Yichao Yu
8.422 Problem Set 5
Recitation Section 1

1.

(a)

(b)

2.

(a)

For atoms in an isotropic environment

$$\begin{aligned}\langle g|\vec{d}|g\rangle =&\langle i|\vec{d}|i\rangle\\ =&0\end{aligned}$$

The first order correction to the energy is 0.
Second order

$$\begin{aligned}\delta E =& -\sum_{i_a,i_b}\frac{|\langle i_ai_b|H_{el}|gg\rangle|^2}{\hbar\omega_{ig}^a+\hbar\omega_{ig}^b}\\ \langle i_ai_b|H_{el}|gg\rangle =&\frac{e^2}{R^3}\left(\vec{r}_{ig}^a\cdot\vec{r}_{ig}^b-3x_{ig}^ax_{ig}^b\right)\end{aligned}$$

Since the system is symmetric for rotation around $\vec{R}$, the "good" states to calculate the energy shift should also have the same symmetry. Therefore $\vec{r^a}$ and $\vec{r^b}$ should be along the $\vec{R}$ (x) direction

$$\begin{aligned}\langle i_ai_b|H_{el}|gg\rangle =& -\frac{2e^2x_{ig}^ax_{ig}^b}{R^3}\\ \delta E =& -\sum_{i_a,i_b}\frac{1}{\hbar\omega_{ig}^a+\hbar\omega_{ig}^b}\left|\frac{2e^2x_{ig}^ax_{ig}^b}{R^3}\right|^2\\ =& -\frac{4e^4}{\hbar R^6}\sum_{i_a,i_b}\frac{\left|x_{ig}^a\right|^2\left|x_{ig}^b\right|^2}{\omega_{ig}^a+\omega_{ig}^b}\end{aligned}$$

(b)

$$\begin{aligned}|x_{ig}|^2 =&\frac{\hbar f_{ig}}{2m\omega_{ig}}\\ \delta E =& -\frac{4e^4}{\hbar R^6}\sum_{i_a,i_b}\frac{1}{\omega_{ig}^a+\omega_{ig}^b}\frac{\hbar f_{ig}^a}{2m\omega_{ig}^a}\frac{\hbar f_{ig}^b}{2m\omega_{ig}^b}\\ =& -\frac{\hbar e^4}{m^2R^6}\sum_{i_a,i_b}\frac{f_{ig}^af_{ig}^b}{(\omega_{ig}^a+\omega_{ig}^b)\omega_{ig}^a\omega_{ig}^b}\end{aligned}$$

(c)

Since the oscillator strength for the ground state is always positive, if the first excited state has $f \approx 1$, the contribution from other transitions are small. With this approximation,

$$
\begin{aligned}
|x_{ig}|^2 =& \frac{\hbar\omega_{ig}}{2e^2}\alpha_g \\
\delta E =& -\frac{4e^4}{\hbar R^6}\frac{1}{\omega_{ig}^a + \omega_{ig}^b}\frac{\hbar\omega_{ig}^a}{2e^2}\alpha_g^a\frac{\hbar\omega_{ig}^b}{2e^2}\alpha_g^b \\
=& -\frac{\hbar}{R^6}\frac{\omega_{ig}^a\omega_{ig}^b}{\omega_{ig}^a + \omega_{ig}^b}\alpha_g^a\alpha_g^b \\
C_6 =& \hbar\frac{\omega_{ig}^a\omega_{ig}^b}{\omega_{ig}^a + \omega_{ig}^b}\alpha_g^a\alpha_g^b
\end{aligned}
$$