Components of polarizability

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1 Two theorems

1.1 Wigner-Eckart theorem

$\langle \alpha jm \mid T_q^{(k)} \mid \alpha' j' m' \rangle = (-1)^{2k} \langle \alpha j \mid\mid \mathbf{T}^{(k)} \mid\mid \alpha' j' \rangle \langle jm \mid j'm'; kq \rangle$
contains Clebsh-Gordon coefficients

1.2 Decomposition rule

For a single subsystem,
$\langle j \mid\mid \mathbf{T}^{(k)} \mid\mid j' \rangle = \delta_{j_2 j_2'} (-1)^{j'+j_1+k+j_2} \sqrt{(2j'+1)(2j_1+1)} \begin{Bmatrix} j_1 & j_1' & k \\ j' & j & j_2 \end{Bmatrix} \langle j_1 \mid\mid \mathbf{T}^{(k)} \mid\mid j_1' \rangle$
Wigner-6j symbol, recoupling of three angular momenta

2 DC Stark shifts

$H_{int} = -\mathbf{d} \cdot \mathbf{E}$
Second order time-independent perturabtion theory gives,
$\Delta E_\alpha = \sum_j \frac{|\langle \alpha | H_{int} | \beta_j \rangle|^2}{E_\alpha - E_{\beta_j}} = \langle \alpha \mid H_{stark} \mid \alpha \rangle$
$H_{stark} = \sum_j \frac{d_\mu | \beta_j \rangle \langle \beta_j | d_\nu}{E_\alpha - E_{\beta_j}} E_\mu E_\nu = S_{\mu\nu} E_\mu E_\nu$
where $S_{\mu\nu} = \sum_j \frac{d_\mu | \beta_j \rangle \langle \beta_j | d_\nu}{E_\alpha - E_{\beta_j}}$
A Cartesian tensor of rank 2 can be decomposed into irreducible spherical tensors of rank 0, 1, 2 as
$M_{\alpha\beta} = \frac{1}{3} M^{(0)} \delta_{\alpha\beta} + \frac{1}{4} M_\mu^{(1)} \epsilon_{\mu\alpha\beta} + M_{\alpha\beta}^{(2)}$
where
$M^{(0)} = M_{\mu\mu}$
$M_\mu^{(1)} = \epsilon_{\mu\sigma\tau}(M_{\sigma\tau} - M_{\tau\sigma})$
$M_{\alpha\beta}^{(2)} = M_{\alpha\beta} - \frac{1}{3} M_{\mu\mu} \delta_{\alpha\beta}$
Same for $S_{\mu\nu}$
$S^{(0)} = S_{\mu\mu}$
$S_\mu^{(1)} = 0$
$S_{\mu\nu}^{(2)} = S_{\mu\nu} - \frac{1}{3} S_{\sigma\sigma} \delta_{\mu\nu}$
$\Delta E_\alpha = \frac{1}{3} \langle \alpha \mid S^{(0)} \mid \alpha \rangle E^2 + \langle \alpha \mid S_{\mu\nu}^{(2)} \mid \alpha \rangle E_\mu E_\nu$
scalar and tensor shift

2.1 Scalar shift

Using Wigner-Eckart theorem, we have...
$\alpha^{(0)}(J) = -\frac{2}{3} \sum_{J'} \frac{|\langle J || \mathbf{d} || J' \rangle|^2}{E_J - E_J'}$
$\Delta E_J^{(0)} = -\frac{1}{2} \alpha^{(0)}(J) E^2$
independent of m_J: orientation-independent shift

2.2 Tensor shift

Switch to spherical basis (Roman indices: spherical components. Greek: Cartesian components)

$\langle\alpha \mid S^{(2)}_{\mu\nu} \mid \alpha\rangle E_\mu E_\nu = \sum_q (-1)^q \langle Jm_J \mid S^{(2)}_q \mid Jm_J\rangle [\mathbf{EE}]^{(2)}_{-q}$

Applying Wigner-Eckart theorem one time, we find the only non-vanishing contribution comes from $q=0$, and

$[\mathbf{EE}]^{(2)}_0 = \frac{1}{\sqrt{6}}(3E_z^2 - E^2)$

We define tensor polarizability as (in order to get the the correct normalization)

$\alpha^{(2)}(J) = -\langle J \mid\mid S^{(2)}_q \mid\mid J\rangle \sqrt{\frac{8J(2J-1)}{3(J+1)(2J+3)}}$

$\Delta E^{(2)}_{J,m_J} = -\frac{1}{4}\alpha^{(2)}(J)(3E_z^2 - E^2)\frac{3m_J^2 - J(J+1)}{J(2J-1)}$

Normalization. Let $\mathbf{E} = E_z\hat{z}$, $\Delta E^{(2)}_{J,\pm J} = -\frac{1}{2}\alpha^{(2)}(J)E_z^2$

depends on m_J

Use one more time Wigner-Eckart theorem, we have

$\alpha^{(2)}(J) = \sum_{J'}(-1)^{J+J'+1}\sqrt{\frac{40J(2J+1)(2J-1)}{3(J+1)(2J+3)}}\begin{Bmatrix}1 & 1 & 2\\ J & J & J'\end{Bmatrix}\frac{|\langle J||\mathbf{d}||J'\rangle|^2}{E_J - E'_J}$

2.3 Note

$J=0$ or $J=\frac{1}{2}$, no tensor shift

3 AC Stark shifts (light shifts)

$\mathbf{E}(\mathbf{r}) = \hat{\varepsilon}E_0^{(+)}(\mathbf{r})e^{-i\omega t} + c.c.$

Second order time-dependent perturbation theory

$\Delta E_\alpha = -\sum_\beta \frac{2\omega_{\beta\alpha}|\langle\alpha|\hat{\varepsilon}\cdot\mathbf{d}|\beta\rangle|^2|E_0^{(+)}|^2}{\hbar(\omega^2_{\beta\alpha}-\omega^2)}$

$\Delta E_\alpha = -\frac{1}{2}\mathbf{d}^{(+)}\cdot\mathbf{E}^{(-)} - \frac{1}{2}\mathbf{d}^{(-)}\cdot\mathbf{E}^{(+)} = -Re[\alpha(\omega)] \mid E_0^{(+)} \mid^2$

$\alpha(\omega) = \sum_\beta \frac{2\omega_{\beta\alpha}|\langle\alpha|\hat{\varepsilon}\cdot\mathbf{d}|\beta\rangle|^2}{\hbar(\omega^2_{\beta\alpha}-\omega^2)}$

Define

$\alpha_{\mu\nu}(\omega) = \sum_\beta \frac{2\omega_{\beta\alpha}\langle\alpha|d_\mu|\beta\rangle\langle\beta|d_\nu|\alpha\rangle}{\hbar(\omega^2_{\beta\alpha}-\omega^2)}$

$\Delta E_\alpha = -Re[\alpha_{\mu\nu}(\omega)](E_0^{(-)})_\mu(E_0^{(+)})_\nu$

$\alpha_{\mu\nu}(J,m_J,\omega) = \sum_{J'}\frac{2\omega_{J'J}T_{\mu\nu}}{\hbar(\omega^2_{J'J}-\omega^2)}$

$T_{\mu\nu} = \sum_{m'_J}\langle Jm_J \mid d_\mu \mid J'm'_J\rangle\langle J'm'_J \mid d_\nu \mid Jm_J\rangle$

3.1 Scalar shift

$T^{(0)} = T_{\mu\mu}$

Using Wigner-Eckart theorem,

$T^{(0)} = \mid \langle J \mid\mid \mathbf{d} \mid\mid J'\rangle \mid^2$

$\alpha^{(0)}(J,\omega) = \sum_{J'}\frac{2\omega_{J'J}|\langle J||\mathbf{d}||J'\rangle|^2}{3\hbar(\omega^2_{J'J}-\omega^2)}$

m_J independent

3.2 Vector shift

$T^{(1)}_\mu = \epsilon_{\mu\sigma\tau}(T_{\sigma\tau} - T_{\tau\sigma}) = 2\epsilon_{\mu\sigma\tau}2T_{\sigma\tau}$

$T^{(1)}_q = (-1)^{J+J'}(-i)\sqrt{\frac{24(2J+1)}{J(J+1)}}\begin{Bmatrix}1 & 1 & 1\\ J & J & J'\end{Bmatrix} \mid \langle J \mid\mid \mathbf{d} \mid\mid J'\rangle \mid^2 m_J\delta_{q0}$

$\alpha^{(1)}(J,\omega) = \sum_{J'}(-1)^{J+J'+1}\sqrt{\frac{6J(2J+1)}{J+1}}\begin{Bmatrix}1 & 1 & 1\\ J & J & J'\end{Bmatrix}\frac{\omega_{J'J}|\langle J||\mathbf{d}||J'\rangle|^2}{\hbar(\omega^2_{J'J}-\omega^2)}$

3.3 Tensor shift

$T^{(2)}_{\alpha\beta} = T_{\alpha\beta} - \frac{1}{3}T_{\mu\mu}\delta_{\alpha\beta}$

$T^{(2)}_q = (-1)^{J+J'}\sqrt{\frac{5(2J+1)}{J(J+1)(2J-1)(2J+3)}}\begin{Bmatrix}1 & 1 & 2\\ J & J & J'\end{Bmatrix} \mid \langle J \mid\mid \mathbf{d} \mid\mid J'\rangle \mid^2 [m_J^2 - J(J+1)]\delta_{q0}$

$\alpha^{(2)}(J,\omega) = \sum_{J'}(-1)^{J+J'}\sqrt{\frac{40J(2J+1)(2J-1)}{3(J+1)(2J+3)}}\begin{Bmatrix}1 & 1 & 2\\ J & J & J'\end{Bmatrix}\frac{\omega_{J'J}|\langle J||\mathbf{d}||J'\rangle|^2}{\hbar(\omega^2_{J'J}-\omega^2)}$

3.4 Total light shift

$\Delta E(J, m_J, \omega) = -\alpha^{(0)}(J,\omega) \mid E_0^{(+)} \mid^2 - \alpha^{(1)}(J,\omega)(i\mathbf{E}_0^{(-)} \times \mathbf{E}_0^{(+)})_z \frac{m_J}{J} - \alpha^{(2)}(J,\omega)\frac{3|E_{0z}^{(+)}|^2-|E_0^{(+)}|^2}{2}\frac{3m_J^2-J(J+1)}{J(2J-1)}$

Normalization. Note $(i\mathbf{E}_0^{(-)} \times \mathbf{E}_0^{(+)})_z = \mid \mathbf{E}_{0,-1}^{(+)} \mid^2 - \mid \mathbf{E}_{0,1}^{(-)} \mid^2$. Then $\sigma^+(\mathbf{E}_0^{(+)} = E_{0,-1}^{(+)})$ has light shift $\Delta E^{(1)}_{J,\pm J} = \mp\alpha^{(1)}(J) \mid E_{0,-1}^{(+)} \mid^2$

3.5 Note

1. Linear polarization drives the scalar and tensor light shifts, thus acts as an effective dc electric field
2. Circurly polarization drives the vector light shift, acts as an effective magnetic field
3. $J = 0$ or $J = \frac{1}{2}$, no tensor light shift
4. $J = 0$, no vector light shift

4 Decay rate and calculation of reduced matrix elements

Wigner-Eckart theorem

$\Gamma_{n'J'\to nJ} = \frac{\omega^3_{n'J'\to nJ}}{3\pi\epsilon_0\hbar c^3}\frac{2J+1}{2J'+1} \mid \langle nJ \mid\mid \mathbf{d} \mid\mid n'J'\rangle \mid^2$

Using the decomposition rule

$\langle nJ \mid\mid \mathbf{d} \mid\mid n'J'\rangle = (-1)^{L'+L+1+S}\sqrt{(2J'+1)(2L+1)}\begin{Bmatrix}L & L' & 1\\ J' & J & S\end{Bmatrix}\langle nL \mid\mid \mathbf{d} \mid\mid nL'\rangle$

$A_T(n'J') = \sum_J \Gamma_{n'J'\to nJ} = \frac{|\langle nL||\mathbf{d}||nL'\rangle|^2}{3\pi\epsilon_0\hbar c^3}\frac{2L+1}{2L'+1}\sum_J \omega^3_{n'J'\to nJ}(2J+1)(2L'+1)\begin{Bmatrix}L & L' & 1\\ J' & J & S\end{Bmatrix}^2$

The branching ratio is then

$$\frac{\Gamma_{n'J'\to nJ}}{A_T(n'J')} = \frac{\omega^3_{n'J'\to nJ}(2J+1)\begin{Bmatrix}L & L' & 1\\ J' & J & S\end{Bmatrix}^2}{\sum_J \omega^3_{n'J'\to nJ}(2J+1)\begin{Bmatrix}L & L' & 1\\ J' & J & S\end{Bmatrix}^2}$$

Then we can compute the corresponding $\mid \langle nJ \mid\mid \mathbf{d} \mid\mid n'J'\rangle \mid^2$

It's the same as Boyd thesis when considering different $m_J, m_{J'}$ states using Clebsch-Gordon coefficients and taking ω^3 term into ζ correction. (Eq 3.9-3.10)

5 References

1. Steck, 'Quantum and Atomic Optics', chapter 7.
2. Boyd thesis
3. Martin thesis

6 Special note

The conjugate of the reduced matric element is
$\langle J^{'} \mid\mid T_q^{(k)} \mid\mid J\rangle = (-1)^{J^{'}-J}\sqrt{\frac{2J+1}{2J^{'}+1}}\langle J \mid\mid T_q^{(k)} \mid\mid J^{'}\rangle^*$
which means specifically $\mid \langle J^{'} \mid\mid \mathbf{d} \mid\mid J\rangle \mid^2 = \frac{2J+1}{2J^{'}+1} \mid \langle J \mid\mid \mathbf{d} \mid\mid J^{'}\rangle \mid^2$
Otherwise it will lead to wrong calculation of excited state polarizability (Sr-88, $^1P_1$ and $^1S_0$).

From Kien2013, we can also define another normalization of reduced matrix as:
(Wiger-Eckart theorem) $\langle \alpha jm \mid T_q^{(k)} \mid \alpha^{'} j^{'} m^{'}\rangle = \frac{\langle \alpha j || \mathbf{T}^{(k)} || \alpha^{'} j^{'}\rangle}{\sqrt{2j+1}}\langle jm \mid j^{'}m^{'}; kq\rangle$
or $\langle \alpha j \mid\mid \mathbf{T}^{(k)} \mid\mid \alpha^{'} j^{'}\rangle = (-1)^{2k}\sqrt{2j+1}\langle \alpha j \mid\mid \mathbf{T}^{(k)} \mid\mid \alpha^{'} j^{'}\rangle$ (Steck, equation 7.238-7.239)
or through Wigner-3j symbol
Then $\mid \langle J^{'} \mid\mid \mathbf{d} \mid\mid J\rangle \mid^2 = \mid \langle J \mid\mid \mathbf{d} \mid\mid J^{'}\rangle \mid^2$
(Decomposition rule) $\langle j \mid\mid \mathbf{T}^{(k)} \mid\mid j^{'}\rangle = \delta_{j_2 j_2^{'}}(-1)^{j^{'}+j_1+k+j_2}\sqrt{(2j^{'}+1)(2j+1)}\begin{Bmatrix} j_1 & j_1^{'} & k \\ j^{'} & j & j_2 \end{Bmatrix}\langle j_1 \mid\mid \mathbf{T}^{(k)} \mid\mid j_1^{'}\rangle$
(Decay rate) $\Gamma_{n^{'}J^{'}\to nJ} = \frac{\omega^3_{n^{'}J^{'}\to nJ}}{3\pi\epsilon_0\hbar c^3}\frac{1}{2J^{'}+1} \mid \langle nJ \mid\mid \mathbf{d} \mid\mid n^{'}J^{'}\rangle \mid^2$
The corresponding polarizabilities are:
$\alpha^{(0)}(J,\omega) = \sum_{J^{'}} \frac{2}{3(2J+1)}\frac{\omega_{J^{'}J}|\langle J||\mathbf{d}||J^{'}\rangle|^2}{\hbar(\omega^2_{J^{'}J}-\omega^2)}$
$\alpha^{(1)}(J,\omega) = \sum_{J^{'}}(-1)^{J+J^{'}+1}\sqrt{\frac{6J}{(J+1)(2J+1)}}\begin{Bmatrix} 1 & 1 & 1 \\ J & J & J^{'} \end{Bmatrix}\frac{\omega_{J^{'}J}|\langle J||\mathbf{d}||J^{'}\rangle|^2}{\hbar(\omega^2_{J^{'}J}-\omega^2)}$
$\alpha^{(2)}(J,\omega) = \sum_{J^{'}}(-1)^{J+J^{'}}\sqrt{\frac{40J(2J-1)}{3(J+1)(2J+1)(2J+3)}}\begin{Bmatrix} 1 & 1 & 2 \\ J & J & J^{'} \end{Bmatrix}\frac{\omega_{J^{'}J}|\langle J||\mathbf{d}||J^{'}\rangle|^2}{\hbar(\omega^2_{J^{'}J}-\omega^2)}$