1 Introduction

In this document, I wish to post my derivation for Equation 11 in Romalis-Fortson. This equation gives the vector shift for Cs, using time-dependent perturbation theory. This typed derivation is derived from a pencil-and-paper version that I made earlier

2 derivation

E-field of the trapping light, close to the center, is given by

$$\overrightarrow{E} = \frac{E_0}{2}(\hat{\epsilon}e^{-\iota\omega t} + \hat{\epsilon}^* e^{\iota\omega t})$$

This creates the time-dependent perturbation:

$$\hat{H}'(t) = eE(t) \cdot \overrightarrow{r}$$

The full hamiltonian is:

$$\hat{H} = \hat{H}_0 + \hat{H}'(t)$$

where $\hat{H}_0$ is the normal Hamiltonian of the atom

The eigenvectors of $\hat{H}_0$ are a set of orthonormal eigenvectors $|i\rangle$ with eigenvectors

$$\hat{H}_0|i\rangle = E_i$$

The total wave function for the Hamiltonian is:

$$\Psi_i(t) = c_i(t)|ie^{-\iota E_i \frac{t}{\hbar}} + \sum_{k \neq i} c_k(t)|ke^{-\iota E_k \frac{t}{\hbar}}$$

where $c_i(0) = 1$, $c_k(0) = 0$

when we introduce the perturbation, we will cause these c_i to change.

using time dependent perturbation theory,

$$\hat{H}\Psi(t) = \iota\hbar\frac{\delta\Psi}{\delta t}$$

$$\hat{H}_0\Psi(t) + \hat{H}'\Psi(t) = \iota\hbar\frac{\delta\Psi}{\delta t}$$

expanding,

$$c_i(t)\hat{H}_0|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \sum_{k \neq i} c_k(t)\hat{H}_0|k\rangle e^{-\iota E_k \frac{t}{\hbar}} + c_i(t)\hat{H}'|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \sum_{k \neq i} c_k t\hat{H}'|k\rangle e^{-\iota E_k \frac{t}{\hbar}}$$

$$= \iota\hbar(\dot{c}_i(t)|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \sum_{k\neq i} \dot{c}_k(t)|k\rangle e^{\iota E_k \frac{t}{\hbar}} + c_i(t)\frac{-\iota}{\hbar}E_i|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \sum_{k\neq i} c_k(t)\frac{-\iota}{\hbar}E_k|k\rangle e^{-\iota E_k \frac{t}{\hbar}})$$

We can then subtract the $\hat{H}_0$ terms:

$$c_i(t)\hat{H}'|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \sum_{k\neq i} c_k t \hat{H}'|k\rangle e^{-\iota E_k \frac{t}{\hbar}} = \iota\hbar\dot{c}_i(t)|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \iota\hbar \sum_{k\neq i} \dot{c}_k(t)|k\rangle e^{-\iota E_k \frac{t}{\hbar}}$$

To first order, we assume:

$$c_i(t) = 1, c_k(t) = 0$$

pluggin in:

$$\hat{H}'|i\rangle e^{-\iota E_i \frac{t}{\hbar}} = \iota\hbar\dot{c}_i(t)|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \iota\hbar \sum_{k\neq i} \dot{c}_k(t)|k\rangle e^{-\iota E_k \frac{t}{\hbar}}$$

Thus,

$$\langle i|\hat{H}'|i\rangle e^{-\iota E_i \frac{t}{\hbar}} = \iota\hbar\dot{c}_i(t) e^{-\iota E_i \frac{t}{\hbar}}$$

Thus,

$$\dot{c}_i(t) = \frac{\langle i|\hat{H}'|i\rangle}{\iota\hbar}$$

for $k \neq i$,

$$\langle j|\hat{H}'|i\rangle e^{-\iota E_i \frac{t}{\hbar}} = \iota\hbar\dot{c}_j e^{-\iota E_j \frac{t}{\hbar}}$$

therefore,

$$\dot{c}_j = \frac{1}{\iota\hbar}\langle j|\hat{H}'|i\rangle e^{\iota(E_j - E_i)\frac{t}{\hbar}}$$

Now, integrate to find the c_i:
For $\hat{H}' = e\overrightarrow{E} \cdot \overrightarrow{r}$,

$$\langle i|\hat{H}'|i\rangle = 0$$

therefore,

$$\frac{dc_i(t')}{dt'} = 0$$

$$dc_i(t') = 0 \times dt'$$

$$\int_{c_i(0)}^{c_i(t)} dc_i(t) = \int_0^t 0 dt'$$

$$c_i(t) - c_i(0) = 0$$

therefore,

$$c_i(t) = c_i(0) = 1$$

to this first order.
For $k \neq i$,

$$\frac{dc_k(t')}{dt'} = \frac{1}{\iota\hbar}\langle j|\hat{H}'|i\rangle e^{\iota(E_k - E_i)\frac{t'}{\hbar}}$$

$$\int_{c_k(0)}^{c_k(t)} dc_j(t') = \frac{1}{\iota\hbar}\int_0^t \langle j|\hat{H}'(t')|i\rangle e^{\iota(E_k - E_i)\frac{t'}{\hbar}} dt'$$

since $c_k(0) = 0$,

$$c_k(t) = \frac{1}{\iota\hbar}\int_0^t \langle k|\hat{H}'(t')|i\rangle e^{\iota(E_k - E_i)\frac{t'}{\hbar}} dt'$$

Now, we plug these values into the equation again

$$\hat{H}'|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \sum_{k\neq i} \frac{1}{\iota\hbar}\int_0^t \langle k|\hat{H}'(t')|i\rangle e^{\iota(E_k - E_i)\frac{t'}{\hbar}} dt' \hat{H}'|k\rangle e^{-\iota E_k \frac{t}{\hbar}}$$

$$= \iota\hbar \dot{c}_i(t)|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \iota\hbar \sum_{k\neq i} \dot{c}_k(t)|k\rangle e^{-\iota E_k \frac{t}{\hbar}}$$

once again, project onto $\langle i|$

$$\iota\hbar\dot{c}_i e^{-\iota E_i \frac{t}{\hbar}} = \langle i|\hat{H}'|i\rangle e^{-\iota E_i \frac{t}{\hbar}} + \sum_{k\neq i} \frac{1}{\iota\hbar}\int_0^t \langle k|\hat{H}'(t')|i\rangle e^{\iota(E_k - E_i)\frac{t'}{\hbar}} dt' \langle i|\hat{H}'|k\rangle e^{-\iota E_k \frac{t}{\hbar}}$$

therefore,

$$\dot{c}_i = \frac{\langle i|\hat{H}'|i\rangle}{\iota\hbar} + \sum_{k\neq i} \frac{-1}{\hbar^2}\int_0^t \langle k|\hat{H}'(t')|i\rangle e^{\iota(E_k - E_i)\frac{t'}{\hbar}} dt' \langle i|\hat{H}'|k\rangle e^{\iota(E_i - E_k)\frac{t}{\hbar}}$$

For $H'(t) = e\overrightarrow{E} \cdot \overrightarrow{r}$, $\langle i|H'|i\rangle = 0$
so,

$$\frac{dc_i(t')}{dt'} = \sum_{k\neq i} \frac{-1}{\hbar^2}\int_0^{t'} \langle k|\hat{H}'(t")|i\rangle e^{\iota(E_k - E_i)\frac{t"}{\hbar}} dt" \langle i|\hat{H}'|k\rangle e^{\iota(E_i - E_k)\frac{t'}{\hbar}}$$

$$\int_{c_i(0)}^{c_i(t)} dc_i = \sum_{k\neq i} \frac{-1}{\hbar^2} \int_0^t \int_0^{t'} \langle k|\hat{H}'(t")|i\rangle e^{\iota(E_k-E_i)\frac{t"}{\hbar}} dt" \langle i|\hat{H}'(t')|k\rangle e^{\iota(E_i-E_k)\frac{t'}{\hbar}} dt'$$

thus,

$$c_i(t) - 1 = \frac{-1}{\hbar^2} \sum_{k\neq i} \int_0^t \int_0^{t'} \langle k|\hat{H}'(t")|i\rangle e^{\iota(E_k-E_i)\frac{t"}{\hbar}} dt" \langle i|\hat{H}'(t')|k\rangle e^{\iota(E_i-E_k)\frac{t'}{\hbar}} dt'$$

thus,

$$c_i(t) = 1 - \frac{1}{\hbar^2} \sum_{k\neq i} \int_0^t \int_0^{t'} \langle k|\hat{H}'(t")|i\rangle e^{\iota(E_k-E_i)\frac{t"}{\hbar}} dt" \langle i|\hat{H}'(t')|k\rangle e^{\iota(E_i-E_k)\frac{t'}{\hbar}} dt'$$

Now, take a look at the actual form of $\hat{H}'(t)$:

$$\int_0^{t'} \langle k|\hat{H}'(t")|i\rangle e^{\iota(E_k-E_i)\frac{t"}{\hbar}} dt"$$

$$= \frac{eE_0}{2} \int_0^{t'} (\langle k|\hat{\epsilon} e^{-\iota\omega t"} \cdot \overrightarrow{r}|i\rangle + \langle k|\hat{\epsilon}^* e^{\iota\omega t"} \cdot \overrightarrow{r}|i\rangle) e^{\iota(E_k-E_i)\frac{t"}{\hbar}} dt"$$

$$= \frac{eE_0}{2} (\int_0^{t'} \langle k|\hat{\epsilon} \cdot \overrightarrow{r}|i\rangle e^{\iota(E_k-E_i-\omega\hbar)\frac{t"}{\hbar}} dt" + \int_0^{t'} \langle k|\hat{\epsilon}^* \cdot \overrightarrow{r}|i\rangle e^{\iota(E_k+\omega\hbar-E_i)\frac{t"}{\hbar}} dt")$$

$$= \frac{eE_0}{2} (\langle k|\hat{\epsilon} \cdot \overrightarrow{r}|i\rangle \frac{e^{\iota(E_k-E_i-\omega\hbar)\frac{t'}{\hbar}} - 1}{\frac{\iota}{\hbar}(E_k-E_i-\omega\hbar)} + \langle k|\hat{\epsilon}^* \cdot \overrightarrow{r}|i\rangle \frac{e^{\iota(E_k-E_i+\omega\hbar)\frac{t'}{\hbar}} - 1}{\frac{\iota}{\hbar}(E_k-E_i+\omega\hbar)})$$

Therefore,

$$c_i(t) - 1 = \frac{-1}{\hbar^2} \sum_{k\neq i} \int_0^t \frac{eE_0}{2} (\langle k|\hat{\epsilon} \cdot \overrightarrow{r}|i\rangle \frac{e^{\iota(E_k-E_i-\omega\hbar)\frac{t'}{\hbar}} - 1}{\frac{\iota}{\hbar}(E_k-E_i-\omega\hbar)} + \langle k|\hat{\epsilon}^* \cdot \overrightarrow{r}|i\rangle \frac{e^{\iota(E_k-E_i+\omega\hbar)\frac{t'}{\hbar}} - 1}{\frac{\iota}{\hbar}(E_k-E_i+\omega\hbar)})$$

$$\times \frac{eE_0}{2} (\langle i|\hat{\epsilon} \cdot \overrightarrow{r}|k\rangle e^{\iota(E_i-E_k-\omega\hbar)\frac{t}{\hbar}} + \langle i|\hat{\epsilon}^* \cdot \overrightarrow{r}|k\rangle e^{\iota(E_i+\omega\hbar-E_k)\frac{t'}{\hbar}}) dt'$$

Thus,

$$c_i(t) = 1 - \frac{e^2 E_0^2}{4\hbar} \int_0^t (\langle k|\hat{\epsilon} \cdot \overrightarrow{r}|i\rangle \langle i|\hat{\epsilon} \cdot \overrightarrow{r}|k\rangle \frac{e^{-2\iota\omega t'} - e^{\iota(E_i-E_k-\omega\hbar)\frac{t'}{\hbar}}}{\frac{\iota}{\hbar}(E_k-E_i-\omega\hbar)}$$

$$+\langle k|\hat{\epsilon}\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}^*\cdot\overrightarrow{r}|k\rangle\frac{1-e^{\iota(E_i+\omega\hbar-E_k)\frac{t'}{\hbar}}}{\frac{\iota}{\hbar}(E_k-E_i-\omega\hbar)}$$

$$+\langle k|\hat{\epsilon}^*\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}\cdot\overrightarrow{r}|k\rangle\frac{1-e^{\iota(E_i-\omega\hbar-E_k)\frac{t'}{\hbar}}}{\frac{\iota}{\hbar}(E_k-E_i+\omega\hbar)}$$

$$+\langle k|\hat{\epsilon}^*\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}^*\cdot\overrightarrow{r}|k\rangle\frac{e^{2\iota\omega t'}-e^{\iota(E_i+\omega\hbar-E_k)\frac{t'}{\hbar}}}{\frac{\iota}{\hbar}(E_k-E_i+\omega\hbar)})dt'$$

Let us now consider what exactly is ΔE:

$$\Delta E=\langle\Psi_i|\hat{H}-\hat{H}_0|\Psi\rangle=\langle i|\hat{H}|\Psi_i\rangle-\langle i|\hat{H}_0|\Psi\rangle$$

$$\hat{H}|\Psi\rangle=\iota\hbar\frac{\delta\Psi}{\delta t}$$

$$=\iota\hbar\dot{c}_i(t)|i\rangle e^{-\iota E_i\frac{t}{\hbar}}+c_i(t)E_i|i\rangle e^{-\iota E_i\frac{t}{\hbar}}+\sum_{k\neq i}\iota\hbar\dot{c}_k(t)|k\rangle e^{-\iota E_k\frac{t}{\hbar}}+c_k(t)E_k|k\rangle e^{-\iota E_k\frac{t}{\hbar}}$$

since

$$\hat{H}_0|\Psi>=c_i(t)E_i|i\rangle e^{-\iota E_i\frac{t}{\hbar}}+c_k(t)E_k|k\rangle e^{-\iota E_k\frac{t}{\hbar}}$$

this means

$$(\hat{H}-\hat{H}_0)|\Psi\rangle=\iota\hbar(\dot{c}_i(t)|i\rangle e^{-\iota E_i\frac{t}{\hbar}}+\sum_{k\neq i}\dot{c}_k(t)|k\rangle e^{-\iota E_k\frac{t}{\hbar}})$$

thus,

$$\langle\Psi_i|\hat{H}-\hat{H}_0|\Psi\rangle=e^{\iota E_i\frac{t}{\hbar}}\langle i|\iota\hbar\dot{c}_i(t)|i\rangle e^{-\iota E_i\frac{t}{\hbar}}=\iota\hbar\dot{c}_i(t)$$

using the 2nd funamental theorem of calculus,

$$\Delta E=\iota\hbar(\frac{-1}{\hbar^2}\sum_{k\neq i}\frac{e^2E_0^2}{4}((\langle k|\hat{\epsilon}\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}\cdot\overrightarrow{r}|k\rangle\frac{e^{-2\iota\omega t}-e^{\iota(E_i-E_k-\omega\hbar)\frac{t}{\hbar}}}{\frac{\iota}{\hbar}(E_k-E_i-\omega\hbar)}$$

$$+\langle k|\hat{\epsilon}\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}^*\cdot\overrightarrow{r}|k\rangle\frac{1-e^{\iota(E_i+\omega\hbar-E_k)\frac{t}{\hbar}}}{\frac{\iota}{\hbar}(E_k-E_i-\omega\hbar)}$$

$$+\langle k|\hat{\epsilon}^*\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}\cdot\overrightarrow{r}|k\rangle\frac{1-e^{\iota(E_i-\omega\hbar-E_k)\frac{t}{\hbar}}}{\frac{\iota}{\hbar}(E_k-E_i+\omega\hbar)}$$

$$+\langle k|\hat{\epsilon}^*\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}^*\cdot\overrightarrow{r}|k\rangle\frac{e^{2\iota\omega t}-e^{\iota(E_i+\omega\hbar-E_k)\frac{t}{\hbar}}}{\frac{\iota}{\hbar}(E_k-E_i+\omega\hbar)})$$

with the rotating wave approximation, anything of the form $e^{\iota\omega t}$ averages out to zero. So,

$$\Delta E = \iota\hbar(\frac{-1}{\hbar^2}\sum_{k\neq i}\frac{e^2E_0^2}{4}\frac{\hbar}{\iota}(\frac{\langle k|\hat{\epsilon}\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}^*\cdot\overrightarrow{r}|k\rangle}{E_k-E_i-\omega\hbar}+\frac{\langle k|\hat{\epsilon}^*\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}\cdot\overrightarrow{r}|k\rangle}{E_k-E_i+\omega\hbar})$$

Thus,

$$\Delta E = -\frac{e^2E_0^2}{4\hbar}\sum_{k\neq i}(\frac{\langle k|\hat{\epsilon}\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}^*\cdot\overrightarrow{r}|k\rangle}{\omega_{ki}-\omega}+\frac{\langle k|\hat{\epsilon}^*\cdot\overrightarrow{r}|i\rangle\langle i|\hat{\epsilon}\cdot\overrightarrow{r}|k\rangle}{\omega_{ki}+\omega})$$

where $\omega_{ki} = \frac{E_k-E_i}{\hbar}$