Mössbauer effect

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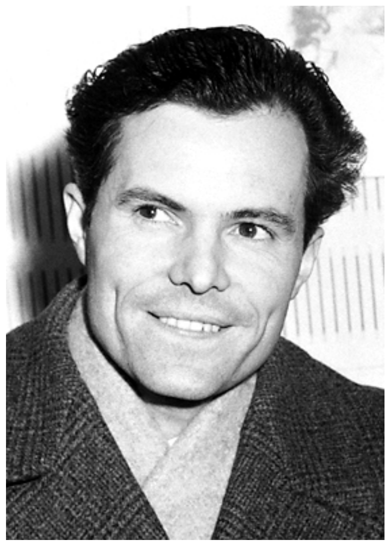
Rudolf Ludwig Mössbauer (German spelling: **Mößbauer**; January 31, 1929 – September 14, 2011) was a German physicist best known for his 1957 discovery of *recoilless nuclear resonance fluorescence* for which he was awarded the 1961 Nobel Prize in Physics. This effect, called the Mössbauer effect, is the basis for Mössbauer spectroscopy.

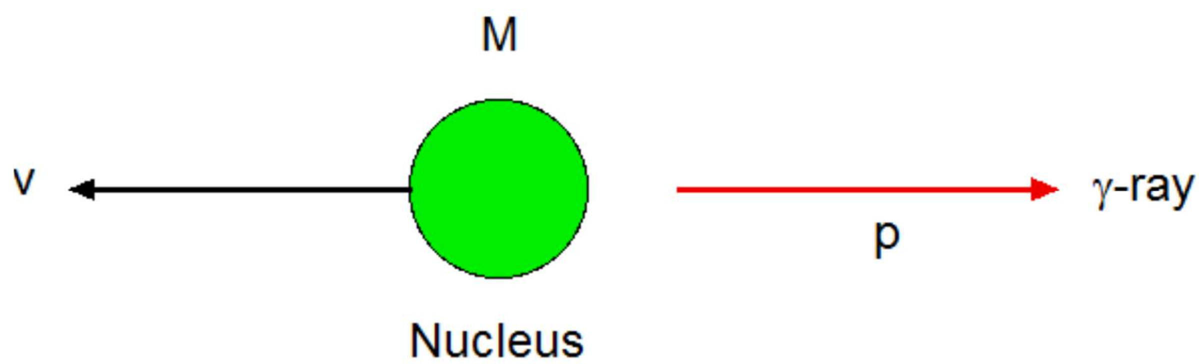


http://en.wikipedia.org/wiki/Rudolf_M%C3%B6ssbauer

1. Recoil

We consider a phenomenon in which the nucleus makes a transition from an excited state to the ground state via γ-ray, and the emitted γ-ray is then absorbed by another nucleus of the same kind to make a resonant transition from the ground state to the excited state. Let the energy difference between the ground state and the excited state be E_γ and the energy of the emitted g-ray be E_γ. The momentum p of the γ-ray is given by E_γ /c. Because of momentum conservation, the isolated nuclear recoils with momentum -p.

Momentum conservation



$$p = \frac{\hbar\omega}{c} = Mv$$

or

$$v = \frac{\hbar\omega}{Mc}$$

The kinetic energy of nucleus, *R*, is

$$R = \frac{1}{2}Mv^2 = \frac{\hbar^2\omega^2}{2Mc^2}$$

where *M* is the mass of nucleus.

The value of R can be evaluated numerically as follows.

M = mass of ^{57}Fe = 56.935396 g/mol
$\hbar\omega = 14.4$ keV
R = 1.95494 meV.
$v = 8.13994 \times 10^3$ m/s

((**Mathematica**))

```
Clear["Global`*"];
rule1 = {NA → 6.02214179 × 10^23, c → 2.99792 × 10^10,
   ℏ → 1.054571628 10^-27, keV → 1.602176487 × 10^-9,
   meV → 1.602176487 × 10^-15, M → 56.935396, E1 → 14.4 keV};
```

$$R = \frac{E1^2}{2 \frac{M}{NA} c^2 \, meV} \text{ //. rule1}$$

1.95494

$$v = \frac{E1}{\frac{M}{NA} c} \text{ //. rule1}$$

8139.94

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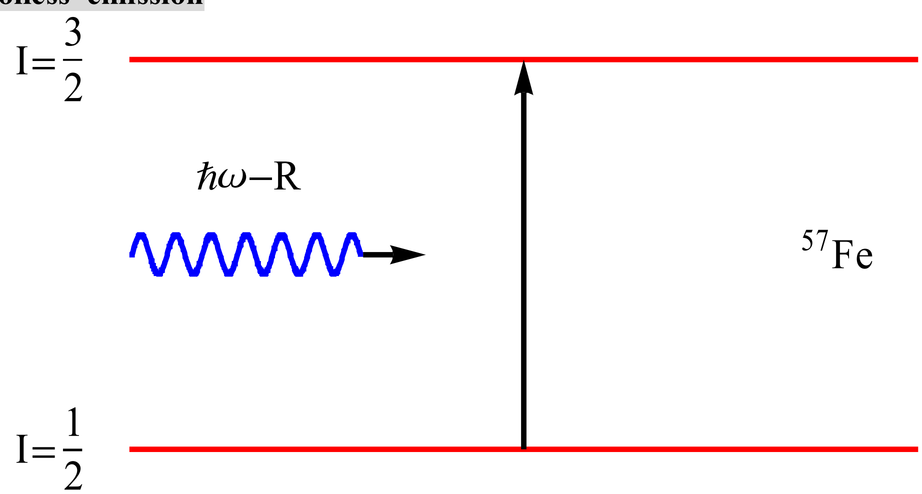
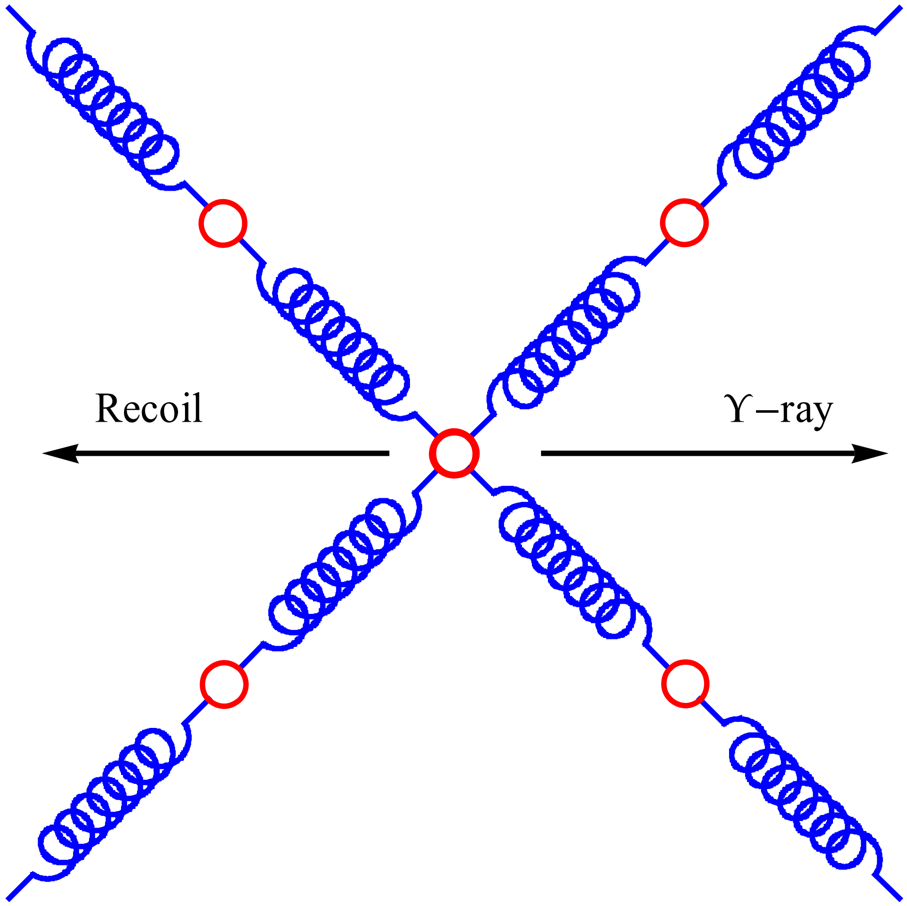
2. Recoiless emission



$\hbar\omega$ - R is a little lower to raise the energy level of nucleus from the ground state to the excited state.

Recoilless emission



In crystals the nucleus interacts with the surrounding nucleus. Since $M \to \infty$, we have R = 0. The probability of the occurrence of recoilless γ-ray with R = 0 is

$$P = \exp(-\frac{3R}{2k_B\Theta})$$

with

$$R = \frac{1}{2}Mv^2 = \frac{\hbar^2\omega^2}{2Mc^2}$$

The value of P can be evaluated numerically as follows.

M = mass of ^{57}Fe = 56.935396 g/mol
$\hbar\omega = 14.4$ keV
R = 1.95494 meV = 22.6861 K
P = 0.922173

((**Mathematica**))

```
Clear["Global`*"];
rule1 = {NA → 6.02214179 × 10^23, c → 2.99792 × 10^10,
  ℏ → 1.054571628 10^-27, keV → 1.602176487 × 10^-9,
  meV → 1.602176487 × 10^-15, M → 56.935396, E1 → 14.4 keV,
  kB → 1.3806504 × 10^-16, Θ → 420};
```

$$R = \frac{E1^2}{2 \frac{M}{NA} c^2} \text{ //. rule1; } R1 = \frac{E1^2}{2 \frac{M}{NA} c^2 kB} \text{ //. rule1}$$

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22.6861
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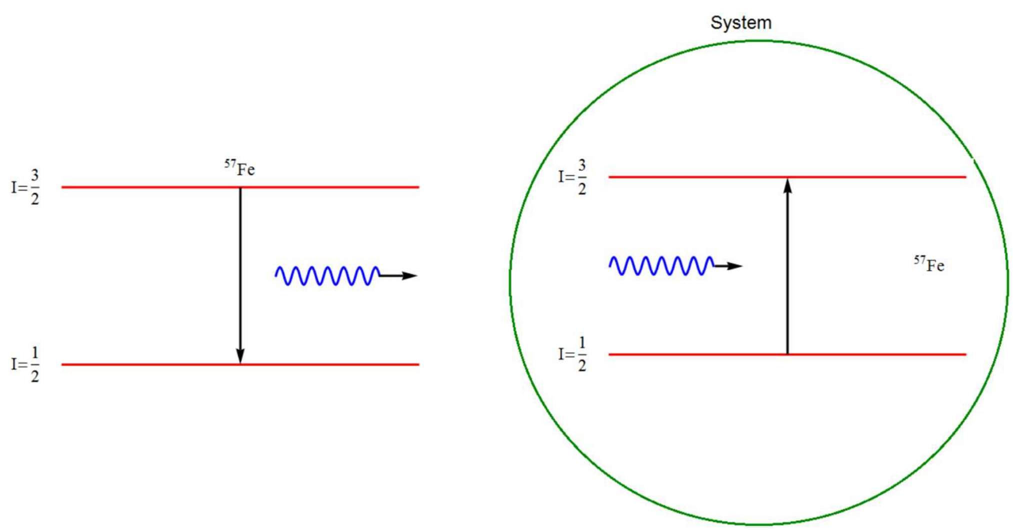
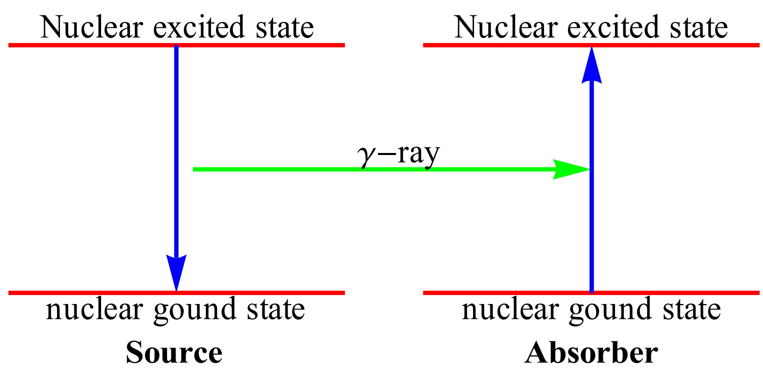
$$P = \mathrm{Exp}\left[-\frac{3 R}{2 kB \Theta}\right] \text{ //. rule1}$$

```
0.922173
```

3. Experiment of Mossbauer effect

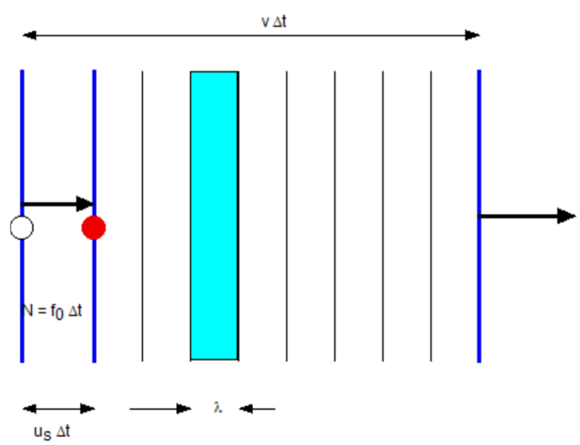




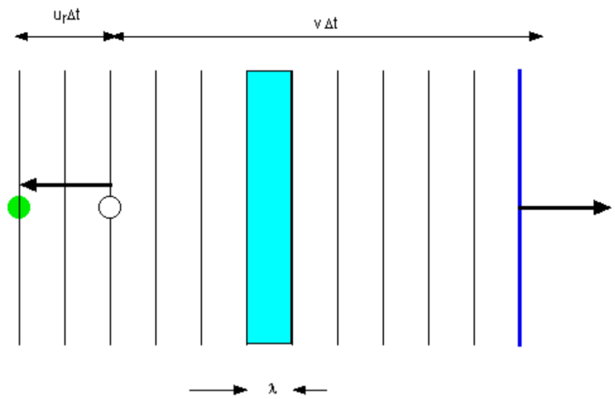
The energy difference between the ground state and the first excited state is different depending on the surrounding interaction of ^{57}Fe. In this case no absorption occurs.

4. Doppler effect

The Doppler effect is the apparent change in frequency (or wavelength) that occurs because of motion of the source or observer of a wave. When the motion of the source or the observer is toward the other, the frequency appears to increase. When the motion of the source or observer is away from the other, the frequency appears to decrease



$$\lambda = \frac{(v-u_s)\Delta t}{N} = \frac{(v-u_s)\Delta t}{f_0 \Delta t} = \frac{v-u_s}{f_0}$$



$$f\Delta t = \frac{(u_r + v)\Delta t}{\lambda}$$

$$f = \frac{(u_r + v)}{\lambda} = \left(\frac{v + u_r}{v - u_s}\right) f_0$$

u_s (>0) is the velocity of sender approaching the receiver.
u_r (>0) is the velocity of the receiver approaching the sender.
f_0 is the frequency of the sender and f is the frequency of the receiver.

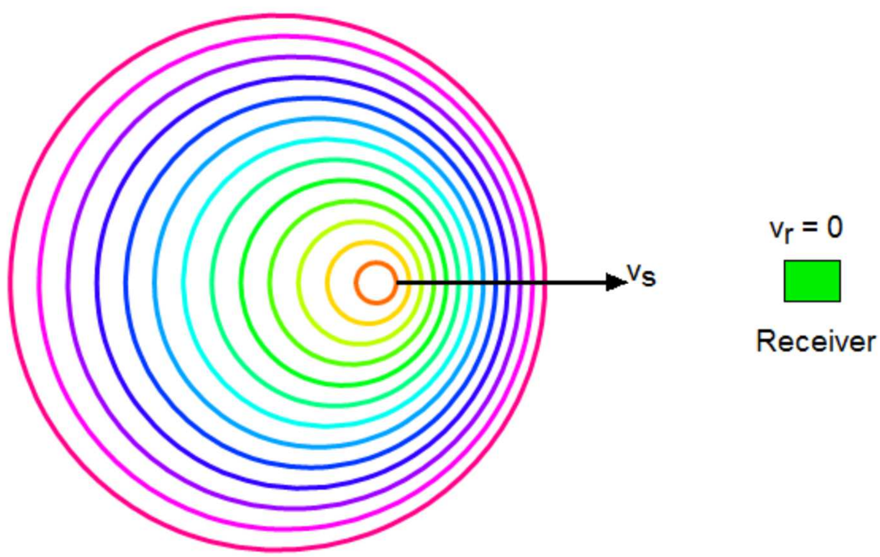


Fig. A receiver is stationary and a source is moving toward the receiver at the velocity v_s. v is the velocity of sound. $v_s < v$.

We consider the Doppler effect

Suppose that the source (emitting γ-ray with the angular frequency w) moves toward the nucleus (receiver) in the system (stationary, $v_r = 0$) at the velocity v. Using the formula of the Doppler effect, we get

$$f_r = \sqrt{\frac{c+v}{c-v}} f_s = \sqrt{\frac{1+\frac{v}{c}}{1-\frac{v}{c}}} f_s \approx (1+\frac{v}{c}) f_s$$

or

$$\hbar\omega_r = \hbar\omega(1+\frac{v}{c}) = \hbar\omega + \delta$$

where

$$\delta = \frac{\hbar\omega v}{c}$$

The value of v can be estimated as follows.

$\hbar\omega = 14.4$ keV

$\delta = 1$ μV.

v = 2.08189 cm/s

6. Isomar shift

The energy of interaction can be computed classically by considering an unifoprmly charged spherical nucleus imbeded in its s-electron charge cloud.

((**Model**))

Electrostatic shift of a nuclear level

The electronic charge density ρ is assumed to be uniform over nuclear dimensions

For the point nucleus the electrostatic potential Vpt is

$$V_{pt} = \frac{Ze}{r}$$

For the finite one,

$$V = \frac{Ze}{R}\left(\frac{3}{2} - \frac{r^2}{2R^2}\right) \qquad \text{for } r<R,$$

$$V = \frac{Ze}{r} \qquad \text{for } r>R,$$

((**Note**)) Using the Gauss's law ($\int \boldsymbol{E}\cdot d\boldsymbol{a} = 4\pi Q_{tot}$, with the total charge Q_{tot})

For $r<R$,

$$E(4\pi r^2) = 4\pi(Ze)\frac{\frac{4\pi}{3}r^3}{\frac{4\pi}{3}R^3} = 4\pi(Ze)\frac{r^3}{R^3} \qquad \text{for } r<R,$$

or

$$E = \frac{Zer}{R^3}$$

For $r>R$,

$$E = \frac{Ze}{r^2}$$

Then the electric potential is obtained as follows.

(i) For $r>R$,

$$V = -\int_{\infty}^{r} Edr = -\int_{\infty}^{r} \frac{Ze}{r^2}dr = \frac{Ze}{r}$$

(ii) For $r<R$,

$$V = -\int^{r} E dr = -\int^{r} \frac{Zer}{R^3} dr = -\frac{Zer^2}{2R^3} + C = \frac{3Ze}{2R} - \frac{Zer^2}{2R^3}$$

where the constant C is obtained from the continuity of V at $r = R$,

$$C = \frac{3Ze}{2R}$$

Then the energy difference is

$$\begin{aligned}
\delta E &= \int_0^R \rho (V - V_{pt}) d\mathbf{r} \\
&= \int_0^R \rho (V - V_{pt}) 4\pi r^2 dr \\
&= \frac{4\pi\rho}{R} Ze \int_0^R \left(\frac{3}{2} - \frac{r^2}{2R^2} - \frac{R}{r}\right) dr \\
&= -\frac{2\pi}{5} Ze\rho R^2 = \frac{2\pi}{5} Ze^2 |\psi(0)|^2 R^2
\end{aligned}$$

where

$$\rho = -e|\psi(0)|^2$$

6. Quadrupole interaction

Isomar shift: nucleus is spherical. The charge density is uniform.

If these conditions are relaed, other effects appear which are in fact higher order term in the multipole expansiuon of the electrostatic interaction. These terms do not shift the nuclear levels ; they split them, i.e., they lift all or partr of their (2I+1)-fold degeneracy (I: nuclear spin quantum number).

Quadrupole coupling⇒ Second nonvanishing term of the electrostatic interaction of a nucleus with its surrounding electronic charge.

The interaction of the nuclear quadrupole moment Q with the gradient of the electric field due to other charges in the crystal.

The nuclear quadrupole moment reflects the deviation of the nucleus from spherical symmetry. An oblate (flattened) nucleus has a negative Q, while a prolate (elengated) one has a positive Q. Nuclear whose spin is 0 or 1/2 are spherically symmetric and have a $Q = 0$. Thus the ground state of ^{57}Fe, with $I = 1/2$ cannot exhibit quadrupole splitting.

We assume that $V(\boldsymbol{r})$ is the electric potential due to electrons around the nucleus site. When $\rho_n(\boldsymbol{r})$ is the nuclear charge distribution, the energy of the nucleus in this potential is given by

$$H = \int d\boldsymbol{r}\rho_n(\boldsymbol{r})V(\boldsymbol{r})$$

The origin is the center of mass of the nucleus. We expand $V(\boldsymbol{r})$ about the origin (Taylor expansion)

$$\begin{aligned} H &= \int d\boldsymbol{r}\rho_n(\boldsymbol{r})\{V_0 + \sum_j x_j \left(\frac{\partial V}{\partial x_j}\right)_0 + \frac{1}{2}\sum_{j,k} x_j x_k \left(\frac{\partial^2 V}{\partial x_j \partial x_k}\right)_0 + \ldots\} \\ &= ZeV_0 + \sum_j P_j \left(\frac{\partial V}{\partial x_j}\right)_0 + \frac{1}{2}\sum_{j,k} Q_{jk}' \left(\frac{\partial^2 V}{\partial x_j \partial x_k}\right)_0 + \ldots\ldots.. \end{aligned}$$

where x_j denotes one of x, y, and z. Here Ze, P_j and Q'_{jk} are defined by

$$Ze = \int d\boldsymbol{r}\rho_n(\boldsymbol{r}): \qquad \text{nuclear charge}$$

$$P_j = \int d\boldsymbol{r}\rho_n(\boldsymbol{r})x_j \qquad \text{electric dipole moment}$$

$$Q'_{jk} = \int d\boldsymbol{r}\rho_n(\boldsymbol{r})x_j x_k \qquad \text{electric quadrupole moment}$$

The first term is constant. The second term is zero. Note that the electric dipole moment P_j vanishes if the nuclear charge distribution has inversion symmetry with respect to the origin, as we assume. We consider only the third term

$$H_Q = \frac{1}{2}\sum_{j,k} Q'_{jk} V_{jk}$$

where

$$V_{jk}=\left(\frac{\partial^2 V}{\partial x_j \partial x_k}\right)_0$$

Here we introduce the traceless tensor

$$Q_{jk}=3Q'_{jk}-\delta_{jk}\sum_i Q'_{ii}$$
$$=\begin{pmatrix} 3Q'_{11}-Q'_{11}-Q'_{22}-Q'_{33} & 3Q'_{12} & 3Q'_{13} \\ 3Q'_{21} & 3Q'_{22}-Q'_{11}-Q'_{22}-Q'_{33} & 3Q'_{23} \\ 3Q'_{31} & 3Q'_{32} & 3Q'_{33}-Q'_{11}-Q'_{22}-Q'_{33} \end{pmatrix}$$

Then H_Q' can be rewritten as

$$H_Q'=\frac{1}{2}\sum_{j,k}[\frac{1}{3}Q_{jk}+\frac{1}{3}\delta_{jk}\sum_i Q'_{ii}]V_{jk}=\frac{1}{6}\sum_{j,k}Q_{jk}V_{jk}+\frac{1}{6}\left(\sum_i Q'_{ii}\right)\sum_j V_{jj}$$

7. Isomar shift

We consider the first term (the isomar shift)

$$\delta E=\frac{1}{6}\left(\sum_i Q'_{ii}\right)\sum_j V_{jj}=\frac{1}{6}(V_{xx}+V_{yy}+V_{zz})\int d\boldsymbol{r}r^2\rho_n(\boldsymbol{r})$$

where

$$(V_{xx}+V_{yy}+V_{zz})=\left(\nabla^2 V\right)_0=-4\pi(-e)|\psi_e(0)|^2 \qquad \text{(Poisson's equation)}$$

where $|\psi_e(0)|^2$ is the electronic probability density at the nucleus. Then we have

$$\delta E=\frac{2\pi}{3}e|\psi(0)|^2\int d\boldsymbol{r}r^2\rho_n(\boldsymbol{r})$$

Suppose that the distribution of charge of proton inside the nucleus is homegeneous for $r<R$.

$$\int d\boldsymbol{r}r^2\rho_n(\boldsymbol{r})=\rho_n\int 4\pi r^4 dr=\frac{4\pi\rho_n}{5}R^5=\frac{4\pi R^5}{5}\frac{Ze}{\frac{4\pi R^3}{3}}=\frac{3}{5}ZeR^2,$$

where R is the radius of nucleus, and the homogeneous charge density is

$$\rho_n = \frac{Ze}{\frac{4\pi R^3}{3}} = \frac{3Ze}{4\pi R^3}.$$

Then we have

$$\delta E = \frac{2\pi}{3} e|\psi(0)|^2 \frac{3}{5} ZeR^2 = \frac{2\pi}{5} Ze^2 R^2 |\psi(0)|^2$$

which is the isomar shift.

8. Electric quadrupole interaction

$$H_Q = H_Q' - \delta E = \frac{1}{6}\sum_{j,k} Q_{jk} V_{jk}$$

We are concerned only with the ground state of a nucleus. The eigenstates of the nucleus are characterized by the total angular momentum I, of each state, $2I+1$ values of a component of angular momentum. According to the Wigner-Eckart theorem (which will be discussed in detail), the Hamiltonian can be rewritten as

$$\langle I,m|Q_{jk}|I,m'\rangle = C\langle I,m|\frac{3}{2}(I_j I_k + I_k I_j) - \delta_{jk}\boldsymbol{I}^2|I,m'\rangle$$

where C is a constant. We define C as follows, using the quadrupole moment eQ,

$$eQ = \langle I,I|Q_{zz}|I,I\rangle = C\langle I,I|3I_z^2 - \boldsymbol{I}^2)|I,I\rangle = C[3I^2 - I(I+1)] = CI(2I-1).$$

or

$$C = \frac{eQ}{I(2I-1)}$$

The quantity eQ is the expectation value of

$$Q_{zz} = 3Q'_{zz} - Q'_{xx} - Q'_{yy} - Q'_{zz} = \int d\boldsymbol{r}\rho_n(\boldsymbol{r})(3z^2 - r^2)$$

over the state in which the z component of $\boldsymbol{I}$ is I. We note that $eQ = 0$ for $I = ½$.

9. Hamiltonian of the electric quadrupole (general case)

We introduce

$$I_{\pm} = I_x \pm iI_y$$

$$V_0 = V_{zz}, \qquad V_{\pm 1} = V_{xz} \pm iV_{yz}, \qquad V_{\pm 2} = \frac{1}{2}(V_{xx} - V_{yy}) \pm iV_{xy}$$

where we take the principal axes as the coordinate system,

$$V_{xx} + V_{yy} + V_{zz} = 0$$

The Hamiltonain can be rewritten as

$$H_Q = \frac{eQ}{4I(2I-1)}[(3I_z{}^2 - \boldsymbol{I}^2)V_0 + (I_+I_z + I_zI_+)V_{-1} + (I_-I_z + I_zI_-)V_1 + \\ + I_+{}^2V_{-2} + I_-{}^2V_2]$$

Here we choose the z, y, and x axes so that

$$|V_{zz}| \geq |V_{yy}| \geq |V_{xx}|$$

and define eq and η (asymmetric parameter)as

$$eq = V_{zz}, \qquad \eta = \frac{V_{xx} - V_{yy}}{V_{zz}} \qquad (0 \leq \eta \leq 1)$$

Then we have

$$H_Q = \frac{e^2qQ}{4I(2I-1)}[(3I_z{}^2 - \boldsymbol{I}^2) + \frac{\eta}{2}(I_+{}^2 + I_-{}^2)] \\ = \frac{e^2qQ}{4I(2I-1)}[3I_z{}^2 - I(I+1) + \frac{\eta}{2}(I_+{}^2 + I_-{}^2)]$$

where $I \geq 1$.

10. Example

Suppose that $I = 3/2$ (^{57}Fe): $Q = 0.21$ barn.

$$I_x = \begin{pmatrix} 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 \end{pmatrix}, \qquad I_y = \begin{pmatrix} 0 & -i\frac{\sqrt{3}}{2} & 0 & 0 \\ i\frac{\sqrt{3}}{2} & 0 & -i & 0 \\ 0 & i & 0 & -i\frac{\sqrt{3}}{2} \\ 0 & 0 & i\frac{\sqrt{3}}{2} & 0 \end{pmatrix}$$

$$I_z = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}$$

$$H_Q = \frac{1}{12} e^2 qQ \begin{pmatrix} 3 & 0 & \sqrt{3}\eta & 0 \\ 0 & -3 & 0 & \sqrt{3}\eta \\ \sqrt{3}\eta & 0 & -3 & 0 \\ 0 & \sqrt{3}\eta & 0 & 3 \end{pmatrix}$$

(i) Eigenvalue

$$-\frac{1}{4} e^2 qQ \sqrt{1 + \frac{\eta^2}{3}} \qquad \text{(degenerate)}$$

with eigenvectors (not normalized) given by

$$\{0, -\frac{\sqrt{3} + \sqrt{3+\eta^2}}{\eta}, 0, 1\}, \qquad \{\frac{\sqrt{3} - \sqrt{3+\eta^2}}{\eta}, 0, 1, 0\}$$

(ii) Eigenvalue

$$\frac{1}{4}e^2 qQ\sqrt{1+\frac{\eta^2}{3}}$$ (degenerate)

with eigenvectors (not normalized) given by

$$\{0,\frac{-\sqrt{3}+\sqrt{3+\eta^2}}{\eta},0,1\}, \qquad \{\frac{\sqrt{3}+\sqrt{3+\eta^2}}{\eta},0,1,0\}$$

The energy level of I = 3/2 splits into the two levels (both degenerate). The energy difference of these two levels is

$$\Delta E_Q = \frac{1}{2}e^2|q|Q\sqrt{1+\frac{\eta^2}{3}}$$

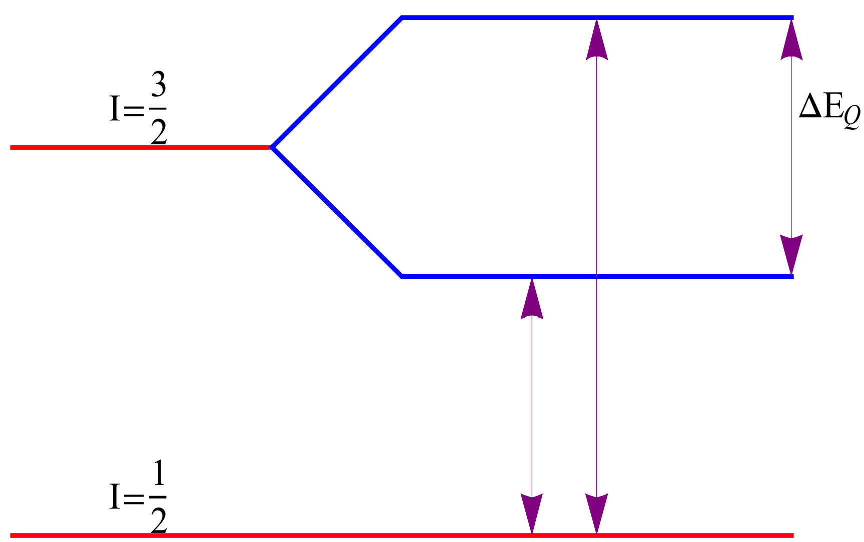


Fig. The splitting of the energy level of I = 3/2 due to the electric quadrupole moment. The hyperfine splitting is neglected. $\Delta E_Q = \frac{1}{2}e^2|q|Q\sqrt{1+\frac{\eta^2}{3}}$

((**Mathematica**))

```
Clear["Global`*"]; j0 = 3/2;

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
Jx[ℓ_, n_, m_] := 1/2 Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] +
  1/2 Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1];
Jy[ℓ_, n_, m_] := -1/2 ⅈ Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] +
  1/2 ⅈ Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1];
Jz[ℓ_, n_, m_] := m KroneckerDelta[n, m];
Jx = Table[Jx[j0, n, m], {n, j0, -j0, -1}, {m, j0, -j0, -1}];
Jy = Table[Jy[j0, n, m], {n, j0, -j0, -1}, {m, j0, -j0, -1}];
Jz = Table[Jz[m0, n, m], {n, j0, -j0, -1}, {m, j0, -j0, -1}];
E1 = IdentityMatrix[4]; Jp = Jx + ⅈ Jy;
Jm = Jx - ⅈ Jy;

A1 = e1^2 q1 Q1 / (4 j0 (2 j0 - 1));
H1 = A1 (3 Jz.Jz - j0 (j0 + 1) E1 + η/2 (Jp.Jp + Jm.Jm)) // Simplify;

H1 // MatrixForm
```

$$\begin{pmatrix} \frac{1}{4}\,\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1} & 0 & \frac{\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1}\,\eta}{4\sqrt{3}} & 0 \\ 0 & -\frac{1}{4}\,\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1} & 0 & \frac{\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1}\,\eta}{4\sqrt{3}} \\ \frac{\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1}\,\eta}{4\sqrt{3}} & 0 & -\frac{1}{4}\,\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1} & 0 \\ 0 & \frac{\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1}\,\eta}{4\sqrt{3}} & 0 & \frac{1}{4}\,\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1} \end{pmatrix}$$

```
Eigensystem[H1] // FullSimplify
```

$$\Big\{\Big\{-\frac{\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1}\sqrt{3+\eta^2}}{4\sqrt{3}},\ -\frac{\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1}\sqrt{3+\eta^2}}{4\sqrt{3}},\ \frac{\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1}\sqrt{3+\eta^2}}{4\sqrt{3}},\ \frac{\mathrm{e1}^2\,\mathrm{q1}\,\mathrm{Q1}\sqrt{3+\eta^2}}{4\sqrt{3}}\Big\},$$

$$\Big\{\Big\{0,\ -\frac{\sqrt{3}+\sqrt{3+\eta^2}}{\eta},\ 0,\ 1\Big\},\ \Big\{\frac{\sqrt{3}-\sqrt{3+\eta^2}}{\eta},\ 0,\ 1,\ 0\Big\},\ \Big\{0,\ \frac{-\sqrt{3}+\sqrt{3+\eta^2}}{\eta},\ 0,\ 1\Big\},\ \Big\{\frac{\sqrt{3}+\sqrt{3+\eta^2}}{\eta},\ 0,\ 1,\ 0\Big\}\Big\}\Big\}$$

((Experimental data))

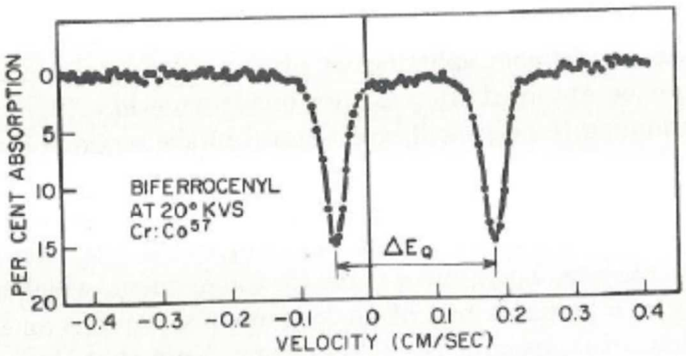


FIG. 1. Quadrupole splitting in Fe^{57}. Data on biferrocenyl from Wertheim and Herber [4].

G.K. Wertheim and R.H. Herber, J. Chem. Phys. **38**, 2106 (1963).

11. Zeeman splitting

$$H_m = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -g\mu_N \boldsymbol{I} \cdot \boldsymbol{B} = -g\mu_N mB$$

with $m = I, I - 1, I\text{-}2, \ldots, -I$. The magnetic moment of the nuclear spin is given by

$$\mu = \gamma\hbar I = g\mu_N I$$

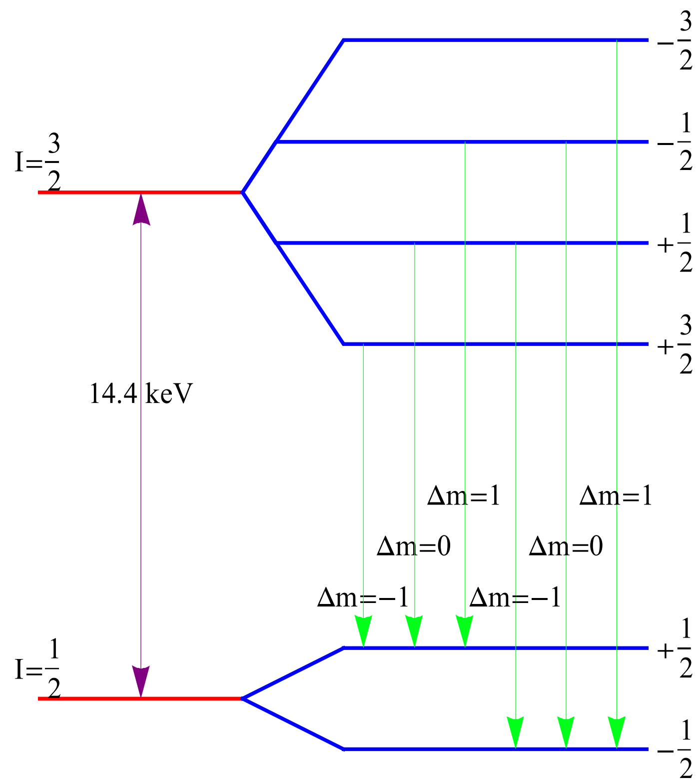
where γ is the gyromagnetic ratio (the ratio of the magnetic moment to the angular momentum),

$$\gamma = \frac{g\mu_N I}{\hbar I} = \frac{g\mu_N}{\hbar}.$$

The Landé g factor: $g_e>0$ (for $I = 3/2$) and $g_g<0$ (for $I = 1/2$); $g_e = 0.103$, $g_g = -0.18$. The selection rule is given by $\Delta m = 0, \pm 1$, and $\Delta I = 1$ (dipolar transition) because of the matrix element

$$\langle \psi_f | H_{dipole} | \psi_i \rangle$$

where H_{dipole} is the dipolar interaction. There are 6 lines observed for the Mössbauer measurement of ^{57}Fe



((**Experimental data**)) O.C. Kistmer and A.W. Sunyar, Phys. Rev. Lett. **4**, 412 (1960).

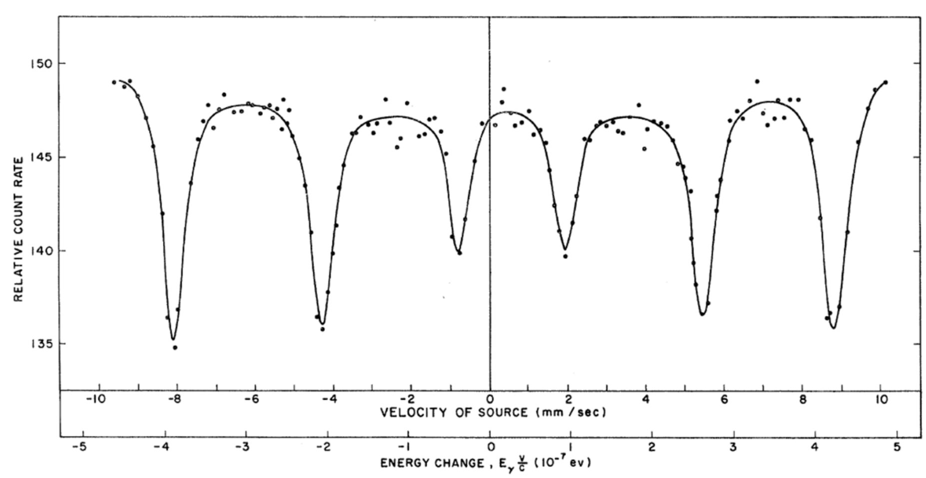


FIG. 1. The absorption by Fe^{57} bound in Fe_2O_3 of the 14.4-kev gamma ray emitted in the decay of Fe^{57m} bound in stainless steel as a function of relative source-absorber velocity. Positive velocity indicates a motion of source toward absorber.

Fig. The data from O. C. Kistmer and A. W. Sunyar, Phys. Rev. Lett., 4, 412(1960). The energy levels of the iron nucleus, contained in an ordinary iron sample, are split by the nuclear Zeeman effect. The spectrum shows the transitions for ^{57}Fe in Fe_2O_3. The splittings are some 11 orders of magnitude smaller than the nuclear transition energy;

$$\frac{10^{-7}eV}{14.4keV} \approx 10^{-11}.$$

12. Magnetic hyperfine interaction

Even in the absence of an external magnetic field, the effective magnetic field $\boldsymbol{H}_{loc}$ arises in the form of molecular magnetic field through a hyperfine interaction.

$$\boldsymbol{H}_{loc} = -\frac{16}{3}\pi\mu_B|\psi(0)|^2\langle \boldsymbol{s}\rangle_{AV} = -\frac{16}{3}\pi\mu_B\lambda_s{}^2\langle \boldsymbol{s}\rangle_{AV}$$

where $\langle \boldsymbol{s}\rangle_{AV}$ is the average of electron spin vector in thermal equilibrium.

$$\lambda_s{}^2 = |\psi(0)|^2$$

10. Selection rules

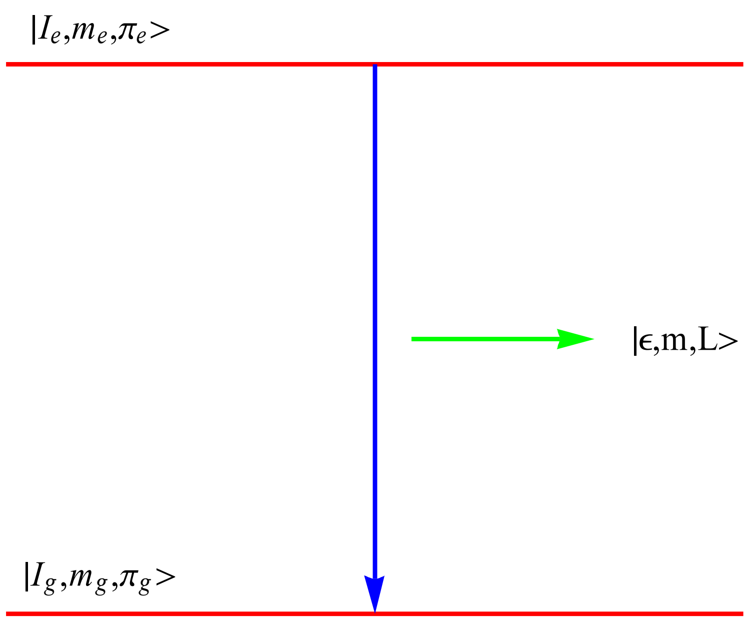


Fig. Transition from the excited state to the ground state and the radiation field.

The γ-ray is emitted on the transition from the excited state to the ground state. The excited state and the grounds state are specified by the angular momentum ($\hbar I$) and the parity. In this transition, the angular momentum is conserved. Suppose that $\hbar L$ is the angular momentum of the γ-ray.

Since γ radiation arises from electromagnetic effects, it can be thought of as changes in the charge and current distributions in nuclei.

Charge distributions resulting electric moments
Current distributions yield magnetic moments

Gamma decay can be classified as magnetic (*M*) or electric (*E*)
E and *M* multipole radiations differ in parity properties
Transition probabilities decrease rapidly with increasing angular-momentum changes as in β-decay

Carries of angular momentum

L = 1,2,3,4

2^L –pole (dipole, quadrupole, octupole…)

Shorthand notation for electric (or magnetic) 2^L –pole radiation

E_1 or M_1
$\rightarrow E_2$ is electric quadrupole

$I_i + I_f \geq I \geq |I_i - I_f|$, where I_i is the initial spin state and I_f is the final spin state. If initial and final state have the same parity electric multipoles of even I and magnetic multipoles of odd I are allowed

If different parity, the opposite is true

In general, a gamma transition between two nuclear levels of spin I_1 and I_2 must conserve the z component of the angular momentum, i.e., the angular momentum, L, carried off by the

$$\left|I_1 - I_2\right| \leq L \leq I_1 + I_2$$

However, L cannot be zero. A transition for which L = 1 is called a dipole transition. If it is accompanied by a change in parity, it is a magnetic dipole M_1 transition. If not, it is a electric dipole, E_1, transition.

For a given L, transitions between sublevels are limited to those with $|\Delta m| \le L$, and of course to those with proper parity change.

Table

2^L-pole	L	Parity change	Transition
Dipole	1	No	E_1
Dipole	1	Yes	M_1
Quadrupole	2	Yes	E_2
Quadrupole	2	No	M_2

11. Clebsch-Gordon co-efficient

Here we have the relation

$$|j_1, j_2; j, m\rangle = \sum_{m_1}\sum_{m_2} |j_1, j_2; m_1, m_2\rangle\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$$

where we use the closure relation.

$$\sum_{m_1}\sum_{m_2} |j_1, j_2; m_1, m_2\rangle\langle j_1, j_2; m_1, m_2| = 1 \ :$$

$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$: Clebsch Gordan co-efficient

(1) The co-efficient vanishes unless $m = m_1 + m_2$.

((**Proof**))

Note that

$$(\hat{J}_z - \hat{J}_{1z} - \hat{J}_{2z})|j_1, j_2; j, m\rangle = 0$$

$$\langle j_1, j_2; m_1, m_2 | \hat{J}_z - \hat{J}_{1z} - \hat{J}_{2z} | j_1, j_2; j, m\rangle = 0$$

or

$$(m - m_1 - m_2)\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = 0$$

For $m - m_1 - m_2 \neq 0$,

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = 0$$

(2) The co-efficieny vanishes unless

$$|j_1 - j_2| \leq j \leq j_1 + j_2$$

triangle inequality, which tells us the possible range of values of j when we add two angular momenta j_1 and j_2 whose values are fixed.

((Proof))

For a proof of the triangle rule, let us consider the possible values of m. Since $m = m_1 + m_2$, its maximum value is $j_1 + j_2$. The value is realized for the single state $|j_1, j_2; j_1, j_2\rangle$. The total J of this state is $j = j_1 + j_2$. The next highest value of m, $j_1 + j_2 - 1$ is realized for the linear combinations of two states in the uncoupled representations; $|j_1, j_2; j_1 - 1, j_2\rangle$ and $|j_1, j_2; j_1, j_2 - 1\rangle$. One of the linear combinations belongs to $j = j_1 + j_2$ and the second one to $j = j_1 + j_2 - 1$.

For $m = j_1 + j_2 - 2$, there are three linear combinations of the three uncoupled states; $|j_1, j_2; j_1 - 2, j_2\rangle$, $|j_1, j_2; j_1 - 1, j_2 - 1\rangle$, and $|j_1, j_2; j_1, j_2 - 2\rangle$, corresponding to three of j, $j = j_1 + j_2$, $j = j_1 + j_2 - 1$, and $j = j_1 + j_2 - 2$.

If we continue this process, we can see that each time we lower m by 1, a new value of j appears. The argument continues until we reach a stage where we can no longer go one more step down in one of them to make new states. We assume that $j_1 > j_2$.

$j = j_1 + j_2$; $m = j_1 + j_2, j_1 + j_2 - 1, ..., -(j_1 + j_2)$

$j = j_1 + j_2 - 1$, $m = j_1 + j_2 - 1, j_1 + j_2 - 2, ... -(j_1 + j_2 - 1)$,

....

$j = j_1 - j_2$, $m = j_1 - j_2, j_1 - j_2 - 1, \ldots\ldots, -(j_1 - j_2)$.

Here we show that if the triangle rule is valid, then the dimension of the space spanned by $\{|j_1, j_2; j, m\rangle\}$ is the same as that of the space spanned by $\{|j_1, j_2; m_1, m_2\rangle\}$.

For the (m_1, m_2) way of counting, we obtain $N = (2j_1 + 1)(2j_2 + 1)$.

As for the $\{j, m)$ way of counting, note that for each j, there are $(2j+1)$ states. According to the inequality ($|j_1 - j_2| \leq j \leq j_1 + j_2$), j runs (we assume $j_1 > j_2$) from $j_1 - j_2$ to $j_1 + j_2$.

$$\begin{aligned} N &= \sum_{j=j_1-j_2}^{j_1+j_2} (2j+1) = \sum_{j=0}^{j_1+j_2} (2j+1) - \sum_{j=0}^{j_1-j_2} (2j+1) \\ &= (j_1 + j_2 + 1)^2 - (j_1 - j_2)^2 = (2j_1 + 1)(2j_2 + 1) \end{aligned}$$

((Note))

$$D_{j_1} \times D_{j_2} = D_{j_1+j_2} + D_{j_1+j_2-1} + \ldots + D_{|j_1-j_2|}$$

where

$D_{j_1+j_2}$; $j = j_1 + j_2$; $m = j_1 + j_2, j_1 + j_2 - 1, \ldots, -(j_1 + j_2)$,

$D_{j_1+j_2-1}$; $j = j_1 + j_2 - 1$; $m = j_1 + j_2 - 1, j_1 + j_2 - 2, \ldots, -(j_1 + j_2 - 1)$,

....

$D_{|j_1-j_2|}$; $j = |j_1 - j_2|$; $m = |j_1 - j_2|, |j_1 - j_2| - 1, \ldots, -|j_1 - j_2|$,

The Clebsch-Gordan coefficients form an unitary matrix. Furthermore, the matrix elements are taken to be real by convention. A real unitary matrix is orthogonal. We have the orthogonal condition.

$$\langle j_1, j_2, j, m | j_1, j_2, m_1, m_2\rangle = \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle^* = \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$$

Closure relation

$$\langle j_1, j_2, m_1, m_1 | j_1, j_2, m_1', m_2' \rangle = \sum_{j,m} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; j, m | j_1, j_2; m_1', m_2' \rangle$$
$$= \sum_{j,m} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; m_1', m_2' | j_1, j_2; j, m \rangle = \delta_{m_1, m_1'} \delta_{m_2, m_2'}$$

or

$$\sum_{j,m} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; m_1', m_2' | j_1, j_2; j, m \rangle = \delta_{m_1, m_1'} \delta_{m_2, m_2'}$$

Similarly,

$$\sum_{m_1, m_2} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; m_1, m_2 | j_1, j_2; j', m' \rangle = \delta_{j, j'} \delta_{m, m'}$$

As a special case of this, we may set $j = j'$, $m' = m = m_1 + m_2$.

$$\sum_{\substack{m_1, m_2 \\ m = m_1 + m_2}} \left| \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \right|^2 = 1$$

which is just the normalization condition of $| j_1, j_2; j, m \rangle$.

13. Addition of angular momentum: Mathematica

In Mathematica we use the notation given by

$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \rightarrow$ ClebschGordan[{j_1,m_1},{j_2,m_2},{j,m}]

$| j_1, j_2; j, m \rangle \rightarrow$ CG[{j, m}, j_1,j_2]

$| j_1, j_2; m_1, m_2 \rangle$ $a(j_1, m_1) b(j_2, m_2)$

For example, we consider the case of j_1=3/2 and j_2=1/2; j = 2 and j = 1.

$$D_{3/2} \times D_{1/2} = D_2 + D_1$$

j1=3/2 and j2=1/2

```
Clear["Global`*"];

CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], 0]]

CG[{j_, m_}, j1_, j2_] :=
 Sum[CCGG[{j1, m1}, {j2, m - m1}, {j, m}] a[j1 , m1] b[j2, m - m1], {m1, -j1, j1}]

CG[{2, 2}, 3 / 2, 1 / 2]
```

$a\left[\frac{3}{2}, \frac{3}{2}\right] b\left[\frac{1}{2}, \frac{1}{2}\right]$

```
CG[{2, 1}, 3 / 2, 1 / 2]
```

$\frac{1}{2} a\left[\frac{3}{2}, \frac{3}{2}\right] b\left[\frac{1}{2}, -\frac{1}{2}\right] + \frac{1}{2} \sqrt{3} a\left[\frac{3}{2}, \frac{1}{2}\right] b\left[\frac{1}{2}, \frac{1}{2}\right]$

```
CG[{2, 0}, 3 / 2, 1 / 2]
```

$\frac{a\left[\frac{3}{2}, \frac{1}{2}\right] b\left[\frac{1}{2}, -\frac{1}{2}\right]}{\sqrt{2}} + \frac{a\left[\frac{3}{2}, -\frac{1}{2}\right] b\left[\frac{1}{2}, \frac{1}{2}\right]}{\sqrt{2}}$

```
CG[{2, -1}, 3 / 2, 1 / 2]
```

$\frac{1}{2} \sqrt{3} a\left[\frac{3}{2}, -\frac{1}{2}\right] b\left[\frac{1}{2}, -\frac{1}{2}\right] + \frac{1}{2} a\left[\frac{3}{2}, -\frac{3}{2}\right] b\left[\frac{1}{2}, \frac{1}{2}\right]$

```
CG[{2, -2}, j1, j2]
```

$a\left[\frac{1}{2}, -\frac{1}{2}\right] b\left[\frac{3}{2}, -\frac{3}{2}\right]$

```
CG[{2, 1}, j1, j2]
```

$\frac{1}{2}\sqrt{3}\, a\left[\frac{1}{2}, \frac{1}{2}\right] b\left[\frac{3}{2}, \frac{1}{2}\right] + \frac{1}{2}\, a\left[\frac{1}{2}, -\frac{1}{2}\right] b\left[\frac{3}{2}, \frac{3}{2}\right]$

```
CG[{2, 0}, j1, j2]
```

$\frac{a\left[\frac{1}{2}, \frac{1}{2}\right] b\left[\frac{3}{2}, -\frac{1}{2}\right]}{\sqrt{2}} + \frac{a\left[\frac{1}{2}, -\frac{1}{2}\right] b\left[\frac{3}{2}, \frac{1}{2}\right]}{\sqrt{2}}$

```
CG[{2, -1}, j1, j2]
```

$\frac{1}{2}\, a\left[\frac{1}{2}, \frac{1}{2}\right] b\left[\frac{3}{2}, -\frac{3}{2}\right] + \frac{1}{2}\sqrt{3}\, a\left[\frac{1}{2}, -\frac{1}{2}\right] b\left[\frac{3}{2}, -\frac{1}{2}\right]$

```
CG[{1, 1}, j1, j2]
```

$\frac{1}{2}\, a\left[\frac{1}{2}, \frac{1}{2}\right] b\left[\frac{3}{2}, \frac{1}{2}\right] - \frac{1}{2}\sqrt{3}\, a\left[\frac{1}{2}, -\frac{1}{2}\right] b\left[\frac{3}{2}, \frac{3}{2}\right]$

```
CG[{1, 0}, j1, j2]
```

$\frac{a\left[\frac{1}{2}, \frac{1}{2}\right] b\left[\frac{3}{2}, -\frac{1}{2}\right]}{\sqrt{2}} - \frac{a\left[\frac{1}{2}, -\frac{1}{2}\right] b\left[\frac{3}{2}, \frac{1}{2}\right]}{\sqrt{2}}$

```
CG[{1, -1}, j1, j2]
```

$\frac{1}{2}\sqrt{3}\, a\left[\frac{1}{2}, \frac{1}{2}\right] b\left[\frac{3}{2}, -\frac{3}{2}\right] - \frac{1}{2}\, a\left[\frac{1}{2}, -\frac{1}{2}\right] b\left[\frac{3}{2}, -\frac{1}{2}\right]$

---

14. Conventional notations of ket vector.

For $j = 2$,

$$\left| j = 2, m = 2 \right\rangle = \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle \qquad \text{for } m = 2$$

$$\left| j = 2, m = 1 \right\rangle = \frac{1}{2} \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle + \frac{\sqrt{3}}{2} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle \qquad \text{for } m = 1$$

$$\left| j = 2, m = 0 \right\rangle = \frac{1}{\sqrt{2}} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle + \frac{1}{\sqrt{2}} \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle \qquad \text{for } m = 0$$

$$\left| j=2, m=-1 \right\rangle = \frac{\sqrt{3}}{2}\left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle + \frac{1}{2}\left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle \qquad \text{for } m = -1$$

$$\left| j=2, m=-2 \right\rangle = \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \qquad \text{for } m = -2$$

For $j = 1$

$$\left| j=1, m=1 \right\rangle = \frac{\sqrt{3}}{2}\left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle - \frac{1}{2}\left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle \qquad \text{for } m = 1$$

$$\left| j=1, m=0 \right\rangle = \frac{1}{\sqrt{2}}\left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle - \frac{1}{\sqrt{2}}\left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle \qquad \text{for } m = 0$$

$$\left| j=1, m=-1 \right\rangle = \frac{1}{2}\left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle - \frac{\sqrt{3}}{2}\left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle \qquad \text{for } m = -1$$

15. Symmetry relation for the Clebsch-Gordan coefficient

We replace the operator equation

$$\boldsymbol{J}_1 + \boldsymbol{J}_2 = \boldsymbol{J}$$

by

$$\boldsymbol{J}_2 = -\boldsymbol{J}_1 + \boldsymbol{J} = \bar{\boldsymbol{J}}_1 + \boldsymbol{J}$$

is the time reversed angular momentum. These results suggest that the Clebsch-Gordon coefficient $\langle j_1, j; -m_1, m | j_1, j; j_2, m_2 \rangle$ may be related to $\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle$. In fact, we have the symmetry relation (I),

$$\begin{aligned}
\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle &= (-1)^{j_1 - m_1} \sqrt{\frac{2j+1}{2j_2+1}} \langle j_1, j; m_1, -m | j_1, j; j_2, -m_2 \rangle \\
&= (-1)^{j_1 - m_1} \sqrt{\frac{2j+1}{2j_2+1}} (-1)^{j_1 + j - j_2} \langle j_1, j; -m_1, m | j_1, j; j_2, m_2 \rangle \\
&= (-1)^{2j_1 + j - j_2 - m_1} \sqrt{\frac{2j+1}{2j_2+1}} \langle j_1, j; -m_1, m | j_1, j; j_2, m_2 \rangle
\end{aligned}$$

or

$$\langle j_1, j; -m_1, m | j_1, j; j_2, m_2 \rangle = (-1)^{-2j_1 - j + j_2 + m_1} \sqrt{\frac{2j_2+1}{2j+1}} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle$$

((Note)) The detail of this formula is presented in the following reference.

M.E. Rose, Elementary Theory of Angular Momentum (Dover, New York, 1957, 1995).
A.R. Edmonds, Angular momentum in quantum mechanics p.42 (Princeton University Press, 1957)

((**Mathematica**))
The proof is given here for the case of j_1=3/2 and j_2 = 1/2. l = 1, m = 1, 0, and -1.

- **j1=3/2 and j2=1/2**

```
Clear["Global`*"]; CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], 0]]; j1 = 3 / 2;
j2 = 1 / 2;

L = 1;

Table[{m1, m2, m1 + m2, CCGG[{j1, -m1}, {L, m1 + m2}, {j2, m2}],
   (-1)^(-2 j1-L+j2 +m1) Sqrt[2 j2 + 1]/Sqrt[2 L + 1] CCGG[{j1, m1}, {j2, m2}, {L, m1 + m2}]}, {m1, -j1, j1, 1},
 {m2, -j2, j2, 1}]
```

```
L = 1;
Table[{m1, m2, m1 + m2, CCGG[{j1, -m1}, {L, m1 + m2}, {j2, m2}],
  (-1)^(-2 j1-L+j2 +m1) Sqrt[2 j2 + 1]/Sqrt[2 L + 1] CCGG[{j1, m1}, {j2, m2}, {L, m1 + m2}]}, {m1, -j1, j1, 1},
 {m2, -j2, j2, 1}]
```

$$\left\{\left\{\left\{-\frac{3}{2}, -\frac{1}{2}, -2, 0, 0\right\}, \left\{-\frac{3}{2}, \frac{1}{2}, -1, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}\right\},\right.$$
$$\left\{\left\{-\frac{1}{2}, -\frac{1}{2}, -1, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{6}}\right\}, \left\{-\frac{1}{2}, \frac{1}{2}, 0, -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right\}\right\},$$
$$\left\{\left\{\frac{1}{2}, -\frac{1}{2}, 0, -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right\}, \left\{\frac{1}{2}, \frac{1}{2}, 1, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{6}}\right\}\right\},$$
$$\left.\left\{\left\{\frac{3}{2}, -\frac{1}{2}, 1, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \left\{\frac{3}{2}, \frac{1}{2}, 2, 0, 0\right\}\right\}\right\}$$

```
L = 2;
Table[{m1, m2, m1 + m2, CCGG[{j1, -m1}, {L, m1 + m2}, {j2, m2}],
  (-1)^(-2 j1-L+j2 +m1) Sqrt[2 j2 + 1]/Sqrt[2 L + 1] CCGG[{j1, m1}, {j2, m2}, {L, m1 + m2}]}, {m1, -j1, j1, 1},
 {m2, -j2, j2, 1}]
```

$$\left\{\left\{\left\{-\frac{3}{2}, -\frac{1}{2}, -2, \sqrt{\frac{2}{5}}, \sqrt{\frac{2}{5}}\right\}, \left\{-\frac{3}{2}, \frac{1}{2}, -1, \frac{1}{\sqrt{10}}, \frac{1}{\sqrt{10}}\right\}\right\},\right.$$
$$\left\{\left\{-\frac{1}{2}, -\frac{1}{2}, -1, -\sqrt{\frac{3}{10}}, -\sqrt{\frac{3}{10}}\right\}, \left\{-\frac{1}{2}, \frac{1}{2}, 0, -\frac{1}{\sqrt{5}}, -\frac{1}{\sqrt{5}}\right\}\right\},$$
$$\left\{\left\{\frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{\sqrt{5}}, \frac{1}{\sqrt{5}}\right\}, \left\{\frac{1}{2}, \frac{1}{2}, 1, \sqrt{\frac{3}{10}}, \sqrt{\frac{3}{10}}\right\}\right\},$$
$$\left.\left\{\left\{\frac{3}{2}, -\frac{1}{2}, 1, -\frac{1}{\sqrt{10}}, -\frac{1}{\sqrt{10}}\right\}, \left\{\frac{3}{2}, \frac{1}{2}, 2, -\sqrt{\frac{2}{5}}, -\sqrt{\frac{2}{5}}\right\}\right\}\right\}$$

(ii) We replace the operator equation

$$\boldsymbol{J}_1 + \boldsymbol{J}_2 = \boldsymbol{J}$$

by

$$\bar{\boldsymbol{J}} = \bar{\boldsymbol{J}}_1 + \bar{\boldsymbol{J}}_2$$

These results suggest that the Clebsch-Gordon coefficient $\langle j_1, j_2; -m_1, -m_2 | j_1, j_2; j, -m\rangle$ may be related to $\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$. In fact, we have the symmetry relation (II),

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = (-1)^{j_1+j_2-j}\langle j_1, j_2; -m_1, -m_2 | j_1, j_2; j, -m\rangle$$

((**Formula**)) M.E. Rose Elementary theory of angular momentum, p.38 (Dover)

$$\begin{aligned}\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle &= (-1)^{j_1+j_2-j}\langle j_1, j_2; -m_1, -m_2 | j_1, j_2; j, -m\rangle \\ &= (-1)^{j_1+j_2-j}\langle j_2, j_1; m_2, m_1 | j_2, j_1; j, m\rangle \\ &= (-1)^{j_1-m_1}\sqrt{\frac{2j+1}{2j_2+1}}\langle j_1, j; m_1, -m | j_1, j; j_2, -m_2\rangle\end{aligned}$$

---

16. Intensity of the the γ-ray transition

If the γ-ray transition is between two levels of nuclear spin I_1 and I_2, and furthermore between the two substates with I_z values of m_1 and m_2, respectively, then the angular-independent probability term is given by the square of the appropriate Clebsch-Gordon coefficient,

$$\text{Intensity} \propto |\langle j_1, j; -m_1, m, | j_1, j; j_2, m_2\rangle|^2 = |\langle I_1, L; -m_1, m, | I_1, L; I_2, m_2\rangle|^2$$

L = 1 is a dipole transition and L = 2 is a quadratic transition. If there is no change in parity during the decay it is classified as magnetic dipole (M_1) or electric quadrupole (E_2). Electric dipole (E1) transitions with a change in parity also come within our scope.

Using the above formula (symmetry rule), we get

$$|\langle I_1, I_2; m_1, m_2 | I_1, I_2; L, m\rangle|^2 = \frac{2L+1}{2I_2+1}|\langle I_1, L; -m_1, m, | I_1, L; I_2, m_2\rangle|^2,$$

or

$$|\langle I_1, L; -m_1, m, | I_1, L; I_2, m_2\rangle|^2 = \frac{2I_2+1}{2L+1}|\langle I_1, I_2; m_1, m_2 | I_1, I_2; L, m\rangle|^2$$

The results of the Clebsch-Gordan co-efficient are summarized as follows.

Table-1 $l = 1.$

l	m	m_1	m_2	$\left\langle I_1 = \frac{3}{2}, l; -m_1, m \middle| I_1, l; I_2 = \frac{1}{2}, m_2 \right\rangle^2$
1	1	$\frac{3}{2}$	$-\frac{1}{2}$	$\frac{3}{6}$
1	1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{6}$
1	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{2}{6}$
1	0	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{6}$
1	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{6}$
1	-1	$-\frac{3}{2}$	$\frac{1}{2}$	$\frac{3}{6}$

Table-2 $l = 2.$

l	m	m_1	m_2	$\left\langle I_1 = \frac{3}{2}, l; -m_1, m \middle| I_1, l; I_2 = \frac{1}{2}, m_2 \right\rangle^2$
2	2	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{4}{10}$
2	1	$\frac{3}{2}$	$-\frac{1}{2}$	$\frac{1}{10}$
2	1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{10}$
2	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{2}{10}$
2	0	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{10}$
2	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{3}{10}$
2	-1	$-\frac{3}{2}$	$\frac{1}{2}$	$\frac{1}{10}$
2	-2	$-\frac{3}{2}$	$-\frac{1}{2}$	$\frac{4}{10}$

17. Angular dependence for $l = 1$

The intensity including the angular dependence is given by

$$\left| \left\langle I_1 = \frac{3}{2}, l; -m_1, m, \middle| I_1 = \frac{3}{2}, l; I_2 = \frac{1}{2}, m_2 \right\rangle \right|^2 \Theta(l,m)$$

where $\Theta(l,m)$ is defined by

$$\Theta(l,m) = \sum_{\xi=\pm1} \left| d_{\xi m}^{(l)} \right|^2 = \left| d_{1m}^{(l)} \right|^2 + \left| d_{-1m}^{(l)} \right|^2$$

$d_{\xi m}^{(l)}$ is the element of the rotation matrix for the right-handed (+1) and left-handed (-1) polarization. For m = 1, 0, and -1, we have

$$\Theta(l=1, m=1) = \left| d_{11}^{(1)} \right|^2 + \left| d_{-11}^{(1)} \right|^2 = \frac{1+\cos^2\theta}{2}$$

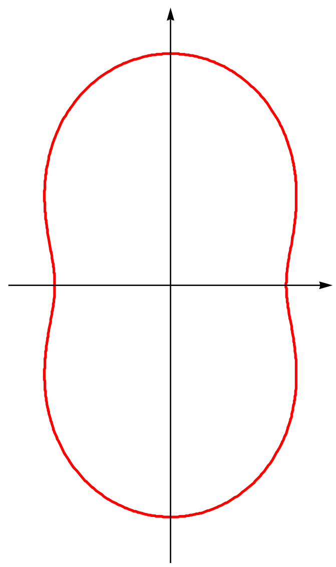
$$\Theta(l=1, m=0) = \left| d_{10}^{(1)} \right|^2 + \left| d_{-10}^{(1)} \right|^2 = 2\frac{\sin^2\theta}{2} = \sin^2\theta$$

$$\Theta(l=1, m=-1) = \left| d_{1-1}^{(1)} \right|^2 + \left| d_{-1-1}^{(1)} \right|^2 = \frac{1+\cos^2\theta}{2}$$

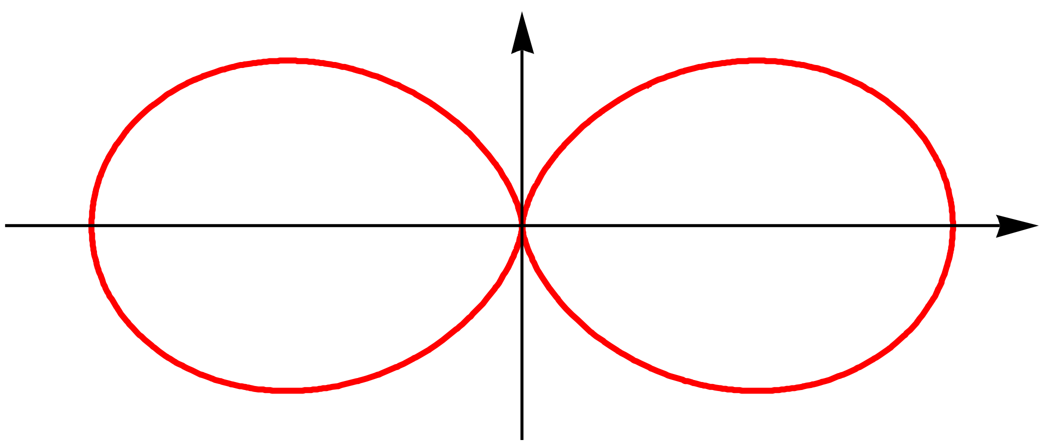
where the rotation operator for $l = 1$ is given by

$$D^{(1)}(\theta,\phi) = \begin{pmatrix} e^{-i\phi}(\frac{1+\cos\theta}{2}) & -e^{-i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{-i\phi}(\frac{1-\cos\theta}{2}) \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ e^{i\phi}(\frac{1-\cos\theta}{2}) & e^{i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{i\phi}(\frac{1+\cos\theta}{2}) \end{pmatrix}$$

(1) $\quad \Theta(l=1, m=\pm1) = \dfrac{1+\cos^2\theta}{2}$



(2) $\Theta(l=1, m=0) = \sin^2\theta$



For $\phi = 0$, we have the rotation matrix as

$$D^{(1)}(\theta, \phi = 0) = \begin{pmatrix} d_{11}^{(1)}(\theta) & d_{10}^{(1)}(\theta) & d_{1-1}^{(1)}(\theta) \\ d_{01}^{(1)}(\theta) & d_{00}^{(1)}(\theta) & d_{0-1}^{(1)}(\theta) \\ d_{-11}^{(1)}(\theta) & d_{-10}^{(1)}(\theta) & d_{-1-1}^{(1)}(\theta) \end{pmatrix} = \begin{pmatrix} \frac{1+\cos\theta}{2} & -\frac{\sin\theta}{\sqrt{2}} & \frac{1-\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} & \frac{\sin\theta}{\sqrt{2}} & \frac{1+\cos\theta}{2} \end{pmatrix}$$

18. Angular dependence for $l = 2$

$$\Theta(l=2,m) = \sum_{\xi=\pm 1} \left| d_{\xi m}^{(2)} \right|^2 = \left| d_{1m}^{(2)} \right|^2 + \left| d_{-1m}^{(2)} \right|^2$$

$$D^{(2)}(\theta,\phi=0) = \begin{pmatrix} d_{22}^{(2)}(\theta) & d_{21}^{(2)}(\theta) & d_{20}^{(2)}(\theta) & d_{2-1}^{(2)}(\theta) & d_{2-2}^{(2)}(\theta) \\ d_{12}^{(2)}(\theta) & d_{11}^{(2)}(\theta) & d_{10}^{(2)}(\theta) & d_{1-1}^{(2)}(\theta) & d_{1-2}^{(2)}(\theta) \\ d_{02}^{(2)}(\theta) & d_{01}^{(2)}(\theta) & d_{00}^{(2)}(\theta) & d_{0-1}^{(2)}(\theta) & d_{0-2}^{(2)}(\theta) \\ d_{-12}^{(2)}(\theta) & d_{-11}^{(2)}(\theta) & d_{-10}^{(2)}(\theta) & d_{-1-1}^{(2)}(\theta) & d_{-1-2}^{(2)}(\theta) \\ d_{-22}^{(2)}(\theta) & d_{-21}^{(2)}(\theta) & d_{-20}^{(2)}(\theta) & d_{-2-1}^{(2)}(\theta) & d_{-2-2}^{(2)}(\theta) \end{pmatrix}$$

$$\Theta(l=2,m=2) = \sum_{\xi=\pm 1} \left| d_{\xi 2}^{(2)} \right|^2 = \left| d_{12}^{(2)} \right|^2 + \left| d_{-12}^{(2)} \right|^2 = \frac{1}{4}[3+\cos(2\theta)]\sin^2\theta$$

$$\Theta(l=2,m=1) = \sum_{\xi=\pm 1} \left| d_{\xi 1}^{(2)} \right|^2 = \left| d_{11}^{(2)} \right|^2 + \left| d_{-11}^{(2)} \right|^2 = \frac{1}{2}[\cos^2\theta+\cos^2(2\theta)]$$

$$\Theta(l=2,m=0) = \sum_{\xi=\pm 1} \left| d_{\xi 0}^{(2)} \right|^2 = \left| d_{10}^{(2)} \right|^2 + \left| d_{-10}^{(2)} \right|^2 = \frac{3}{4}\sin^2(2\theta)$$

$$\Theta(l=2,m=-1) = \sum_{\xi=\pm 1} \left| d_{\xi -1}^{(2)} \right|^2 = \left| d_{1-1}^{(2)} \right|^2 + \left| d_{-1-1}^{(2)} \right|^2 = \frac{1}{2}[\cos^2\theta+\cos^2(2\theta)]$$

$$\Theta(l=2,m=-2) = \sum_{\xi=\pm 1} \left| d_{\xi -2}^{(2)} \right|^2 = \left| d_{1-2}^{(2)} \right|^2 + \left| d_{-1-2}^{(2)} \right|^2 = \frac{1}{4}[3+\cos(2\theta)]\sin^2\theta$$

where

$$d_{12}^{(2)} = -2\cos^3\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right), \qquad d_{-12}^{(2)} = \frac{1}{4}[-2\sin\theta+\sin(2\theta)]$$

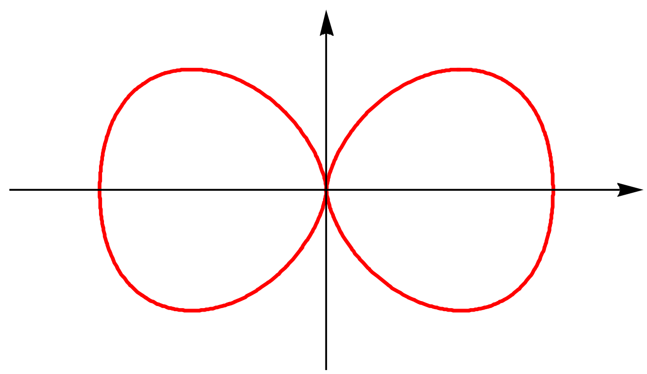
$$d_{11}^{(2)} = \frac{1}{2}[\cos\theta+\cos(2\theta)], \qquad d_{-11}^{(2)} = \frac{1}{2}[\cos\theta-\cos(2\theta)]$$

$$d_{10}^{(2)} = \sqrt{\frac{3}{2}}\sin\theta\cos\theta\,, \qquad d_{-10}^{(2)} = -\sqrt{\frac{3}{2}}\sin\theta\cos\theta$$

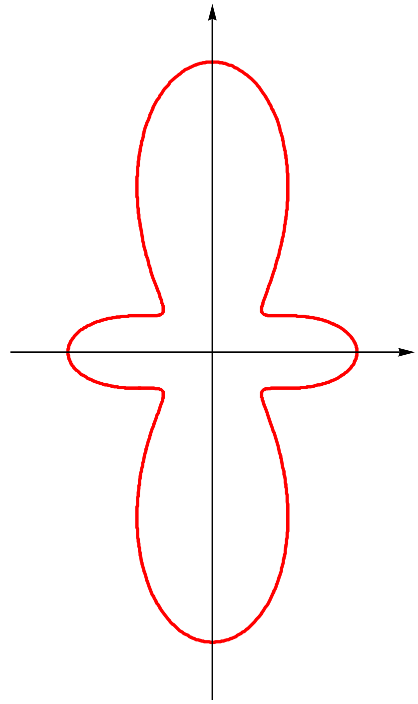
$$d_{1-1}^{(2)} = \frac{1}{2}[\cos\theta - \cos(2\theta)]\,, \qquad d_{-1-1}^{(2)} = \frac{1}{2}[\cos\theta + \cos(2\theta)]$$

$$d_{1-2}^{(2)} = \sin^2\left(\frac{\theta}{2}\right)\sin\theta\,, \qquad d_{-1-2}^{(2)} = \frac{1}{2}[1+\cos\theta]\sin\theta$$

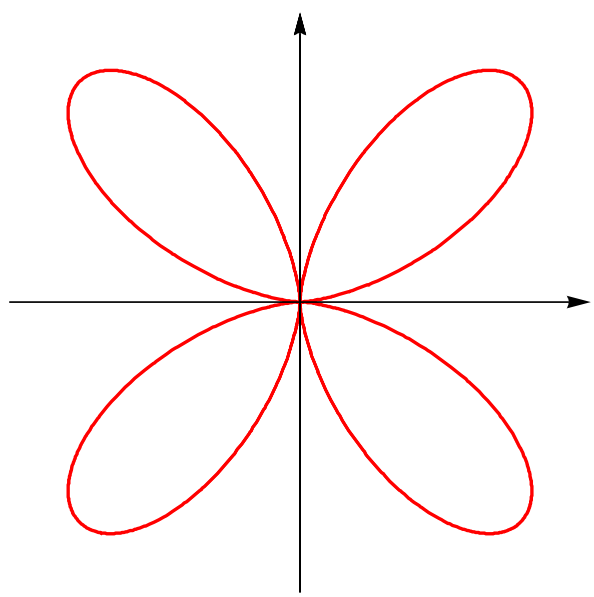
(1) $\Theta(l=2, m=\pm 2) = \frac{1}{4}[3+\cos(2\theta)]\sin^2\theta$



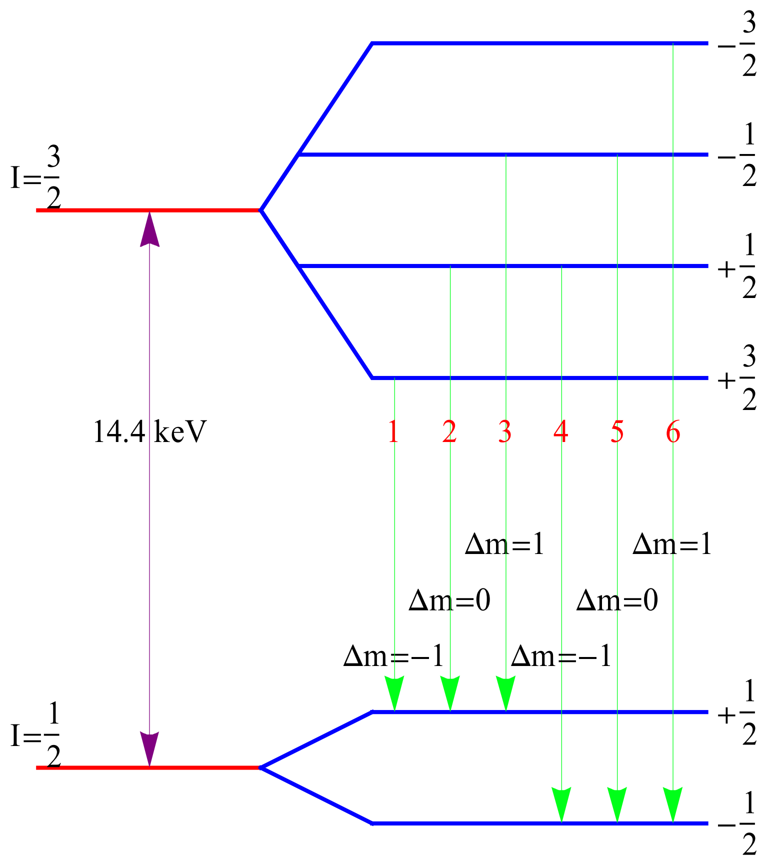
(2) $\Theta(l=2, m=1) = \frac{1}{2}[\cos^2\theta + \cos^2(2\theta)]$



(3) $\Theta(l=2, m=0) = \frac{3}{4}\sin^2(2\theta)$



19. Selection rules



The parity of the state $I = 3/2$; π_i

The parity of the state $I = 1/2$, π_j

Magnetic: $\pi_i \pi_j = (-1)^{l+1}$

Electric: $\pi_i \pi_j = (-1)^{l}$

For $\pi_i = \pi_j$ (the same parity), $l = 1, 3, 5$, (magnetic) and $l = 2, 4, 6$ (electric).

For $\pi_i \neq \pi_j$ (different parity), $l = 1, 3, 5$, (electric) and $l = 2, 4, 6$ (magnetic).

Table-1 $l = 1$

l	m	$-m_1$	m_2	Relative intensity I

1	1	$-\frac{3}{2}$	$-\frac{1}{2}$	$I_6 = 3(1+\cos^2\theta)$
1	1	$-\frac{1}{2}$	$\frac{1}{2}$	$I_3 = 1+\cos^2\theta$
1	0	$-\frac{1}{2}$	$-\frac{1}{2}$	$I_5 = 4\sin^2\theta$
1	0	$\frac{1}{2}$	$\frac{1}{2}$	$I_2 = 4\sin^2\theta$
1	-1	$\frac{1}{2}$	$-\frac{1}{2}$	$I_4 = 1+\cos^2\theta$
1	-1	$\frac{3}{2}$	$\frac{1}{2}$	$I_1 = 3(1+\cos^2\theta)$

The intensity ratio is given by

$$I_1 : I_2 : I_3 : I_4 : I_5 : I_6 = 3(1+\cos^2\theta) : 4\sin^2\theta : 1+\cos^2\theta : 1+\cos^2\theta : 4\sin^2\theta : 3(1+\cos^2\theta)$$

(i) When $\theta = 0$,

$$I_1 : I_2 : I_3 : I_4 : I_5 : I_6 = 3:0:1:1:0:3$$

(ii) When $\theta = \pi/2$,

$$I_1 : I_2 : I_3 : I_4 : I_5 : I_6 = 3:4:1:1:4:3$$

(iii) Powder pattern

Using the average values

$$\overline{\cos^2\theta} = \frac{1}{4\pi}\int_0^\pi \cos^2\theta(2\pi\sin\theta)d\theta = \frac{1}{2}\int_0^\pi \cos^2\theta\sin\theta d\theta = \frac{1}{3}$$

$$\overline{\sin^2\theta} = \frac{1}{4\pi}\int_0^\pi \sin^2\theta(2\pi\sin\theta)d\theta = \frac{1}{2}\int_0^\pi \sin^3\theta d\theta = \frac{2}{3}$$

we get the intensity ratio for the powder sample as

$$I_1 : I_2 : I_3 : I_4 : I_5 : I_6 = 3:2:1:1:2:3$$

20. Resultant intensity for l = 2.

l	m	m_1	m_2	Relative intensity
2	2	$\frac{3}{2}$	$\frac{1}{2}$	$4\sin^2\theta+\sin^2(2\theta)$
2	1	$\frac{3}{2}$	$-\frac{1}{2}$	$\cos^2\theta+\cos^2(2\theta)$
2	1	$\frac{1}{2}$	$\frac{1}{2}$	$3[\cos^2\theta+\cos^2(2\theta)]$
2	0	$\frac{1}{2}$	$-\frac{1}{2}$	$3\sin^2(2\theta)$
2	0	$-\frac{1}{2}$	$\frac{1}{2}$	$3\sin^2(2\theta)$
2	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$3[\cos^2\theta+\cos^2(2\theta)]$
2	-1	$-\frac{3}{2}$	$\frac{1}{2}$	$\cos^2\theta+\cos^2(2\theta)$
2	-2	$-\frac{3}{2}$	$-\frac{1}{2}$	$2[3+\cos(2\theta)]\sin^2\theta$

APPENDIX

1 Rotation operator with j = 1

((**Mathematica**)) Rotation matrix with j = 1

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};

Jx[ℓ_, n_, m_] := 1/2 Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] + 1/2 Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1];

Jy[ℓ_, n_, m_] := -1/2 ⅈ Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] + 1/2 ⅈ Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1];

Jz[ℓ_, n_, m_] := m KroneckerDelta[n, m];

j = 1;

Jx = Table[Jx[j, p, q], {p, j, -j, -1}, {q, j, -j, -1}]; Jy = Table[Jy[j, p, q], {p, j, -j, -1}, {q, j, -j, -1}];
Jz = Table[Jz[j, p, q], {p, j, -j, -1}, {q, j, -j, -1}]; Ry[θ_] := MatrixExp[-ⅈ Jy θ];
Rz[ϕ_] := MatrixExp[-ⅈ Jz ϕ];

R1 = Rz[ϕ].Ry[θ];

R1 /. ϕ → 0 // Simplify // TableForm
```

$\cos\left[\frac{\theta}{2}\right]^2$	$-\frac{\sin[\theta]}{\sqrt{2}}$	$\sin\left[\frac{\theta}{2}\right]^2$
$\frac{\sin[\theta]}{\sqrt{2}}$	$\cos[\theta]$	$-\frac{\sin[\theta]}{\sqrt{2}}$
$\sin\left[\frac{\theta}{2}\right]^2$	$\frac{\sin[\theta]}{\sqrt{2}}$	$\cos\left[\frac{\theta}{2}\right]^2$

The rotation operator with $l = 1$ is given by

$$\hat{R} = D^{(1)}(\theta,\phi) = \begin{pmatrix} e^{-i\phi}(\frac{1+\cos\theta}{2}) & -e^{-i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{-i\phi}(\frac{1-\cos\theta}{2}) \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ e^{i\phi}(\frac{1-\cos\theta}{2}) & e^{i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{i\phi}(\frac{1+\cos\theta}{2}) \end{pmatrix}$$

The eigenkets $|1\rangle_n$, $|0\rangle_n$, and $|-1\rangle_n$ are obtained as

$$|1\rangle_n = \hat{R}|1\rangle = \begin{pmatrix} \frac{1+\cos\theta}{2}e^{-i\phi} \\ \frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2}e^{i\phi} \end{pmatrix},$$

$$|0\rangle_n = \hat{R}|0\rangle = \begin{pmatrix} -\frac{\sin\theta}{\sqrt{2}}e^{-i\phi} \\ \cos\theta \\ \frac{\sin\theta}{\sqrt{2}}e^{i\phi} \end{pmatrix},$$

$$\left|-1\right\rangle_n = \hat{R}\left|-1\right\rangle = \begin{pmatrix} \frac{1-\cos\theta}{2}e^{-i\phi} \\ -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1+\cos\theta}{2}e^{i\phi} \end{pmatrix},$$

For $\phi = 0$, the rotation operator is given by

$$\hat{R} = d^{(1)}(\theta) = \begin{pmatrix} \frac{1+\cos\theta}{2} & -\frac{\sin\theta}{\sqrt{2}} & \frac{1-\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} & \frac{\sin\theta}{\sqrt{2}} & \frac{1+\cos\theta}{2} \end{pmatrix}$$

and

$$\left|1\right\rangle_n = \hat{R}\left|1\right\rangle = \begin{pmatrix} \frac{1+\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} \end{pmatrix}$$

$$\left|0\right\rangle_n = \hat{R}\left|0\right\rangle = \begin{pmatrix} -\frac{\sin\theta}{\sqrt{2}} \\ \cos\theta \\ \frac{\sin\theta}{\sqrt{2}} \end{pmatrix}$$

$$\left|-1\right\rangle_n = \hat{R}\left|-1\right\rangle = \begin{pmatrix} \frac{1-\cos\theta}{2} \\ -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1+\cos\theta}{2} \end{pmatrix}$$

2. **Mathematica** Rotation operator for $l = 2$.

```
Clear["Global`*"];

exp_* := exp /. {Complex[re_, im_] :→ Complex[re, -im]};
Jx[ℓ_, n_, m_] := 1/2 Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] + 1/2 Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1];
Jy[ℓ_, n_, m_] := -1/2 ⅈ Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] + 1/2 ⅈ Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1];
Jz[ℓ_, n_, m_] := m KroneckerDelta[n, m];

j = 2;

Jx = Table[Jx[j, p, q], {p, j, -j, -1}, {q, j, -j, -1}]; Jy = Table[Jy[j, p, q], {p, j, -j, -1}, {q, j, -j, -1}];
Jz = Table[Jz[j, p, q], {p, j, -j, -1}, {q, j, -j, -1}]; Ry[θ_] := MatrixExp[-ⅈ Jy θ];
Rz[ϕ_] := MatrixExp[-ⅈ Jz ϕ];

R1 = Rz[ϕ] . Ry[θ];

R1 /. ϕ → 0 // Simplify // TableForm
```

$\cos\left[\frac{\theta}{2}\right]^4$	$-2\cos\left[\frac{\theta}{2}\right]^3\sin\left[\frac{\theta}{2}\right]$	$\frac{1}{2}\sqrt{\frac{3}{2}}\sin[\theta]^2$	$\frac{1}{4}(-2\sin[\theta]+\sin[2\theta])$	$\sin\left[\frac{\theta}{2}\right]^4$
$\frac{1}{2}(1+\cos[\theta])\sin[\theta]$	$\frac{1}{2}(\cos[\theta]+\cos[2\theta])$	$-\sqrt{\frac{3}{2}}\cos[\theta]\sin[\theta]$	$\frac{1}{2}(\cos[\theta]-\cos[2\theta])$	$\frac{1}{4}(-2\sin[\theta]+\sin[2\theta])$
$\frac{1}{2}\sqrt{\frac{3}{2}}\sin[\theta]^2$	$\sqrt{\frac{3}{2}}\cos[\theta]\sin[\theta]$	$\frac{1}{4}(1+3\cos[2\theta])$	$-\sqrt{\frac{3}{2}}\cos[\theta]\sin[\theta]$	$\frac{1}{2}\sqrt{\frac{3}{2}}\sin[\theta]^2$
$\sin\left[\frac{\theta}{2}\right]^2\sin[\theta]$	$\frac{1}{2}(\cos[\theta]-\cos[2\theta])$	$\sqrt{\frac{3}{2}}\cos[\theta]\sin[\theta]$	$\frac{1}{2}(\cos[\theta]+\cos[2\theta])$	$-2\cos\left[\frac{\theta}{2}\right]^3\sin\left[\frac{\theta}{2}\right]$
$\sin\left[\frac{\theta}{2}\right]^4$	$\sin\left[\frac{\theta}{2}\right]^2\sin[\theta]$	$\frac{1}{2}\sqrt{\frac{3}{2}}\sin[\theta]^2$	$\frac{1}{2}(1+\cos[\theta])\sin[\theta]$	$\cos\left[\frac{\theta}{2}\right]^4$

3. Spherical Harmonics as rotator matrices

Using the relation

$$\left|\Re\boldsymbol{r}\right\rangle = \hat{R}\left|\boldsymbol{r}\right\rangle$$

$$\begin{aligned}\left|\boldsymbol{n}\right\rangle &= \left|\Re\boldsymbol{r}\right\rangle \\ &= \hat{R}\left|\boldsymbol{e}_z\right\rangle \\ &= \hat{R}_z(\phi)\hat{R}_y(\theta)\left|\boldsymbol{e}_z\right\rangle \\ &= \sum_{m'}\hat{R}_z(\phi)\hat{R}_y(\theta)\left|lm'\right\rangle\left\langle lm'\right|\boldsymbol{e}_z\left.\right\rangle\end{aligned}$$

Then

$$\left\langle lm\middle|\boldsymbol{n}\right\rangle = \sum_{m'}\left\langle lm\right|\hat{R}_z(\phi)\hat{R}_y(\theta)\left|lm'\right\rangle\left\langle lm'\middle|\boldsymbol{e}_z\right\rangle$$

Here note that

$$\langle \boldsymbol{n} | lm \rangle = Y_\ell^m(\boldsymbol{n}) = Y_\ell^m(\theta,\phi)$$

or

$$\langle lm | \boldsymbol{n} \rangle = [Y_\ell^m(\theta,\phi)]^*$$

$\langle lm | \boldsymbol{e}_z \rangle = [Y_\ell^m(\theta,\phi)]^*$ evaluated at $\theta = 0$ with ϕ undetermined. At $\theta = 0$, $Y_\ell^m(\theta,\phi)$ is known to vanish for $m \neq 0$. Then we get

$$\begin{aligned}
\langle lm | \boldsymbol{e}_z \rangle &= [Y_\ell^m(\theta = 0,\phi)]^* \delta_{m,0} \\
&= \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos\theta = 1)\delta_{m,0} \\
&= \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m,0}
\end{aligned}$$

$$\begin{aligned}
[Y_\ell^m(\theta,\phi)]^* &= \sum_{m'} \langle lm | \hat{R}_z(\phi)\hat{R}_y(\theta) | lm' \rangle \langle lm' | \boldsymbol{e}_z \rangle \\
&= \sqrt{\frac{2\ell+1}{4\pi}} \sum_{m'} \langle lm | \hat{R}_z(\phi)\hat{R}_y(\theta) | lm' \rangle \delta_{m',0} = \sqrt{\frac{2\ell+1}{4\pi}} \langle lm | \hat{R}_z(\phi)\hat{R}_y(\theta) | l0 \rangle
\end{aligned}$$

or

$$\langle lm | \hat{R}_z(\phi)\hat{R}_y(\theta) | l0 \rangle = \sqrt{\frac{4\pi}{2\ell+1}} [Y_\ell^m(\theta,\phi)]^*$$

Since

$$\hat{R}_z(\phi) = \exp[-\frac{i}{\hbar}\hat{J}_z\phi]$$

we have

$$\langle lm | \hat{R}_z(\phi)\hat{R}_y(\theta) | l0 \rangle = \langle lm | \exp[-\frac{i}{\hbar}\hat{J}_z\phi]\hat{R}_y(\theta) | l0 \rangle = e^{-im\phi} \langle lm | \hat{R}_y(\theta) | l0 \rangle$$

or

$$e^{-im\phi}\langle lm|\hat{R}_y(\theta)|l0\rangle = \sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^*$$

or

$$\langle lm|\hat{R}_y(\theta)|l0\rangle = e^{im\phi}\sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^*$$

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