# Scalar and Tensor Polarizabilities of Atoms

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**Abstract**

This is a note written to understand the formulas for scalar and tensor polarizabilities of atoms,

## 1 Basic Formulas

We derive formulas for the scalar and tensor polarizabilities following the outline given by Khadjavi et al. [1]. We assume that the atom is in state $|JM_J\rangle$ and is subject to a perturbation $H^{(1)} = e\,\boldsymbol{r}\cdot E$. Owing to parity conservation, the first-order correction to the unperturbed energy vanishes. The second-order energy is

$$\begin{aligned}\Delta W_{JM_J} &= -e^2 \sum_{K\neq J}\sum_{M_K} \frac{\langle JM_J|\boldsymbol{r}\cdot E|KM_K\rangle\langle KM_K|\boldsymbol{r}\cdot E|JM_J\rangle}{W_K - W_J} \\ &= -e^2 \sum_{K\neq J}\sum_{M_K}\sum_{\mu\nu}(-1)^{\mu+\nu}E_\mu E_\nu \frac{\langle JM_J|r_{-\mu}|KM_K\rangle\langle KM_K|r_{-\nu}|JM_J\rangle}{W_K - W_J},\end{aligned} \tag{1}$$

where $E_\mu$ and $r_\mu$ are components of the vectors $\boldsymbol{E}$ and $\boldsymbol{r}$, respectively, in a spherical basis.

### 1.1 Product Tensor

To put Eq.(1) into a tractable form, we express the product $E_\mu E_\nu$ of two rank 1 irreducible tensor operators $E_\mu$ and $E_\nu$ as a sum of irreducible tensor operators $\mathcal{E}(L, M_L)$ defined by

$$\mathcal{E}(L, M_L) = \sum_{\mu\nu}\sqrt{[L]}(-1)^{M_L}\begin{pmatrix} 1 & 1 & L \\ \mu & \nu & -M_L \end{pmatrix} E_\mu E_\nu \tag{2}$$

Inverting this relation, we find

$$E_\mu E_\nu = \sum_{L=0}^{2} \sum_{M_L=-L}^{L} \sqrt{[L]}(-1)^{M_L} \begin{pmatrix} 1 & 1 & L \\ \mu & \nu & -M_L \end{pmatrix} \mathcal{E}(L, M_L) \tag{3}$$

Explicit formulas for the components of the irreducible tensor operator $\mathcal{E}(L, M_L)$ are as follows:

$$\begin{aligned}
\mathcal{E}(0,0) &= -\frac{1}{\sqrt{3}} \left[E_0^2 - 2E_{-1}E_1\right] = -\frac{1}{\sqrt{3}} E^2 \\
\mathcal{E}(1,\mp 1) &= 0 \qquad \mathcal{E}(1,0) = 0 \\
\mathcal{E}(2,\mp 2) &= E_{\mp 1}^2 \qquad \mathcal{E}(2,\mp 1) = \sqrt{2} E_{\mp 1} E_0 \\
\mathcal{E}(2,0) &= \sqrt{\frac{2}{3}} \left[E_0^2 + E_{-1}E_1\right] = \frac{1}{\sqrt{6}} \left[3E_z^2 - E^2\right]
\end{aligned}$$

## 1.2 Sum over magnetic quantum numbers

As a first step in evaluating the sum over magnetic quantum numbers in Eq.(1), we define

$$S(J, M_J) = \sum_{M_K} \sum_{\mu\nu} (-1)^{\mu+\nu} E_\mu E_\nu \langle J M_J | r_{-\mu} | K M_K \rangle \langle K M_K | r_{-\nu} | J M_J \rangle \tag{4}$$

Substituting for $E_\mu E_\nu$ and writing the dipole matrix elements in terms of reduced matrix elements, Eq.(4) becomes

$$\begin{aligned}
S(J, M_J) = (-1)^{J-K} &\left|\langle J \| r \| K \rangle\right|^2 \\
&\sum_L \sqrt{[L]} \sum_{M_L} \mathcal{E}(L, M_L) \sum_{\mu\nu} (-1)^{\mu+\nu} (-1)^{M_L} \begin{pmatrix} 1 & 1 & L \\ \mu & \nu & -M_L \end{pmatrix} \\
\sum_{M_K} &\left[ (-1)^{J-M_J} \begin{pmatrix} J & 1 & K \\ -M_J & -\mu & M_K \end{pmatrix} (-1)^{K-M_K} \begin{pmatrix} K & 1 & J \\ -M_K & -\nu & M_J \end{pmatrix} \right]
\end{aligned} \tag{5}$$

The sum over $\mu$, $\nu$ and $M_K$ in Eq.(5) is carried out to give

$$\begin{aligned}
\sum_{\mu\nu M_K} &(-1)^{\mu+\nu} (-1)^{M_L} \begin{pmatrix} 1 & 1 & L \\ \mu & \nu & -M_L \end{pmatrix} \\
&(-1)^{J-M_J} \begin{pmatrix} J & 1 & K \\ -M_J & -\mu & M_K \end{pmatrix} (-1)^{K-M_K} \begin{pmatrix} K & 1 & J \\ -M_K & -\nu & M_J \end{pmatrix} \\
&\qquad = (-1)^{2J} (-1)^{J-M_J} \begin{pmatrix} J & L & J \\ -M_J & 0 & M_J \end{pmatrix} \begin{Bmatrix} J & 1 & K \\ 1 & K & L \end{Bmatrix} \delta_{M_L,0}
\end{aligned} \tag{6}$$

Substituting Eq.(6) into Eq.(5), we find

$$S(J,M_J) = (-1)^{J+K} |\langle J\|r\|K\rangle|^2 \sum_L \mathcal{E}(L,0)\sqrt{[L]}(-1)^{J-M_J} \begin{pmatrix} J & L & J \\ -M_J & 0 & M_J \end{pmatrix} \begin{Bmatrix} J & 1 & K \\ 1 & K & L \end{Bmatrix} \quad (7)$$

With the aid of Eq(7) we decompose $\Delta W_{JM_J}$ into a sum over $L$:

$$\Delta W_{JM_J} = \sum_L \Delta W^{(L)}_{JM_J}, \quad (8)$$

where

$$\Delta W^{(L)}_{JM_J} = -e^2 \sum_{K\neq J} \frac{|\langle J\|r\|K\rangle|^2}{W_K - W_J} \mathcal{E}(L,0) \sqrt{[L]}(-1)^{J+K}(-1)^{J-M_J} \begin{pmatrix} J & L & J \\ -M_J & 0 & M_J \end{pmatrix} \begin{Bmatrix} J & 1 & K \\ 1 & K & L \end{Bmatrix}. \quad (9)$$

It should be noted that there are only two nonvanishing components of $\mathcal{E}(L,0)$, $L=0$ and $L=2$.

#### 1.2.1 L=0

For the case $L=0$, we have

$$(-1)^{J-M_J} \begin{pmatrix} J & 0 & J \\ -M_J & 0 & M_J \end{pmatrix} = \frac{1}{\sqrt{[J]}} \quad (10)$$

and

$$\begin{Bmatrix} J & 1 & K \\ 1 & K & 0 \end{Bmatrix} = \frac{(-1)^{J+K+1}}{\sqrt{[J][1]}} \quad (11)$$

We also have

$$\mathcal{E}(0,0) = -\frac{1}{\sqrt{3}} E^2 \quad (12)$$

Therefore

$$\Delta W^{(0)}_{JM_J} = -e^2 E^2 \frac{1}{3(2J+1)} \sum_{K\neq J} \frac{|\langle J\|r\|K\rangle|^2}{W_K - W_J}. \quad (13)$$

#### 1.2.2 L=2

For the case $L=2$, we have

$$(-1)^{J-M_J} \begin{pmatrix} J & 2 & J \\ -M_J & 0 & M_J \end{pmatrix} = \frac{2[3M_J^2 - J(J+1)]}{[(2J+3)(2J+2)(2J+1)(2J)(2J-1)]^{1/2}} \quad (14)$$

and

$$\mathcal{E}(2,0) = \frac{1}{\sqrt{6}}\left(3E_z^2 - E^2\right) \tag{15}$$

It follows that

$$\Delta W^{(2)}_{JM_J} = -e^2(3E_z^2 - E^2)\sqrt{\frac{5J(2J-1)}{6(2J+3)(J+1)(2J+1)}}$$
$$\frac{3M_J^2 - J(J+1)}{J(2J-1)} \sum_{K\neq J} (-1)^{J+K} \left\{ \begin{array}{ccc} J & 1 & K \\ 1 & J & 2 \end{array} \right\} \frac{|\langle J\|r\|K\rangle|^2}{W_K - W_J} \tag{16}$$

Note that $\Delta W^{(2)}_{J,M_J} = 0$ for the cases $J = 0$ and $J = 1/2$.

### 1.3 Definition of Polarizabilities

Let us choose our axis system so that the electric field is directed along the z-axis: $\boldsymbol{E} = E\hat{\boldsymbol{z}}$. We may then write

$$\Delta W^{(2)}_{JM_J} = -\frac{1}{2}e^2E^2\sqrt{\frac{40J(2J-1)}{3(2J+3)(J+1)(2J+1)}}$$
$$\frac{3M_J^2 - J(J+1)}{J(2J-1)} \sum_{K\neq J} (-1)^{J+K} \left\{ \begin{array}{ccc} J & 1 & K \\ 1 & J & 2 \end{array} \right\} . \frac{|\langle J\|r\|K\rangle|^2}{W_K - W_J} \tag{17}$$

We define the scalar and tensor polarizabilities in terms of $\Delta W_{JM_J}$ through the relation

$$\Delta W_{JM_J} = -\frac{1}{2}e^2E^2\left[\alpha_J^{(0)} + \frac{3M_J^2 - J(J+1)}{J(2J-1)}\ \alpha_J^{(2)}\right]. \tag{18}$$

It follows that

$$\alpha_J^{(0)} = \frac{2}{3(2J+1)} \sum_{K\neq J} \frac{|\langle J\|r\|K\rangle|^2}{W_K - W_J} \tag{19}$$

$$\alpha_J^{(2)} = \sqrt{\frac{40J(2J-1)}{3(2J+3)(J+1)(2J+1)}}$$
$$\sum_{K\neq J} (-1)^{J+K} \left\{ \begin{array}{ccc} J & 1 & K \\ 1 & J & 2 \end{array} \right\} \frac{|\langle J\|r\|K\rangle|^2}{W_K - W_J} \tag{20}$$

For a general orientation of the electric field, in which the electric field vector makes an angle $\theta$ with the z-axis, we may write

$$\Delta W_{JM_J} = -\frac{1}{2}e^2E^2\left[\alpha_J^{(0)} + P_2(\cos\theta)\ \frac{3M_J^2 - J(J+1)}{J(2J-1)}\ \alpha_J^{(2)}\right]. \tag{21}$$

Table 1: Values of the coefficients $C_2[J,K]$ for half-integer values of $J$.

| $J$ | $C_2[J,J-1]$ | $C_2[J,J]$ | $C_2[J,J+1]$ |
|---|---|---|---|
| $\frac{3}{2}$ | $-\frac{1}{6}$ | $\frac{2}{15}$ | $-\frac{1}{30}$ |
| $\frac{5}{2}$ | $-\frac{1}{9}$ | $\frac{8}{63}$ | $-\frac{5}{126}$ |
| $\frac{7}{2}$ | $-\frac{1}{12}$ | $\frac{1}{9}$ | $-\frac{7}{180}$ |
| $\frac{9}{2}$ | $-\frac{1}{15}$ | $\frac{16}{165}$ | $-\frac{2}{55}$ |
| $\frac{11}{2}$ | $-\frac{1}{18}$ | $\frac{10}{117}$ | $-\frac{55}{1638}$ |

Table 2: Values of the coefficients $C_2[J,K]$ for integer values of $J$.

| $J$ | $C_2[J,J-1]$ | $C_2[J,J]$ | $C_2[J,J+1]$ |
|---|---|---|---|
| 1 | $-\frac{2}{9}$ | $\frac{1}{9}$ | $-\frac{1}{45}$ |
| 2 | $-\frac{2}{15}$ | $\frac{2}{15}$ | $-\frac{4}{105}$ |
| 3 | $-\frac{2}{21}$ | $\frac{5}{42}$ | $-\frac{5}{126}$ |
| 4 | $-\frac{2}{27}$ | $\frac{14}{135}$ | $-\frac{56}{1485}$ |
| 5 | $-\frac{2}{33}$ | $\frac{1}{11}$ | $-\frac{5}{143}$ |

### 1.4 Useful Simplifications

Let us rewrite the expression for $\alpha_J^{(2)}$ in the form

$$\alpha_J^{(2)} = \sum_{K \neq J} C_2(J,K) \frac{|\langle J \| r \| K \rangle|^2}{W_K - W_J} \tag{22}$$

Values of the coefficients $C_2(J,K)$ are tabulated in Table 1 for half-integer values of $J$ and in Table 2 for integer values of $J$.

## 2 Polarizability of a hyperfine level

In this section, wee derive the formulas for the scalar and tensor polarizabilities of a hyperfine level:

$$|FM_F\rangle = \sum_{M_J M_I} C^{FM_F}_{JM_J\,IM_I} |JM_J\rangle |IM_I\rangle$$

To this end, we must evaluate

$$
\begin{aligned}
S(F,M_F) &= (-1)^{J-K}\, |\langle J\|r\|K\rangle|^2 \\
&\quad \sum_L \sum_{M_L} \mathcal{E}(L,M_L) \sum_{\mu\nu} (-1)^{\mu+\nu} \sum_{M_1 M_2 M_K} C^{FM_F}_{JM_1\, IM_I} C^{FM_F}_{JM_2\, IM_I} C^{LM_L}_{1\mu\, 1_\nu} \\
&\quad (-1)^{J-M_1} \begin{pmatrix} J & 1 & K \\ -M_1 & -\mu & M_K \end{pmatrix} (-1)^{K-M_K} \begin{pmatrix} K & 1 & J \\ -M_K & -\nu & M_2 \end{pmatrix}
\end{aligned} \tag{23}
$$

The sum over $\mu$, $\nu$, $M_1$, $M_2$ and $M_K$ in Eq.(23) becomes

$$
\begin{aligned}
&\sum_{\mu\nu} (-1)^{\mu+\nu} \sum_{M_1 M_2 M_K} C^{FM_F}_{JM_1\, IM_I} C^{FM_F}_{JM_2\, IM_I} C^{LM_L}_{1\mu\, 1_\nu} \\
&\quad (-1)^{J-M_1} \begin{pmatrix} J & 1 & K \\ -M_1 & -\mu & M_K \end{pmatrix} (-1)^{K-M_K} \begin{pmatrix} K & 1 & J \\ -M_K & -\nu & M_2 \end{pmatrix} \\
&\qquad = (-1)^{J-F-I} \sqrt{[L]}[F] (-1)^{F-M_F} \begin{pmatrix} F & L & F \\ -M_F & 0 & M_F \end{pmatrix} \\
&\qquad\qquad \begin{Bmatrix} J & 1 & K \\ 1 & J & L \end{Bmatrix} \begin{Bmatrix} F & J & I \\ J & F & L \end{Bmatrix} \delta_{M_L,0}
\end{aligned} \tag{24}
$$

### 2.1 L=0

For $L = 0$, we have

$$
\begin{aligned}
S(F,M_F) &= (-1)^{J-K}\, |\langle J\|r\|K\rangle|^2 \;\; \mathcal{E}(0,0)\;\; (-1)^{J-F-I}\;\; [F] \\
&\quad (-1)^{F-M_F} \begin{pmatrix} F & 0 & F \\ -M_F & 0 & M_F \end{pmatrix} \begin{Bmatrix} J & 1 & K \\ 1 & J & 0 \end{Bmatrix} \begin{Bmatrix} F & J & I \\ J & F & 0 \end{Bmatrix} \\
&= \frac{1}{3[J]}\; E^2 \;\; |\langle J\|r\|K\rangle|^2 .
\end{aligned} \tag{25}
$$

Note that the above result is independent of $F$ and $M_F$. We may therefore write

$$
\Delta W^{(0)}_{FM_F} = -\frac{1}{2} e^2 E^2 \alpha^{(0)}_J . \tag{26}
$$

## 2.2 L=2

For $L = 2$, we have

$$S(F, M_F) = (-1)^{J-K} \left|\langle J\|r\|K\rangle\right|^2 \ \mathcal{E}(2,0)\ (-1)^{J-F-I}\ [F]\ \sqrt{5}$$
$$(-1)^{F-M_F} \begin{pmatrix} F & 2 & F \\ -M_F & 0 & M_F \end{pmatrix} \begin{Bmatrix} J & 1 & K \\ 1 & j & 2 \end{Bmatrix} \begin{Bmatrix} F & J & I \\ J & F & 2 \end{Bmatrix}$$
$$= E^2 P_2(\cos\theta) \left|\langle J\|r\|K\rangle\right|^2$$
$$[F]\sqrt{\frac{40F(2F-1)}{3(2F+3)(F+1)(2F+1)}} \frac{3M_F^2 - F(F+1)}{F(2F-1)}$$
$$(-1)^{I+J+F} \begin{Bmatrix} F & J & I \\ J & F & 2 \end{Bmatrix} (-1)^{J+K} \begin{Bmatrix} J & 1 & K \\ 1 & J & 2 \end{Bmatrix}. \quad (27)$$

It follows that

$$\Delta W^{(2)}_{FM_F} =$$
$$-\frac{1}{2}e^2 E^2 P_2(\cos\theta)\ [F]\sqrt{\frac{40F(2F-1)}{3(2F+3)(F+1)(2F+1)}} \frac{3M_F^2 - F(F+1)}{F(2F-1)}$$
$$(-1)^{I+J+F} \begin{Bmatrix} F & J & I \\ J & F & 2 \end{Bmatrix} \sum_{K\neq J} (-1)^{J+K} \begin{Bmatrix} J & 1 & K \\ 1 & J & 2 \end{Bmatrix} \frac{\left|\langle J\|r\|K\rangle\right|^2}{W_K - W_J} \quad (28)$$

Defining $\alpha^{(2)}_F$ in terms of the energy shift, we have

$$\Delta W_{FM_F} = -\frac{1}{2}e^2 E^2 \left[\alpha^{(0)}_F + P_2(\cos\theta)\ \frac{3M_F^2 - F(F+1)}{F(2F-1)}\ \alpha^{(2)}_F\right]. \quad (29)$$

It follows that

$$\alpha^{(0)}_F = \alpha^{(0)}_J \quad (30)$$
$$\alpha^{(2)}_F = (-1)^{I+J+F} \sqrt{\frac{40F(2F-1)(2F+1)}{3(2F+3)(F+1)}} \begin{Bmatrix} F & J & I \\ J & F & 2 \end{Bmatrix}$$
$$\times \sum_{K\neq J} (-1)^{J+K} \begin{Bmatrix} J & 1 & K \\ 1 & J & 2 \end{Bmatrix} \frac{\left|\langle J\|r\|K\rangle\right|^2}{W_K - W_J}. \quad (31)$$

It is interesting to note that in the stretched state, $F = I + J$,

$$\alpha^{(2)}_{F=I+J} = \alpha^{(2)}_J$$

for $I \geq 1/2$ and $J \geq 3/2$.

# References


[1] A. Khadjavi, A. Lurio, and W. Happer, Phys. Rev. **167**, 128 (1968).