} k(x_1{}^2 + x_2{}^2)$

$= \frac{1}{2}\,2\,k(x_3 - \frac{x_1 + x_2}{2})^2 + \frac{1}{4} k(x_1 - x_2)^2$

The energy levels for the x_3 degree of freedom is therefore $(n + \frac{1}{2})\,\hbar \sqrt{\frac{2k}{m}}$.

Taking the ground state for the x_3 degree of freedom, the Hamiltonian reduces to

$H_{\text{eff}} = \frac{p_1{}^2}{2M} + \frac{p_2{}^2}{2M} + \frac{1}{2}\,\hbar \sqrt{\frac{2k}{m}} + \frac{1}{4} k(x_1 - x_2)^2.$

Separating the center-of-mass motion with $P = p_1 + p_2$, $X = \frac{x_1 + x_2}{2}$, $p = \frac{p_1 - p_2}{2}$, $x = x_1 - x_2$, it becomes

$H_{\text{eff}} = \frac{P^2}{4M} + \frac{p^2}{M} + \frac{1}{4}\,k\,x^2 + \frac{1}{2}\,\hbar \sqrt{\frac{2k}{m}}.$

Leaving the trivial translational energy aside, the energy levels are therefore

$E = (n' + \frac{1}{2})\,\hbar \sqrt{\frac{k}{M}} + \frac{1}{2}\,\hbar \sqrt{\frac{2k}{m}}.$

(b) Exact Solution

We identify the normal modes of the coupled harmonic oscillators.

One way is to go back to the Lagrangian,

$L = \frac{1}{2} M \dot{x}_1{}^2 + \frac{1}{2} M \dot{x}_2{}^2 + \frac{1}{2} m \dot{x}_3{}^2 - \frac{1}{2} k(x_3 - x_1)^2 - \frac{1}{2} k(x_2 - x_3)^2.$

We rescale the coordinates to make the kinetic terms the same for all three, $x_1 = \frac{1}{\sqrt{M}} q_1$, $x_2 = \frac{1}{\sqrt{M}} q_2$, $x_3 = \frac{1}{\sqrt{m}} q_3$. Then

$L = \frac{1}{2} \dot{q}_1{}^2 + \frac{1}{2} \dot{q}_2{}^2 + \frac{1}{2} \dot{q}_3{}^2 - \frac{1}{2} k\left(\frac{1}{\sqrt{m}} q_3 - \frac{1}{\sqrt{M}} q_1\right)^2 - \frac{1}{2} k\left(\frac{1}{\sqrt{m}} q_3 - \frac{1}{\sqrt{M}} q_2\right)^2.$

We can write the potential term as

$$V = \frac{1}{2} k(q_1,\ q_3,\ q_2) \begin{pmatrix} 1/M & -1\big/\sqrt{m\,M} & 0 \\ -1\big/\sqrt{m\,M} & 2/m & -1\big/\sqrt{m\,M} \\ 0 & -1\big/\sqrt{m\,M} & 1/M \end{pmatrix} \begin{pmatrix} q_1 \\ q_3 \\ q_2 \end{pmatrix}.$$

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In[5]:= Eigenvalues[{{1/M, -1/√(m M), 0}, {-1/√(m M), 2/m, -1/√(m M)}, {0, -1/√(m M), 1/M}}]
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Out[5]= {0, 1/M, (m + 2 M)/(m M)}
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Therefore, it is given by three independent harmonic oscillators of frequencies 0, $\sqrt{k/M}$, and $\sqrt{k(2M+m)/mM}$. The zero-frequency mode corresponds to the overall translation, while the other two give the harmonic oscillator levels,
$E = (n' + \frac{1}{2})\hbar\sqrt{\frac{k}{M}} + (n + \frac{1}{2})\hbar\sqrt{\frac{k(2M+m)}{mM}}$.

(c) Comparison

Taking $n = 0$ in the exact result, we find
$E = (n' + \frac{1}{2})\hbar\sqrt{\frac{k}{M}} + \frac{1}{2}\hbar\sqrt{\frac{k(2M+m)}{mM}}$,
while the Born-Oppenheimer approximation gives
$E = (n' + \frac{1}{2})\hbar\sqrt{\frac{k}{M}} + \frac{1}{2}\hbar\sqrt{\frac{2k}{m}}$.
Therefore the Born-Oppenheimer approximation gives the correct result up to a correction suppressed by m/M as expected.

2. A=14

Looking at the nitrogen, the levels with spin/parity that appear together in carbon and nitrogen with similar excitation energies are identified as $I = 1$, wihle those that appear only in nitrogen as $I = 0$.

From the ground state and up,

J^P	I	
1^+	0	
0^+	1	
1^+	0	
0^-	0	
2^-	0	
1^-	0	
3^-	0	
1^+	0	
3^+	0	
2^+	0	
2^-	0	
1^-	1	$8062 - 2313 = 5749$, in rough accordance with the excitation energies in carbon and oxygen
4^-	0	
0^+	1	
0^-	0	
3^-	1	
5^-	0	
2^+	0	appears too close to 3^- with $I = 1$ compared to carbon and oxygen
3^+	0	
2^+	1	$9172 - 8907 = 265$, in rough accordance with the $2^+ - 3^-$ splittings in carbon and oxygen

etc