Electric dipole selectrion rules
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Here we collect all the topics on the commutation relations related to the orbital angular momentum, which play an important rule for the electric dipole selection rules. Several topics are discussed in the previous chapters. We now consider how to calculate the matrix element of the electric dipole,

$$\langle n'l'm'|\hat{\boldsymbol{r}}|nlm\rangle .$$

1. Commutation relations of angular momentum

1.1 Commutation relation-I

The orbital angular momentum is defined as

$$\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$

We consider the commutation relation:

$$\hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = i\hbar \hat{\boldsymbol{L}}$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x , \qquad [\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y , \qquad [\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$[\hat{L}_z, \hat{z}] = [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{z}] = 0 ,$$

$$[\hat{L}_z, \hat{x}] = [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{x}] = -[\hat{y}\hat{p}_x, \hat{x}] = -\hat{y}[\hat{p}_x, \hat{x}] = i\hbar \hat{y}$$

$$[\hat{L}_z, \hat{y}] = [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{y}] = [\hat{x}\hat{p}_y, \hat{y}] = -i\hbar\hat{x}$$

or

$$[\hat{L}_z, \hat{x} + i\hat{y}] = [\hat{L}_z \hat{x}] + i[\hat{L}_z, \hat{y}] = i\hbar\hat{y} + i(-i\hbar\hat{x}) = \hbar(\hat{x} + i\hat{y})$$

$$[\hat{L}_z, \hat{x} - i\hat{y}] = [\hat{L}_z \hat{x}] - i[\hat{L}_z, \hat{y}] = i\hbar\hat{y} - i(-i\hbar\hat{x}) = -\hbar(\hat{x} - i\hat{y})$$

1.2 Proof of the above commutation relations by using Mathematica

((**Mathematica**)) Proof

```
Clear["Global`"];

ux = {1, 0, 0}; uy = {0, 1, 0}; uz = {0, 0, 1};
r = {x, y, z};

Lx := (ℏ ux.(-ⅈ Cross[r, Grad[#, {x, y, z}]]) &) // Simplify
Ly := (ℏ uy.(-ⅈ Cross[r, Grad[#, {x, y, z}]]) &) // Simplify
Lz := (ℏ uz.(-ⅈ Cross[r, Grad[#, {x, y, z}]]) &) // Simplify
Lsq := (Lx[Lx[#]] + Ly[Ly[#]] + Lz[Lz[#]] &);

eq2 = Lsq[Lsq[x ψ[x, y, z]]] - Lsq[x Lsq[ψ[x, y, z]]] -
    Lsq[x Lsq[ψ[x, y, z]]] + x Lsq[Lsq[ψ[x, y, z]]] //
   FullSimplify;

eq3 = 2 ℏ^2 (x Lsq[ψ[x, y, z]] + Lsq[x ψ[x, y, z]]) //
   FullSimplify;

eq2 - eq3 // Simplify

0
```

1.3 Commutation relation-II

We also note that

$$[\hat{\boldsymbol{L}}^2,[\hat{\boldsymbol{L}}^2,\hat{x}]] = 2\hbar^2\{\hat{x},\hat{\boldsymbol{L}}^2\}$$

where

$$\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

$$[\hat{\boldsymbol{L}}^2,[\hat{\boldsymbol{L}}^2,\hat{z}] = 2\hbar^2(\hat{z}\hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{L}}^2\hat{z})$$

((**Proof**)) Griffiths, Introduction to Quantum Mechanics

We prove this by using a various kind of commutation relations.

$$\begin{aligned}[\hat{\boldsymbol{L}}^2,\hat{z}] &= [\hat{L}_x{}^2,\hat{z}] + [\hat{L}_y{}^2,\hat{z}] + [\hat{L}_z{}^2,\hat{z}] \\ &= \hat{L}_x[\hat{L}_x,\hat{z}] + [\hat{L}_x,\hat{z}]\hat{L}_x + \hat{L}_y[\hat{L}_y,\hat{z}] + [\hat{L}_y,\hat{z}]\hat{L}_y + \hat{L}_z[\hat{L}_z,\hat{z}] + [\hat{L}_z,\hat{z}]\hat{L}_z \\ &= i\hbar(-\hat{L}_x\hat{y} - \hat{y}\hat{L}_x + \hat{L}_y\hat{x} + \hat{x}\hat{L}_y)\end{aligned}$$

We note that

$$\hat{L}_x\hat{y} = [\hat{L}_x,\hat{y}] + \hat{y}\hat{L}_x = i\hbar\hat{z} + \hat{y}\hat{L}_x$$

$$\hat{L}_y\hat{x} = [\hat{L}_y,\hat{x}] + \hat{x}\hat{L}_y = -i\hbar\hat{z} + +\hat{x}\hat{L}_y$$

Then we get

$$\begin{aligned}[\hat{\boldsymbol{L}}^2,\hat{z}] &= i\hbar[-(i\hbar\hat{z} + \hat{y}\hat{L}_x) - \hat{y}\hat{L}_x + (-i\hbar\hat{z} + \hat{x}\hat{L}_y) + \hat{x}\hat{L}_y) \\ &= 2i\hbar(\hat{x}\hat{L}_y - \hat{y}\hat{L}_x - i\hbar\hat{z})\end{aligned}$$

Similarly,

$$[\hat{\boldsymbol{L}}^2,\hat{x}] = 2i\hbar(\hat{y}\hat{L}_z - \hat{z}\hat{L}_y - i\hbar\hat{x})$$

and

$$[\hat{\boldsymbol{L}}^2,y] = 2i\hbar(z\hat{L}_x - x\hat{L}_z - i\hbar\hat{y})$$

where

$$[\hat{L}_x, \hat{z}] = [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}] = [\hat{y}\hat{p}_z, \hat{z}] - [\hat{z}\hat{p}_y, \hat{z}] = \hat{y}[\hat{p}_z, \hat{z}] = -i\hbar\hat{y} .$$

$$[\hat{L}_y, \hat{z}] = [\hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \hat{z}] = -[x\hat{p}_z, \hat{z}] = -\hat{x}[\hat{p}_z, \hat{z}] = -\frac{\hbar}{i}\hat{x} = i\hbar\hat{x} .$$

$$[\hat{L}_z, \hat{z}] = [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{z}] = -[\hat{y}\hat{p}_x, \hat{z}] = 0 .$$

$$[\hat{L}_x, \hat{x}] = [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{x}] = 0 .$$

$$[\hat{L}_y, \hat{x}] = [\hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \hat{x}] = [\hat{z}\hat{p}_x, \hat{x}] = \frac{\hbar}{i}\hat{z} = -i\hbar\hat{z} .$$

$$[\hat{L}_z, \hat{x}] = [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{x}] = -[\hat{y}\hat{p}_x, \hat{x}] = i\hbar\hat{y} .$$

$$[\hat{L}_x, \hat{y}] = [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{y}] = i\hbar\hat{z} .$$

$$[\hat{L}_y, \hat{y}] = [\hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \hat{y}] = 0 .$$

$$[\hat{L}_z, \hat{y}] = [\hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \hat{y}] = -i\hbar\hat{x} .$$

Then we get

$$
\begin{aligned}
[\hat{\boldsymbol{L}}^2,[\hat{\boldsymbol{L}}^2,\hat{z}]] &= 2i\hbar\{[\hat{\boldsymbol{L}}^2,\hat{x}\hat{L}_y]-[\hat{\boldsymbol{L}}^2,\hat{y}\hat{L}_x]-i\hbar[\hat{\boldsymbol{L}}^2,\hat{z}]\} \\
&= 2i\hbar\{[\hat{\boldsymbol{L}}^2,\hat{x}]\hat{L}_y+\hat{x}[\hat{\boldsymbol{L}}^2,\hat{L}_y]-[\hat{\boldsymbol{L}}^2,\hat{y}]\hat{L}_x-\hat{y}[\hat{\boldsymbol{L}}^2,\hat{L}_x]-i\hbar[\hat{\boldsymbol{L}}^2,\hat{z}]\} \\
&= 2i\hbar\{2i\hbar(\hat{y}\hat{L}_z-\hat{z}\hat{L}_y-i\hbar\hat{x})\hat{L}_y-2i\hbar(\hat{z}\hat{L}_x-\hat{x}\hat{L}_z-i\hbar\hat{y})\hat{L}_x \\
&\quad -i\hbar(\hat{\boldsymbol{L}}^2\hat{z}-\hat{z}\hat{\boldsymbol{L}}^2)\} \\
&= -2\hbar^2\{2(\hat{y}\hat{L}_z\hat{L}_y-\hat{z}\hat{L}_y{}^2-i\hbar\hat{x}\hat{L}_y)-2(\hat{z}\hat{L}_x{}^2-\hat{x}\hat{L}_z\hat{L}_x-i\hbar\hat{y}\hat{L}_x) \\
&\quad -(\hat{\boldsymbol{L}}^2\hat{z}-\hat{z}\hat{\boldsymbol{L}}^2\} \\
&= -2\hbar^2\{2(\hat{y}\hat{L}_z-i\hbar\hat{x})\hat{L}_y-2\hat{z}(\hat{L}_x{}^2+\hat{L}_y{}^2)+2(\hat{x}\hat{L}_z+i\hbar\hat{y})\hat{L}_x) \\
&\quad -(\hat{\boldsymbol{L}}^2\hat{z}-\hat{z}\hat{\boldsymbol{L}}^2)\} \\
&= -2\hbar^2\{2\hat{L}_z\hat{y}\hat{L}_y-2\hat{z}(\hat{\boldsymbol{L}}^2-\hat{L}_z{}^2)+2\hat{L}_z\hat{x}\hat{L}_x \\
&\quad -(\hat{\boldsymbol{L}}^2\hat{z}-\hat{z}\hat{\boldsymbol{L}}^2)\} \\
&= -2\hbar^2\{2\hat{L}_z(\hat{x}\hat{L}_x+\hat{y}\hat{L}_y+\hat{z}\hat{L}_z)-2\hat{L}_z\hat{z}\hat{L}_z-2\hat{z}(\hat{\boldsymbol{L}}^2-\hat{L}_z{}^2)-(\hat{\boldsymbol{L}}^2\hat{z}-\hat{z}\hat{\boldsymbol{L}}^2\}
\end{aligned}
$$

or

$$
\begin{aligned}
[\hat{\boldsymbol{L}}^2,[\hat{\boldsymbol{L}}^2,\hat{z}]] &= -2\hbar^2\{-2\hat{L}_z\hat{z}\hat{L}_z-2\hat{z}\hat{\boldsymbol{L}}^2+2\hat{z}\hat{L}_z{}^2-(\hat{\boldsymbol{L}}^2\hat{z}-\hat{z}\hat{\boldsymbol{L}}^2\} \\
&= 2\hbar^2(\hat{z}\hat{\boldsymbol{L}}^2+\hat{\boldsymbol{L}}^2\hat{z})
\end{aligned}
$$

where we use the relations,

$$\hat{x}\hat{L}_x+\hat{y}\hat{L}_y+\hat{z}\hat{L}_z=0$$

$$[\hat{\boldsymbol{L}}^2,\hat{L}_x]=[\hat{\boldsymbol{L}}^2,\hat{L}_y]=[\hat{\boldsymbol{L}}^2,\hat{L}_z]=0$$

$$[\hat{L}_z,\hat{z}]=0$$

and

$$
\begin{aligned}
[\hat{\boldsymbol{L}}^2,\hat{z}] &= 2i\hbar(\hat{x}\hat{L}_y-\hat{y}\hat{L}_x-i\hbar\hat{z}) \\
[\hat{\boldsymbol{L}}^2,\hat{x}] &= 2i\hbar(\hat{y}\hat{L}_z-\hat{z}\hat{L}_y-i\hbar\hat{x}) \\
[\hat{\boldsymbol{L}}^2,\hat{y}] &= 2i\hbar(\hat{z}\hat{L}_x-\hat{x}\hat{L}_z-i\hbar\hat{y})
\end{aligned}
$$

1.4 Proof of the above commutation relation by using Mathematica

Using the Mathematica, we show that the above commutations are valid.

$$[\hat{L}_z, \hat{z}] = 0 .$$

$$[\hat{L}_z, \hat{x}] = i\hbar\hat{y} . \quad [\hat{L}_z, \hat{y}] = -i\hbar\hat{x} .$$

$$[\hat{\boldsymbol{L}}^2, [\hat{\boldsymbol{L}}^2, \hat{\boldsymbol{r}}]] = 2\hbar^2(\hat{\boldsymbol{L}}^2\hat{\boldsymbol{r}} + \hat{\boldsymbol{r}}\hat{\boldsymbol{L}}^2)$$

((**Mathematica**))

```
Clear["Global`"];

<< VectorAnalysis`;

SetCoordinates[Cartesian[x, y, z]];

ux = {1, 0, 0}; uy = { 0, 1, 0}; uz = {0, 0, 1}; r = {x, y, z};

Lx := (ux.(-ⅈ ℏ Cross[r, Grad[#]]) &) // Simplify;
Ly := (uy.(-ⅈ ℏ Cross[r, Grad[#]]) &) // Simplify;
Lz := (uz.(-ⅈ ℏ Cross[r, Grad[#]]) &) // Simplify;

Lsq := (Nest[Lx, #, 2] + Nest[Ly, #, 2] + Nest[Lz, #, 2]) &;

eq1 = (Lz[z χ[x, y, z]] - z Lz[χ[x, y, z]]) // FullSimplify
0

eq2 = Lz[x χ[x, y, z]] - x Lz[ χ[x, y, z]] - ⅈ ℏ y χ[x, y, z] // Simplify
0

eq3 = Lz[y χ[x, y, z]] - y Lz[ χ[x, y, z]] + ⅈ ℏ x χ[x, y, z] // Simplify
0

eq4 = 2 ℏ^2 (Lsq[x χ[x, y, z]] + x Lsq[χ[x, y, z]]) // Simplify;

eq5 = Lsq[Lsq[x χ[x, y, z]]] - Lsq[x Lsq[χ[x, y, z]]] - Lsq[x Lsq[χ[x, y, z]]] +
    x Lsq[ Lsq[χ[x, y, z]]] // Simplify;

eq4 - eq5
0
```

2. Eigenkets of angular momentum

$$\hat{\boldsymbol{L}}^2 |n,l,m\rangle = \hbar^2 l(l+1)|n,l,m\rangle$$

$$\hat{L}_z|n,l,m\rangle = \hbar m|n,l,m\rangle$$

$$\hat{L}_+|n,l,m\rangle = \hbar\sqrt{(l-m)(l+m+1)}|n,l,m+1\rangle$$

$$\hat{L}_-|n,l,m\rangle = \hbar\sqrt{(l+m)(l-m+1)}|n,l,m-1\rangle$$

where

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y, \qquad \hat{L}_- = \hat{L}_x - i\hat{L}_y$$

3. Selection rule-I

Using the relation

$$\hat{L}_z|n,l,m\rangle = \hbar m|n,l,m\rangle$$

we have

$$\langle n',l',m'|[\hat{L}_z,\hat{z}]|n,l,m\rangle = 0,$$

or

$$\langle n',l',m'|\hat{L}_z\hat{z} - \hat{z}\hat{L}_z|n,l,m\rangle = 0$$

or

$$(m'-m)\langle n',l',m'|\hat{z}|n,l,m\rangle = 0$$

Then we get the relation

$m' = m$, for the dipole ion the z direction.

4. Selection rule-II

Using the relation

$$\hat{L}_z|n,l,m\rangle = \hbar m|n,l,m\rangle$$

we have

$$\langle n,l',m'|[\hat{L}_z,\hat{x}+i\hat{y}]|n,l,m\rangle = \hbar\langle n,l',m'|\hat{x}+i\hat{y}|n,l,m\rangle,$$

or

$$\langle n',l',m'|\hat{L}_z(\hat{x}+i\hat{y})-(\hat{x}+i\hat{y})\hat{L}_z|n,l,m\rangle = \hbar\langle n',l',m'|\hat{x}+i\hat{y}|n,l,m\rangle$$

or

$$(m'-m-1)\langle n',l',m'|\hat{x}+i\hat{y}|n,l,m\rangle = 0$$

Then we get the relation

$m'=m+1$, for the dipole ion the x, y direction.

5. Selection rule-III

Using the relation

$$\hat{L}_z|n,l,m\rangle = \hbar m|n,l,m\rangle$$

we have

$$\langle n',l',m'|[\hat{L}_z,\hat{x}-i\hat{y}]|n,l,m\rangle = -\hbar\langle n',l',m'|\hat{x}-i\hat{y}|n,l,m\rangle,$$

or

$$\langle n',l',m'|\hat{L}_z(\hat{x}-i\hat{y})-(\hat{x}-i\hat{y})\hat{L}_z|n,l,m\rangle = -\hbar\langle n',l',m'|\hat{x}-i\hat{y}|n,l,m\rangle$$

or

$$(m'-m+1)\langle n,l',m'|\hat{x}-i\hat{y}|n,l,m\rangle = 0$$

Then we get the relation

$m'=m-1$, for the dipole ion the x, y direction.

6. Selection rule-IV

Using the commutation relation

$$[\hat{\boldsymbol{L}}^2,[\hat{\boldsymbol{L}}^2,\hat{x}]]=2\hbar^2\{\hat{x},\hat{\boldsymbol{L}}^2\}=2\hbar^2(\hat{x}\hat{\boldsymbol{L}}^2+\hat{\boldsymbol{L}}^2\hat{x})$$

we get the following equation,

$$\langle n',l',m'|[\hat{\boldsymbol{L}}^2,[\hat{\boldsymbol{L}}^2,\hat{x}]]|n,l,m\rangle=2\hbar^2\langle n',l',m'|\{\hat{x},\hat{\boldsymbol{L}}^2\}|n,l,m\rangle$$

or

$$\langle n',l',m'|\hat{\boldsymbol{L}}^2\hat{\boldsymbol{L}}^2\hat{x}-2\hat{\boldsymbol{L}}^2\hat{x}\hat{\boldsymbol{L}}^2+\hat{x}\hat{\boldsymbol{L}}^2\hat{\boldsymbol{L}}^2|n,l,m\rangle=2\hbar^2\langle n',l',m'|\hat{x}\hat{\boldsymbol{L}}^2+\hat{\boldsymbol{L}}^2\hat{x}|n,l,m\rangle$$

Here we use the relation

$$\hat{\boldsymbol{L}}^2|n,l,m\rangle=\hbar^2 l(l+1)|n,l,m\rangle, \qquad \text{and} \qquad \langle n',l',m'|\hat{\boldsymbol{L}}^2=\hbar^2 l'(l'+1)\langle n',l',m'|$$

Then we have

$$\hbar^4[l'^2(l'+1)^2-2l'(l'+1)l(l+1)+l^2(l+1)^2-2l'(l'+1)-2l(l+1)]\langle n',l',m'|\hat{x}|n,l,m\rangle=0$$

or

$$(l'-l-1)(l'-l+1)(l'+l)(l'+l+2)\langle n',l',m'|\hat{x}|n,l,m\rangle=0$$

The last factor yields the selection rule

$$l'=l\pm 1$$

Since l' and l are both non-negative, the $(l'+l+2)$ term cannot vanish, and the $(l'+l)$ term can only vanish for $l'=l=0$. However, this selection rule cannot be satisfied, since the states with $l'=l=0$ are independent of direction, and therefore these matrix elements of $\hat{x}$ vanish. Formally, one easily shows this

$$\langle n,0,0|\hat{x}|n,0,0\rangle = 0$$

using the parity operator.

((Proof))

$$\hat{\pi}\hat{x}\hat{\pi} = -\hat{x}$$

where the parity operator satisfies the relations,

$$\hat{\pi}^{+} = \hat{\pi}\ , \qquad \hat{\pi}^{2} = \hat{1}$$

$$\langle n,0,0|\hat{\pi}\hat{x}\hat{\pi}|n,0,0\rangle = -\langle n,0,0|\hat{x}|n,0,0\rangle$$

or

$$\langle n,0,0|\hat{x}|n,0,0\rangle = 0$$

where

$$\hat{\pi}|n,l,m\rangle = (-1)^{l}|n,l,m\rangle\ ,$$

and

$$\hat{\pi}|n,0,0\rangle = |n,0,0\rangle\ , \qquad \text{and} \qquad \langle n,0,0|\hat{\pi} = \langle n,0,0|$$

7. Wigner-Eckart theorem

We need to calculate the matrix element

$$I = |\langle n',l',m'|\hat{\boldsymbol{r}}|n,m,l\rangle|^{2}$$

where

$$\langle n'l'm'|\hat{\boldsymbol{r}}|n,l,m\rangle = \langle n'l'm'|\hat{x}|n,l,m\rangle\boldsymbol{e}_x + \langle n'l'm'|\hat{y}|n,l,m\rangle\boldsymbol{e}_y + \langle n'l'm'|\hat{z}|n,l,m\rangle\boldsymbol{e}_z$$

is a vector. Then we have

$$I = \left|\left\langle n',l',m'\middle|\hat{\boldsymbol{r}}\middle|n,l,m\right\rangle\right|^2 = \left|\left\langle n',l',m'\middle|\hat{x}\middle|n,l,m\right\rangle\right|^2 + \left|\left\langle n',l',m'\middle|\hat{y}\middle|n,l,m\right\rangle\right|^2 + \left|\left\langle n',l',m'\middle|\hat{z}\middle|n,l,m\right\rangle\right|^2$$

Here we note that

$$\begin{aligned}\left|\left\langle n',l',m'\middle|\hat{x}+i\hat{y}\middle|n,l,m\right\rangle\right|^2 &= \left\langle n',l',m'\middle|\hat{x}+i\hat{y}\middle|n,l,m\right\rangle^* \left\langle n',l',m'\middle|\hat{x}+i\hat{y}\middle|n,l,m\right\rangle \\ &= \left\langle n,l,m\middle|\hat{x}-i\hat{y}\middle|n',l',m'\right\rangle \left\langle \varphi_f\middle|\hat{x}+i\hat{y}\middle|n,l,m\right\rangle\end{aligned}$$

or

$$\left|\left\langle n',l',m'\middle|\hat{x}+i\hat{y}\middle|n,l,m\right\rangle\right|^2 = \left|\left\langle n',l',m'\middle|\hat{x}\middle|n,l,m\right\rangle\right|^2 + \left|\left\langle n',l',m'\middle|\hat{y}\middle|n,l,m\right\rangle\right|^2$$

Similarly we have

$$\left|\left\langle n',l',m'\middle|\hat{x}-i\hat{y}\middle|n,l,m\right\rangle\right|^2 = \left|\left\langle n',l',m\middle|\hat{x}\middle|n,l,m\right\rangle\right|^2 + \left|\left\langle n',l',m\middle|\hat{y}\middle|n,l,m\right\rangle\right|^2$$

Then we have

$$\begin{aligned}I &= \left|\left\langle n',l',m'\middle|\hat{\boldsymbol{r}}\middle|n,l,m\right\rangle\right|^2 \\ &= \frac{1}{2}\left|\left\langle n',l',m'\middle|\hat{x}+i\hat{y}\middle|n,l,m\right\rangle\right|^2 + \frac{1}{2}\left|\left\langle n',l',m'\middle|\hat{x}-i\hat{y}\middle|n,l,m\right\rangle\right|^2 + \left|\left\langle n',l',m'\middle|\hat{z}\middle|n,l,m\right\rangle\right|^2\end{aligned}$$

Spherical tensor of rank 1

$$T_1^{(1)} = -\left(\frac{\hat{x}+i\hat{y}}{\sqrt{2}}\right) = \hat{r}_+$$

$$T_0^{(1)} = \hat{z}$$

$$T_{-1}^{(1)} = \left(\frac{\hat{x}-i\hat{y}}{\sqrt{2}}\right) = \hat{r}_-$$

From the Wigner-Eckart theorem,

$\left\langle n',l',m'\middle|\hat{T}_q^{(1)}\middle|n,l,m\right\rangle \neq 0$ for $m' = m+q$ and for $l' = l+1, l, l-1$

$\hat{T}_q^{(1)}$ is the odd parity operator,

$$\hat{\pi}\hat{T}_q^{(1)}\hat{\pi} = -\hat{T}_q^{(1)}$$

and

$$\hat{\pi}|n,l,m\rangle = (-1)^l |n,l,m\rangle$$

Then the matrix element $\langle n',l',m'|\hat{T}_q^{(1)}|n,l,m\rangle$ is equal to zero for $l'=l$.

Then we have

(i)

$$\begin{aligned}\langle n',l',m'|\hat{T}_1^{(1)}|n,l,m\rangle &= -\frac{1}{\sqrt{2}}\langle n',l',m'|\hat{x}+i\hat{y}|n,l,m\rangle \\ &= \langle n',l',m'|\hat{r}_+|n,l,m\rangle \\ &\neq 0\end{aligned}$$

for $m'=m+1$ and for $l'=l\pm 1$

(ii)

$$\begin{aligned}\langle n',l',m'|\hat{T}_{-1}^{(1)}|n,l,m\rangle &= \frac{1}{\sqrt{2}}\langle n',l',m'|\hat{x}-i\hat{y}|n,l,m\rangle \\ &= \langle n',l',m'|\hat{r}_-|n,l,m\rangle \\ &\neq 0\end{aligned}$$

for $m'=m-1$ and for $l'=l\pm 1$.

(iii)

$$\langle n',l',m'|\hat{T}_0^{(1)}|n,l,m\rangle = \langle n',l',m'|\hat{z}|n,l,m\rangle =\neq 0$$

for $m'=m$ and for $l'=l\pm 1$.

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8. Dipole selection rule

The dipole radiation is emitted if

$$M = \langle n',l',m'|\boldsymbol{\varepsilon}\cdot\hat{\boldsymbol{r}}|n,l,m\rangle = \boldsymbol{\varepsilon}\cdot\langle n',l',m'|\hat{\boldsymbol{r}}|n,l,m\rangle = \boldsymbol{\varepsilon}\cdot\boldsymbol{D}_{fi}$$

does not vanish, where $\boldsymbol{\varepsilon}$ is the polarization vector of photon, and

$$\boldsymbol{D}_{fi} = \langle n',l',m'|\hat{\boldsymbol{r}}|n,l,m\rangle$$

Then we have

$$\boldsymbol{D}_{fi} = \langle n',l',m'|\hat{x}|n,l,m\rangle\boldsymbol{e}_x + \langle n',l',m'|\hat{y}|n,l,m\rangle\boldsymbol{e}_y + \langle n',l',m'|\hat{z}|n,l,m\rangle\boldsymbol{e}_z,$$

(i) For $m' = m$

$$\langle n',l',m'|\hat{z}|n,l,m\rangle \neq 0, \qquad \langle n',l',m'|\hat{x}|n,l,m\rangle = 0, \qquad \langle n',l',m'|\hat{y}|n,l,m\rangle = 0$$

$$\begin{aligned}\boldsymbol{D}_{fi} &= \langle n',l',m'|\hat{x}|n,l,m\rangle\boldsymbol{e}_x + \langle n',l',m'|\hat{y}|n,l,m\rangle\boldsymbol{e}_y + \langle n',l',m'|\hat{z}|n,l,m\rangle\boldsymbol{e}_z \\ &= \langle n',l',m'|\hat{z}|n,l,m\rangle\boldsymbol{e}_z\end{aligned}$$

$\boldsymbol{D}_{fi}$ is directed along the z axis.

(a) Suppose that the wavevector $\boldsymbol{k}$ of the emitted photon is along the z axis. There is no radiation in the z-direction since the polarization vector $\boldsymbol{\varepsilon}$ is perpendicular to $\boldsymbol{D}_{fi}$ (the z axis).

(b) For example, we consider light going in the x direction. It can have two directions of polarization, either in the z or in the y direction. A transition in which $\Delta m = 0$, can produce only light which is polarized in the z direction.

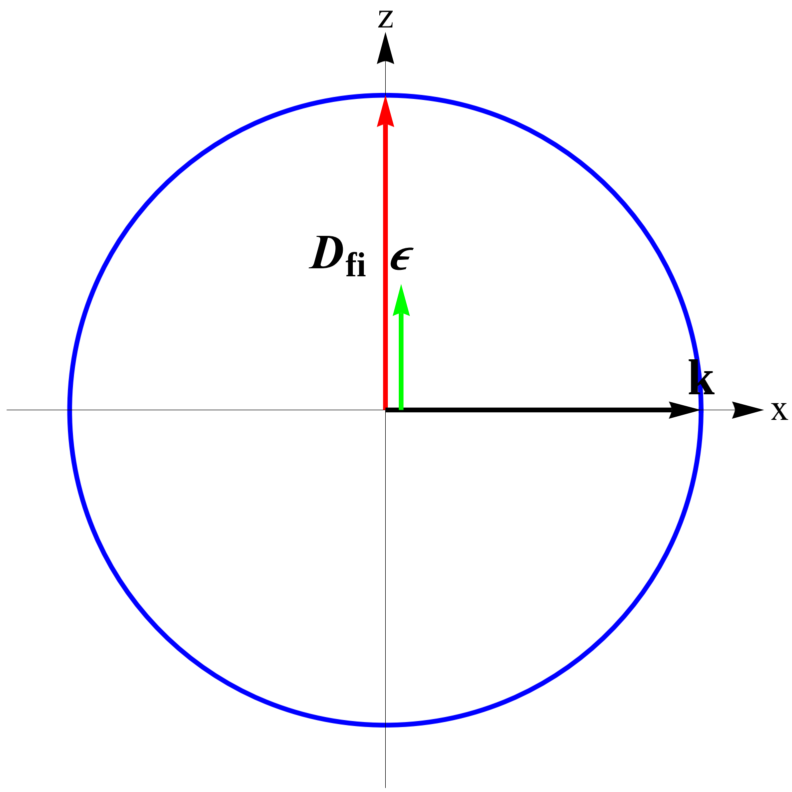

Fig. $m' = m$. $\boldsymbol{D}_{fi} // z$. The light propagating along the x direction. It is a linearly polarized wave (along the z axis).

We assume that

$$\hat{r}_+ = -\frac{\hat{x} + i\hat{y}}{\sqrt{2}}, \qquad \hat{r}_- = \frac{\hat{x} - i\hat{y}}{\sqrt{2}}$$

or

$$\hat{x} = -\frac{1}{\sqrt{2}}(\hat{r}_+ - \hat{r}_-), \qquad \hat{y} = \frac{i}{\sqrt{2}}(\hat{r}_+ + \hat{r}_-)$$

(ii) For $m' = m + 1$

$$\langle l', m' | \hat{r}_- | l, m \rangle = 0, \qquad \langle l', m' | \hat{z} | l, m \rangle = 0.$$

(iii) For $m' = m - 1$

$$\langle l',m'|\hat{r}_+|l,m\rangle = 0, \qquad \langle l',m'|\hat{z}|l,m\rangle = 0.$$

We now consider the matrix element with $m' = m \pm 1$.

$$\begin{aligned}
\boldsymbol{D}_{fi} &= \langle l',m'|\hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y + \hat{z}\boldsymbol{e}_z|l,m\rangle \\
&= \langle l',m'|\hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y|l,m\rangle \\
&= -\langle l',m'|\hat{r}_+\boldsymbol{e}_- + \hat{r}_-\boldsymbol{e}_+|l,m\rangle \\
&= -\boldsymbol{e}_-\langle l',m'|\hat{r}_+|l,m\rangle - \boldsymbol{e}_+\langle l',m'|\hat{r}_-|l,m\rangle
\end{aligned}$$

where the spherical basis vectors are defined by

$$\boldsymbol{e}_+ = -\left(\frac{\boldsymbol{e}_x + i\boldsymbol{e}_y}{\sqrt{2}}\right), \qquad \boldsymbol{e}_- = \frac{\boldsymbol{e}_x - i\boldsymbol{e}_y}{\sqrt{2}}$$

or

$$\boldsymbol{e}_x = -\frac{1}{\sqrt{2}}(\boldsymbol{e}_+ - \boldsymbol{e}_-), \quad \boldsymbol{e}_y = \frac{i}{\sqrt{2}}(\boldsymbol{e}_+ + \boldsymbol{e}_-)$$

and

$$\hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y = -(\hat{r}_+\boldsymbol{e}_- + \hat{r}_-\boldsymbol{e}_+)$$

Note that

$$\boldsymbol{e}_+ \cdot \boldsymbol{e}_+ = 0. \qquad \boldsymbol{e}_- \cdot \boldsymbol{e}_- = 0$$

$$\boldsymbol{e}_+ \cdot \boldsymbol{e}_- = -1. \qquad \boldsymbol{e}_- \cdot \boldsymbol{e}_+ = -1$$

(a) When $m' = m + 1$ (σ^+ circularly polarized photon)

$$\begin{aligned}
\boldsymbol{D}_{fi} &= \langle l',m'|\hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y|l,m\rangle \\
&= -\langle l',m'|(\hat{r}_+\boldsymbol{e}_- + \hat{r}_-\boldsymbol{e}_+)|l,m\rangle \\
&= -\boldsymbol{e}_-\langle l',m'|\hat{r}_+|l,m\rangle
\end{aligned}$$

has the same direction of the left circularly polarization vector ($\boldsymbol{e}_-$). Then the emitted photon which is right circularly polarized ($\boldsymbol{e}_+$), can propagate along the z axis. A photon with right-hand circular polarization carries a spin $+\hbar$ in the z direction (the propagation direction).

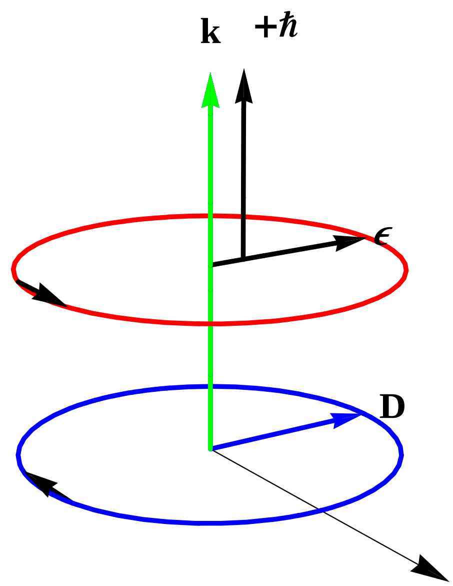

Fig. The case of $m' = m+1$ (right circularly polarization). A right circularly polarized photon ($\boldsymbol{e}_+$) propagates with a wavevector $\boldsymbol{k}$ in the z direction. Note that the electric field is denoted by $\cos(kz-\omega t)\boldsymbol{e}_x + \sin(kz-\omega t)\boldsymbol{e}_y$. This electric field rotates in clock-wise sense with time t, and rotates in counter clock-wise sense with z (as the wave propagates forward). The corresponding spin of the photon is directed in the positive z direction ($\hbar$). $\boldsymbol{D}_{fi}(\approx -\boldsymbol{e}_-)$. $\boldsymbol{E}(\approx \boldsymbol{e}_+)$. ($\boldsymbol{e}_+ \cdot \boldsymbol{e}_- = -1$, $\boldsymbol{e}_- \cdot \boldsymbol{e}_- = 0$).

(b) When $m' = m-1$ (σ^- circularly polarized photon)

$$
\begin{aligned}
\boldsymbol{D}_{fi} &= \langle l', m' | \hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y | l, m \rangle \\
&= -\langle l', m' | (\hat{r}_+\boldsymbol{e}_- + \hat{r}_-\boldsymbol{e}_+) | l, m \rangle \\
&= -\boldsymbol{e}_+ \langle l', m' | \hat{r}_- | l, m \rangle]
\end{aligned}
$$

is parallel to the right circularly polarization vector (-$\boldsymbol{e}_+$). The emitted photon with left circularly polarization ($\boldsymbol{e}_-$) can propagate along the z axis, since $(-\boldsymbol{e}_+)\cdot\boldsymbol{e}_- = 1$. A photon with the left-hand polarization carries a spin (-$\hbar$), that is, a spin direction opposite to the z direction.

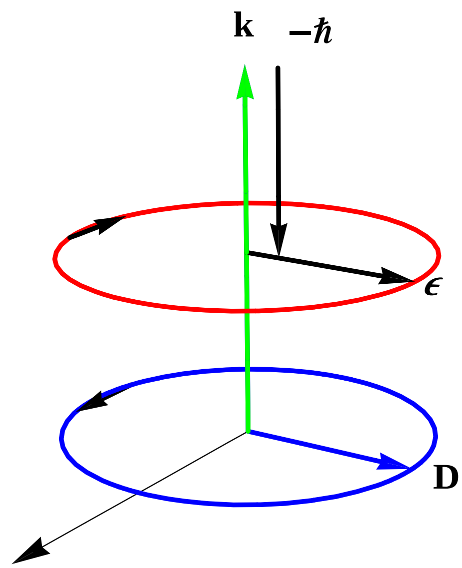

Fig. The case of $m' = m-1$ (left circularly polarization). A left circularly polarized photon ($\boldsymbol{e}_-$) propagates with a wavevector $\boldsymbol{k}$ in the z direction. Note that the electric field is given by $\cos(kz-\omega t)\boldsymbol{e}_x - \sin(kz-\omega t)\boldsymbol{e}_y$. This electric field rotates in counter clock-wise sense with time t, and rotates in clock-wise sense with z (as the wave propagates forward). The corresponding spin of the photon is directed in the negative z direction, as -$\hbar$. $\boldsymbol{D}_{fi}(\approx -\boldsymbol{e}_+)$. $\boldsymbol{E}(\approx \boldsymbol{e}_-)$. ($\boldsymbol{e}_+\cdot\boldsymbol{e}_- = -1$, $\boldsymbol{e}_+\cdot\boldsymbol{e}_+ = 0$).

((Note))

The rules on Δm can be understood by realizing that σ^+ and σ^- circularly polarized photons carry angular momenta of $+\hbar$ and -$\hbar$, respectively, along the z axis, and hence m must change by one unit to conserve angular momentum. For linearly polarized light along the z axis, the photons carry no z-component of momentum, implying $\Delta m = 0$, while x or y-polarized light can be considered as a equal combination of σ^+ and σ^- photons, giving $\Delta m = \pm 1$.

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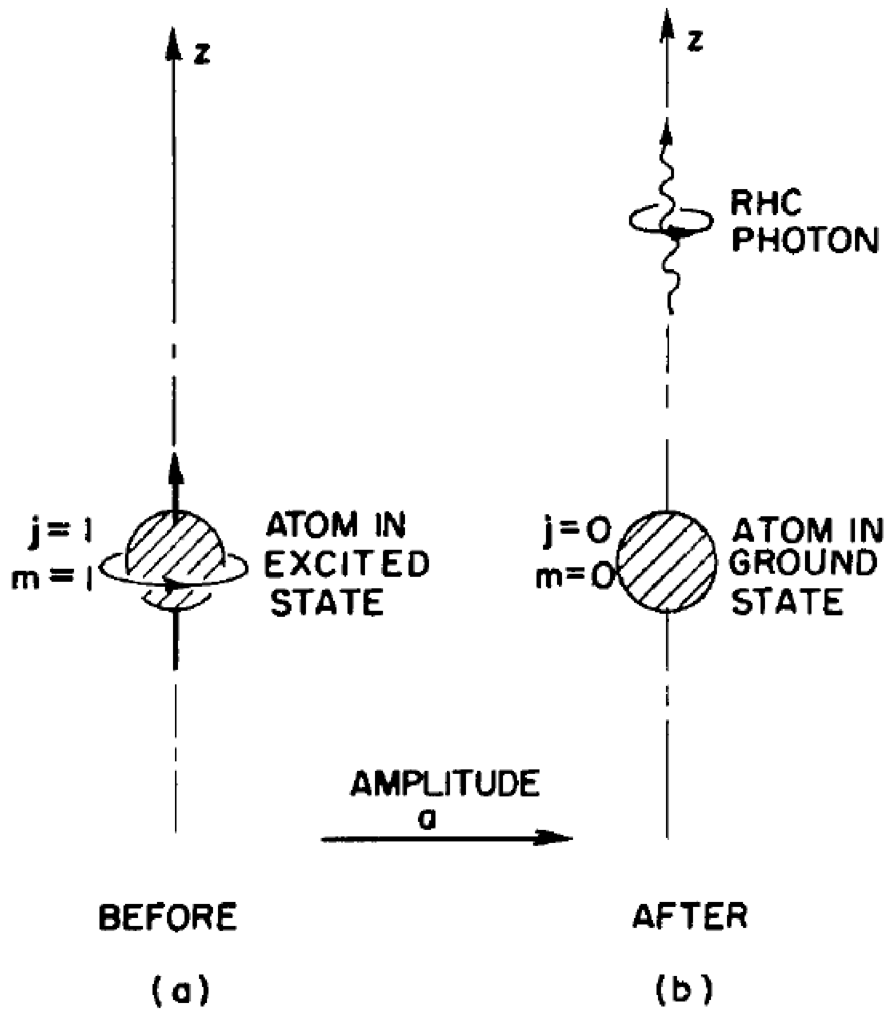
APPENDIX-I
from Feynman book (



Emission of right-hand circularly photon (Feynman et al.)

APPENDIX-II
The dipole selection rule for the Jones vector

We assume that

$$\hat{r}_+ = \frac{\hat{x} + i\hat{y}}{\sqrt{2}}, \qquad \hat{r}_- = \frac{\hat{x} - i\hat{y}}{\sqrt{2}}$$

$$\boldsymbol{e}_+ = \frac{1}{\sqrt{2}}(\boldsymbol{e}_x + i\boldsymbol{e}_y), \qquad \boldsymbol{e}_- = \frac{1}{\sqrt{2}}(\boldsymbol{e}_x - i\boldsymbol{e}_y)$$

or

$$\hat{x} = \frac{1}{\sqrt{2}}(\hat{r}_+ + \hat{r}_-), \qquad \hat{y} = \frac{1}{\sqrt{2}i}(\hat{r}_+ - \hat{r}_-)$$

$$\boldsymbol{e}_x = \frac{1}{\sqrt{2}}(\boldsymbol{e}_+ + \boldsymbol{e}_-), \qquad \boldsymbol{e}_y = \frac{1}{\sqrt{2}i}(\boldsymbol{e}_+ - \boldsymbol{e}_-)$$

$$\boldsymbol{e}_+ \cdot \boldsymbol{e}_- = 1, \qquad \boldsymbol{e}_+ \cdot \boldsymbol{e}_+ = 0, \qquad \boldsymbol{e}_- \cdot \boldsymbol{e}_- = 0$$

(ii) For $m' = m + 1$

$$\langle l', m' | \hat{r}_- | l, m \rangle = 0, \qquad \langle l', m' | \hat{z} | l, m \rangle = 0.$$

(iii) For $m' = m - 1$

$$\langle l', m' | \hat{r}_+ | l, m \rangle = 0, \qquad \langle l', m' | \hat{z} | l, m \rangle = 0.$$

We now consider the matrix element with $m' = m \pm 1$.

$$\begin{aligned}
\boldsymbol{D}_{fi} &= \langle l', m' | \hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y + \hat{z}\boldsymbol{e}_z | l, m \rangle \\
&= \langle l', m' | \hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y | l, m \rangle \\
&= \langle l', m' | \hat{r}_+\boldsymbol{e}_- + \hat{r}_-\boldsymbol{e}_+ | l, m \rangle \\
&= \boldsymbol{e}_- \langle l', m' | \hat{r}_+ | l, m \rangle + \boldsymbol{e}_+ \langle l', m' | \hat{r}_- | l, m \rangle
\end{aligned}$$

(a) When $m' = m + 1$ (σ^+ circularly polarized photon)

$$\begin{aligned}
\boldsymbol{D}_{fi} &= \langle l', m' | \hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y | l, m \rangle \\
&= \langle l', m' | (\hat{r}_+\boldsymbol{e}_- + \hat{r}_-\boldsymbol{e}_+) | l, m \rangle \\
&= \boldsymbol{e}_- \langle l', m' | \hat{r}_+ | l, m \rangle
\end{aligned}$$

has the same direction of the left circularly polarization vector ($\boldsymbol{e}_-$). Then the emitted photon which is right circularly polarized ($\boldsymbol{e}_+$), can propagate along the *z* axis. A photon with right-hand circular polarization carries a spin $+\hbar$ in the *z* direction (the propagation direction).

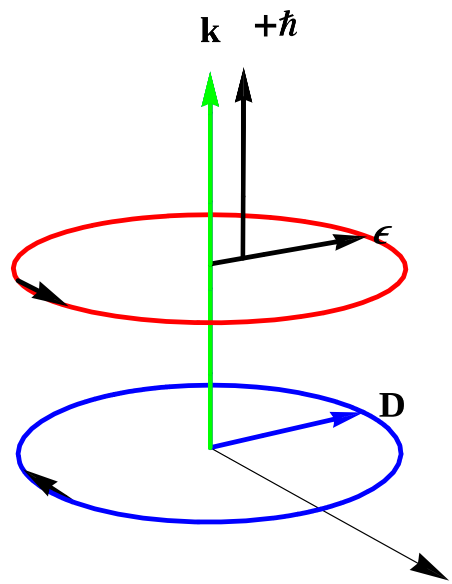


Fig. The case of $m' = m + 1$ (right circularly polarization). A right circularly polarized photon ($\boldsymbol{e}_+$) propagates with a wavevector $\boldsymbol{k}$ in the z direction. Note that the electric field is denoted by $\cos(kz - \omega t)\boldsymbol{e}_x + \sin(kz - \omega t)\boldsymbol{e}_y$. This electric field rotates in clock-wise sense with time t, and rotates in counter clock-wise sense with z (as the wave propagates forward). The corresponding spin of the photon is directed in the positive z direction ($\hbar$). $\boldsymbol{D}_{f_i}(\approx \boldsymbol{e}_-)$. $\boldsymbol{E}(\approx \boldsymbol{e}_+)$. ($\boldsymbol{e}_+ \cdot \boldsymbol{e}_- = 1$, $\boldsymbol{e}_- \cdot \boldsymbol{e}_- = 0$).

(b) When $m' = m - 1$ (σ^- circularly polarized photon)

$$\begin{aligned}
\boldsymbol{D}_{fi} &= \langle l', m' | \hat{x}\boldsymbol{e}_x + \hat{y}\boldsymbol{e}_y | l, m \rangle \\
&= \langle l', m' | (\hat{r}_+\boldsymbol{e}_- + \hat{r}_-\boldsymbol{e}_+) | l, m \rangle \\
&= \boldsymbol{e}_+ \langle l', m' | \hat{r}_- | l, m \rangle]
\end{aligned}$$

is parallel to the right circularly polarization vector ($\boldsymbol{e}_+$). The emitted photon with left circularly polarization ($\boldsymbol{e}_-$) can propagate along the z axis, since $\boldsymbol{e}_+ \cdot \boldsymbol{e}_- = 1$. A photon with the left-hand polarization carries a spin (-$\hbar$), that is, a spin direction opposite to the z direction.

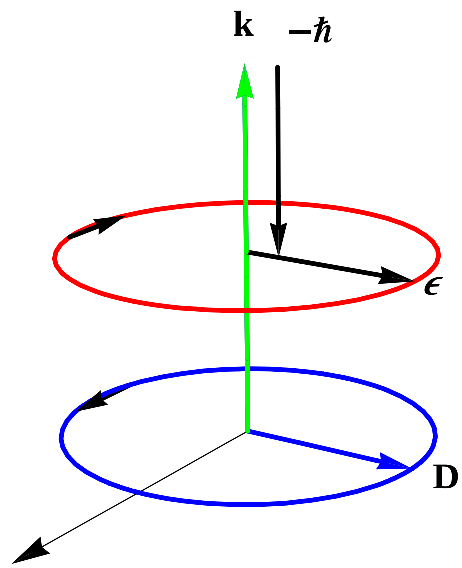
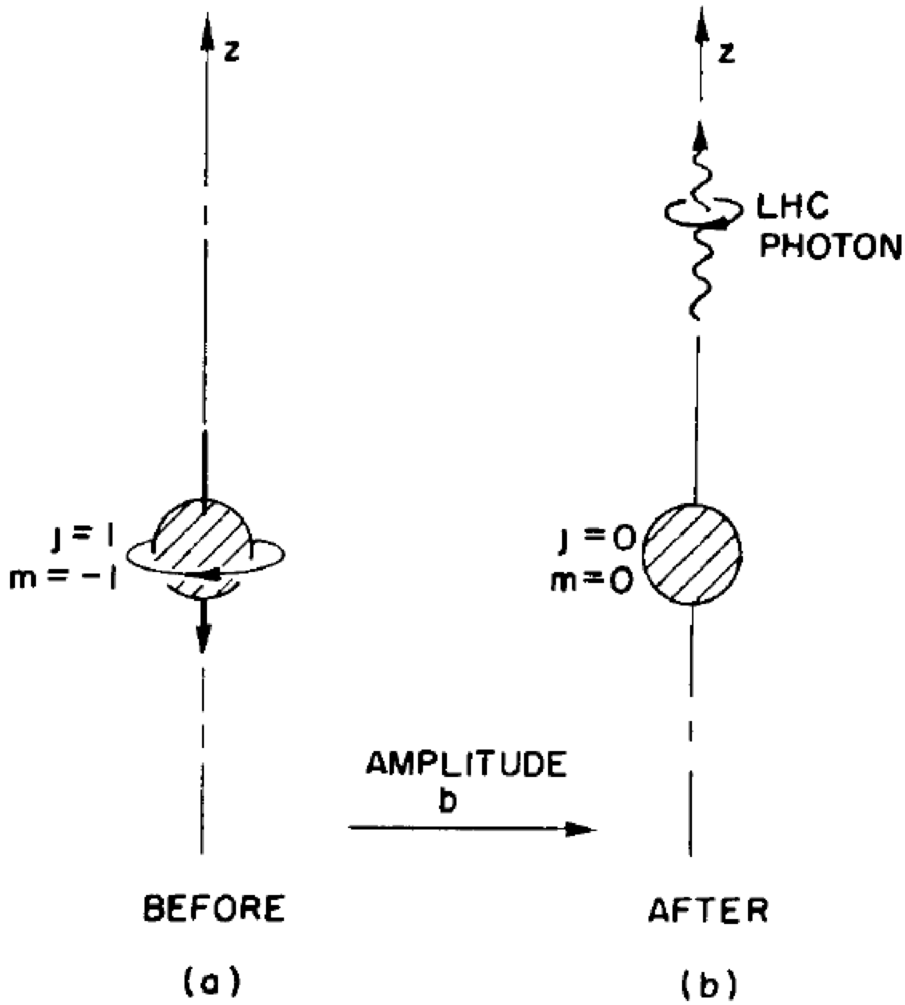


Fig. The case of $m' = m - 1$ (left circularly polarization). A left circularly polarized photon ($\boldsymbol{e}_-$) propagates with a wavevector $\boldsymbol{k}$ in the z direction. Note that the electric field is given by $\cos(kz - \omega t)\boldsymbol{e}_x - \sin(kz - \omega t)\boldsymbol{e}_y$. This electric field rotates in counter clock-wise sense with time t, and rotates in clock-wise sense with z (as the wave propagates forward). The corresponding spin of the photon is directed in the negative z direction, as $-\hbar$. $\boldsymbol{D}_{fi}(\approx \boldsymbol{e}_+)$. $\boldsymbol{E}(\approx \boldsymbol{e}_-)$. ($\boldsymbol{e}_+ \cdot \boldsymbol{e}_- = 1, \boldsymbol{e}_+ \cdot \boldsymbol{e}_+ = 0$).



Emission of left-hand circularly photon