One and two photon absorption matrix elements

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Abstract

The relation between length and velocity forms of matrix elements in resonant one-photon absorption and non-resonant two-photon absorption is discussed.

The interaction Hamiltonian for a charge e in an electromagnetic field described by the vector potential

$$\boldsymbol{A} = \boldsymbol{\epsilon} e^{ikz} \approx \boldsymbol{\epsilon}$$

is

$$H_{\rm int} = -\frac{e}{mc} \boldsymbol{A} \cdot \boldsymbol{p} + \frac{e^2}{2mc^2} A^2$$

One-Photon Transitions

The matrix element describing absorption of a photon leading from state $|a\rangle$ to state $|b\rangle$ with $E_b - E_a = \omega$ (units $\hbar = 1$) is given by

$$M_{ba} = -\frac{e}{mc} \langle b | \, \boldsymbol{\epsilon} \cdot \boldsymbol{p} \, | a \rangle \tag{1}$$

With the aid of the operator identity $\boldsymbol{p} = im \, [H, \boldsymbol{r}]$ this may be rewritten in the form

$$M_{ba} = -i \frac{e}{c} (E_b - E_a) \langle b | \, \boldsymbol{\epsilon} \cdot \boldsymbol{r} \, | a \rangle \equiv -i \frac{e}{c} \omega \langle b | \, \boldsymbol{\epsilon} \cdot \boldsymbol{r} \, | a \rangle. \tag{2}$$

These two forms for the single photon transition matrix element are referred to as velocity and length forms, respectively. The transition between velocity and length forms is accomplished in the one-photon (resonant) case by the substitution

$$\frac{1}{m} \boldsymbol{p} \equiv \boldsymbol{v} \rightarrow i \, \omega \, \boldsymbol{r},$$

where ω is the photon frequency. The purpose in this note is to show that this same transformation is also proper in the non-resonant two-photon case.

Two-Photon Transitions

The (2nd-order) matrix element describing non-resonant absorbtion of two photons leading from from state $|a\rangle$ to state $|b\rangle$ is

$$\begin{aligned} M_{ba} = &\left(\frac{e}{mc}\right)^2 \sum_n \left[\frac{\langle b|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{p}\, |n\rangle\langle n|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{p}\, |a\rangle}{E_a + \omega_1 - E_n} + \frac{\langle b|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{p}\, |n\rangle\langle n|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{p}\, |a\rangle}{E_a + \omega_2 - E_n} \right] \\ &+ \frac{e^2}{2mc^2} \langle b|\boldsymbol{\epsilon}_1 \cdot \boldsymbol{\epsilon}_2|a\rangle, \end{aligned} \tag{3}$$

where $E_b = E_a + \omega_1 + \omega_2$. States $|a\rangle$ and $|b\rangle$ are orthogonal so the term on the second line vanishes.

Now, we make use of $\boldsymbol{p} = im\,[H, \boldsymbol{r}]$ to obtain the following identities:

$$\begin{aligned} \frac{\langle n|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{p}\, |a\rangle}{E_a + \omega_1 - E_n} &= im \frac{E_n - E_a}{E_a + \omega_1 - E_n} \langle n|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |a\rangle \\ &= im \left[-1 + \frac{\omega_1}{E_a + \omega_1 - E_n} \right] \langle n|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |a\rangle, \end{aligned} \tag{4}$$

$$\begin{aligned} \frac{\langle b|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{p}\, |n\rangle}{E_a + \omega_2 - E_n} &= im \frac{E_b - E_n}{E_a + \omega_2 - E_n} \langle n|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |a\rangle \\ &= im \left[1 + \frac{\omega_1}{E_a + \omega_2 - E_n} \right] \langle b|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |n\rangle. \end{aligned} \tag{5}$$

Let us demonstrate that the contribution from the first terms in the two square brackets above vanishes:

$$\begin{aligned} M_{ba}^{(1)} &= i \frac{e^2}{mc^2} \sum_n \left[-\langle b|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{p}\, |n\rangle\langle n|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |a\rangle + \langle b|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |n\rangle\langle n|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{p}\, |a\rangle \right] \\ &= -im \left(\frac{e}{mc}\right)^2 \sum_{ij} \epsilon_{1i} \epsilon_{2j} \langle b|[p_j, x_i]|a\rangle \\ &= -\frac{e^2}{mc^2} \langle b|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{\epsilon}_2\, |a\rangle = 0 \end{aligned} \tag{6}$$

It follows that

$$M_{ba} = i\omega_1 \frac{e^2}{mc^2} \sum_n \left[\frac{\langle b|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{p}\, |n\rangle\langle n|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |a\rangle}{E_a + \omega_1 - E_n} + \frac{\langle b|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |n\rangle\langle n|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{p}\, |a\rangle}{E_a + \omega_2 - E_n} \right] \tag{7}$$

Next, we introduce the identities

$$\begin{aligned} \frac{\langle b|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{p}\, |n\rangle}{E_a + \omega_1 - E_n} &= im \frac{E_b - E_n}{E_a + \omega_1 - E_n} \langle b|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{r}\, |n\rangle \\ &= im \left[1 + \frac{\omega_2}{E_a + \omega_1 - E_n} \right] \langle b|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{r}\, |n\rangle, \end{aligned} \tag{8}$$

$$\begin{aligned} \frac{\langle n|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{p}\, |a\rangle}{E_a + \omega_2 - E_n} &= im \frac{E_n - E_a}{E_a + \omega_2 - E_n} \langle n|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{r}\, |a\rangle \\ &= im \left[-1 + \frac{\omega_2}{E_a + \omega_2 - E_n} \right] \langle n|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{r}\, |a\rangle. \end{aligned} \tag{9}$$

The first terms inside the two square brackets above are easily seen to cancel, leading to the following (length-form) expression for the two-photon matrix element:

$$M_{ba} = -e^2 \frac{\omega_1\omega_2}{c^2} \sum_n \left[\frac{\langle b|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{r}\, |n\rangle\langle n|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |a\rangle}{E_a + \omega_1 - E_n} + \frac{\langle b|\, \boldsymbol{\epsilon}_1 \cdot \boldsymbol{r}\, |n\rangle\langle n|\, \boldsymbol{\epsilon}_2 \cdot \boldsymbol{r}\, |a\rangle}{E_a + \omega_2 - E_n} \right]. \tag{10}$$

For the case of absorbtion of two identical photons, there is a factor of $1/\sqrt{2}$ from the two-photon state vector, so we have

$$M_{ba} = \frac{2}{\sqrt{2}} \left(\frac{e}{mc}\right)^2 \sum_n \frac{\langle b|\, \boldsymbol{\epsilon} \cdot \boldsymbol{p}\, |n\rangle\langle n|\, \boldsymbol{\epsilon} \cdot \boldsymbol{p}\, |a\rangle}{E_a + \omega - E_n} \qquad \text{(velocity-form)}$$

$$M_{ba} = -\frac{2}{\sqrt{2}}\, e^2 \frac{\omega^2}{c^2} \sum_n \frac{\langle b|\, \boldsymbol{\epsilon} \cdot \boldsymbol{r}\, |n\rangle\langle n|\, \boldsymbol{\epsilon} \cdot \boldsymbol{r}\, |a\rangle}{E_a + \omega - E_n} \qquad \text{(length-form)}$$

The lesson from these two examples is that one safely transforms between two equivalent forms of the transition matrix element using

$$\frac{1}{m}\boldsymbol{p} \rightarrow i\,\omega\,\boldsymbol{r},$$

where ω is the photon frequency in either resonant or non resonant cases.