Magnetic neutron scattering

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1. Magnetic moment of neutron

The neutron has a magnetic moment given by

$$\boldsymbol{\mu} = -\gamma \mu_N \boldsymbol{\sigma},$$

μ_N : the nuclear magneton,

$$\mu_N = \frac{e\hbar}{2m_p c} = 5.05079 \text{ x } 10^{-24} \text{ emu (cgs units)}$$

$\mu_N = 5.05078324 \times 10^{-24}$ emu (cgs units), emu = erg/Gauss=emu/Oe

$\mu_N = 5.05078324 \times 10^{-27}$ J/T (SI units)

γ gyromagnetic ratio, $\gamma =$ 1.913 for neutron

m_p : the proton rest mass.

σ: the Pauli spin operator for the neutron (= ±1).

e: the charge of proton (e>0)

2. Spin magnetic moment of electrons

The operator corresponding to the magnetic dipole moment of the electron is

$$\boldsymbol{\mu}_e = -2\mu_B \frac{\boldsymbol{s}_e}{\hbar} = -\mu_B \boldsymbol{\sigma}_e.$$

$\boldsymbol{s}_e$ the spin angular momentum,

$$\boldsymbol{s}_s = \frac{\hbar}{2}\boldsymbol{\sigma}_e$$

σ_e: the Pauli spin operator for the electron (= ±1).

μ_B the Bohr magneton

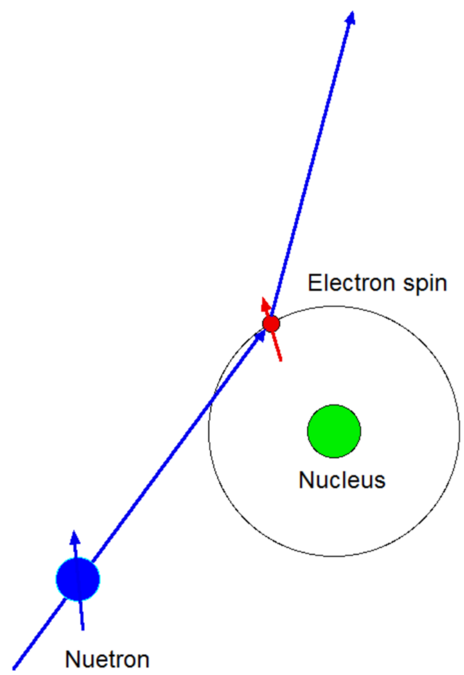
$$\mu_B = \frac{e\hbar}{2m_e c} = 0.27400915 \text{ x } 10^{-21} \text{ emu (cgs)}$$

m_e the mass of electron

$-e$: the charge of electron (we assume $e>0$).

3. Interaction between nutron spin and electron spin

This scattering arises from the interaction of the neutron magnetic moment μ_n with the local magnetic field $\boldsymbol{B}$. The local field due to an electron at position $\boldsymbol{R}$ with momentum $\boldsymbol{p}_e$ and magnetic moment μ_e arising from the electron spin is



$$\boldsymbol{B} = \boldsymbol{B}_S + \boldsymbol{B}_L .$$

The first term ($\boldsymbol{B}_S$): electron spin angular moment

$$\mathbf{A} = \frac{\boldsymbol{\mu}_e \times \mathbf{R}}{R^3}, \qquad \boldsymbol{B}_s = \nabla \times \boldsymbol{A} = \nabla \times \left(\frac{\boldsymbol{\mu}_e \times \boldsymbol{R}}{R^3} \right) = -\frac{2\mu_B}{\hbar} \nabla \times \left(\frac{\boldsymbol{s}_e \times \boldsymbol{R}}{R^3} \right),$$

where $\boldsymbol{R}$ is the distance from the electron to the point at which the field is measured.

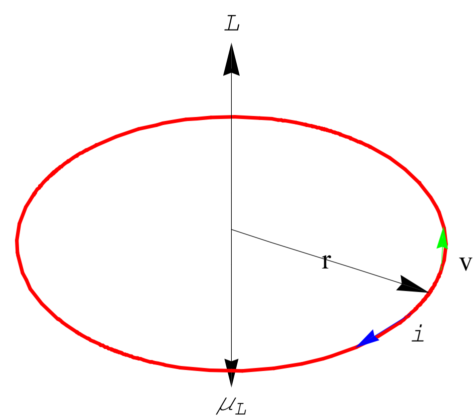
The second term ($\boldsymbol{B}_L$):electron orbital angular momentum

$$\boldsymbol{B}_L = \int d\boldsymbol{B}_L = \int \frac{id\boldsymbol{l} \times \boldsymbol{R}}{cR^3} = \frac{-e(\boldsymbol{p}_e \times \boldsymbol{R})}{m_e cR^3} = -\frac{2\mu_B}{\hbar}\frac{\boldsymbol{p}_e \times \boldsymbol{R}}{R^3},$$

(Biot-Savart law)

where i is the current due to the orbital motion of electron,

$$\oint id\boldsymbol{l} = \left(\frac{-e\boldsymbol{v}}{2\pi r}\right)2\pi r = -e\boldsymbol{v} = -\frac{e}{m_e}\boldsymbol{p}_e = -2\frac{\mu_B}{\hbar}\boldsymbol{p}_e,$$



Then we get

$$\boldsymbol{B} = -\frac{2\mu_B}{\hbar}[\nabla \times \left(\frac{\boldsymbol{s}_e \times \boldsymbol{R}}{R^3}\right) + \frac{\boldsymbol{p}_e \times \boldsymbol{R}}{R^3}]$$
$$= \nabla \times \left(\frac{\boldsymbol{\mu}_e \times \boldsymbol{R}}{R^3}\right) - \frac{2\mu_B}{\hbar}\frac{\boldsymbol{p}_e \times \boldsymbol{R}}{R^3}]$$

The interaction potential with the neutron is given by

$$\begin{aligned}
V &= -\boldsymbol{\mu}\cdot\boldsymbol{B} \\
&= -(-\gamma\mu_N\boldsymbol{\sigma})(-\frac{2\mu_B}{\hbar})[\nabla\times\left(\frac{\boldsymbol{s}_e\times\boldsymbol{R}}{R^3}\right)+\frac{\boldsymbol{p}_e\times\boldsymbol{R}}{R^3}]] \\
&= -\gamma\mu_N\frac{2\mu_B}{\hbar}[\boldsymbol{\sigma}\cdot\nabla\times\left(\frac{\boldsymbol{s}_e\times\boldsymbol{R}}{R^3}\right)+\boldsymbol{\sigma}\cdot\left(\frac{\boldsymbol{p}_e\times\boldsymbol{R}}{R^3}\right)] \\
&= -\gamma\mu_N 2\mu_B[\frac{1}{\hbar}\boldsymbol{\sigma}\cdot\nabla\times\left(\frac{\boldsymbol{s}_e\times\boldsymbol{R}}{R^3}\right)-\frac{1}{\hbar}\boldsymbol{p}_e\cdot\left(\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}\right)]
\end{aligned}$$

The first term is arising from the spin of the electron. The second term is arising from its orbital motion. In order to take proper account of the operator of the momentum of the electron (quantum mechanically), V should be changed as follows.

$$V = -2\gamma\mu_N\mu_B[\frac{1}{\hbar}\boldsymbol{\sigma}\cdot\nabla\times\left(\frac{\boldsymbol{s}_e\times\boldsymbol{R}}{R^3}\right)-\frac{1}{2\hbar}\left(\boldsymbol{p}_e\cdot\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}+\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}\cdot\boldsymbol{p}_e\right)]$$

where

$$\boldsymbol{p}_e = \frac{\hbar}{i}\nabla .$$

4. Differential cross section

The cross section for the scattering of neutrons through the interaction potential V is

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = \frac{k'}{k}\left(\frac{m_n}{2\pi\hbar^2}\right)^2 (2\gamma\mu_N\mu_B)^2 \sum_{\lambda,\lambda',\sigma} P_\lambda P_\sigma$$

$$|(2\pi)^3 \langle \boldsymbol{k}'\lambda'\sigma'| \sum_i [\frac{1}{\hbar}\boldsymbol{\sigma}\cdot\nabla\times\left(\frac{\boldsymbol{s}_i\times\boldsymbol{R}}{R^3}\right) - \frac{1}{2\hbar}\left(\boldsymbol{p}_i\cdot\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3} + \frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}\cdot\boldsymbol{p}_i\right) |\boldsymbol{k}\lambda\sigma\rangle|^2$$

$$\times\delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

$$= \frac{k'}{k}\frac{(\gamma r_0)^2}{16\pi^2}\sum_{\lambda,\lambda',\sigma} P_\lambda P_\sigma$$

$$|(2\pi)^3 \langle \boldsymbol{k}'\lambda'\sigma'| \sum_i [\frac{1}{\hbar}\boldsymbol{\sigma}\cdot\nabla\times\left(\frac{\boldsymbol{s}_i\times\boldsymbol{R}}{R^3}\right) - \frac{1}{2\hbar}\left(\boldsymbol{p}_i\cdot\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3} + \frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}\cdot\boldsymbol{p}_i\right) |\boldsymbol{k}\lambda\sigma\rangle|^2$$

$$\times\delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

where

$$\left(\frac{m_n}{2\pi\hbar^2}\right)^2 (2\gamma\mu_N\mu_B)^2 = \frac{1}{16\pi^2}(\gamma r_0)^2$$

where we assume that $m_n = m_p$. r_0 is defined as

$$r_0 = \frac{e^2}{m_0 c^2} = 2.81795 \text{ x } 10^{-13} \text{ cm} \qquad \text{(classical radius of electron)}$$

and

γr_0=0.539 x 10^{-12} cm.

$\lvert\lambda\rangle$:	initial state of the target.
E_λ:	the energy of initial state of the target
$\lvert\lambda'\rangle$:	the final state of the target
$E_{\lambda'}$:	the energy of final state of the target
$\boldsymbol{s}_i$	the spin angular momentum of the *i*-th electron
$\boldsymbol{p}_i$	the linear momentum of the *i*-th electron
P_σ	incident neutron spin probability
P_λ	probability distribution for initial target states

P_λ has the Boltzmann form

$$P_\lambda = \frac{\exp(-\frac{E_\lambda}{k_B T})}{\sum_\lambda \exp(-\frac{E_\lambda}{k_B T})}$$

5. Matrix calculation (I)

We use the formula

$$\frac{\boldsymbol{R}}{R^3} = -\nabla\left(\frac{1}{R}\right)$$

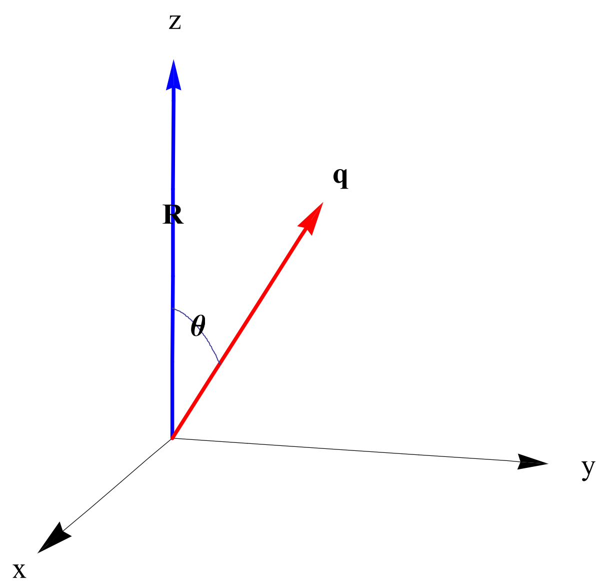
and

$$\frac{1}{R} = \frac{1}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\exp(i\boldsymbol{q}\cdot\boldsymbol{R})$$

where

$$R = |\boldsymbol{R}|$$

and we need to apply the Cauchy theorem for the upper half-plane of the complex plane and use the residue theorem).



$$I = \int d\boldsymbol{q} \frac{1}{q^2} e^{i\boldsymbol{q}\cdot\boldsymbol{R}} = \int_0^\infty 2\pi q^2 dq \int_0^\pi \sin\theta d\theta \frac{1}{q^2} e^{iqR\cos\theta} = \int_0^\infty 2\pi dq \int_0^\pi \sin\theta d\theta e^{iqR\cos\theta}$$

or

$$I = \frac{1}{iR}\int_0^\infty 2\pi dq \frac{e^{iqR} - e^{-iqR}}{q} = \frac{4\pi}{R}\int_0^\infty dq \frac{\sin(qR)}{q} = \frac{4\pi}{R}\int_0^\infty \frac{\sin(x)}{x} dx = \frac{4\pi}{R}\frac{\pi}{2} = \frac{2\pi^2}{R}$$

Then we get

$$\nabla\times\left(\frac{\boldsymbol{s}_i\times\boldsymbol{R}}{R^3}\right)=-\nabla\times\left(\boldsymbol{s}_i\times\nabla\frac{1}{R}\right)$$

$$=-\nabla\times(\boldsymbol{s}_i\times\nabla)\frac{1}{R}$$

$$=-\frac{1}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{\nabla\times(\boldsymbol{s}_i\times\nabla)\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R})$$

$$=-\frac{i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{\nabla\times(\boldsymbol{s}_i\times\boldsymbol{q})\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R})$$

$$=\frac{1}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{\boldsymbol{q}\times(\boldsymbol{s}_i\times\boldsymbol{q})\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R})$$

Then the matrix element can be evaluated as

$$(2\pi)^3\langle\boldsymbol{k}'|\frac{1}{\hbar}\boldsymbol{\sigma}\cdot\nabla\times\left(\frac{\boldsymbol{s}_i\times\boldsymbol{R}}{R^3}\right)|\boldsymbol{k}\rangle=(2\pi)^3\int d\boldsymbol{r}''\int d\boldsymbol{r}'\langle\boldsymbol{k}'|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\frac{1}{2\pi^2\hbar}\int d\boldsymbol{q}\frac{1}{q^2}\boldsymbol{\sigma}\cdot\{\boldsymbol{q}\times(\boldsymbol{s}_i\times\boldsymbol{q})\}e^{i\boldsymbol{q}\cdot\boldsymbol{R}}|\boldsymbol{r}''\rangle\langle\boldsymbol{r}''|\boldsymbol{k}\rangle$$

$$=\frac{1}{2\pi^2\hbar}(2\pi)^3\int d\boldsymbol{r}''\int d\boldsymbol{r}'\langle\boldsymbol{k}'|\boldsymbol{r}'\rangle\int d\boldsymbol{q}\frac{1}{q^2}\boldsymbol{\sigma}\cdot\{\boldsymbol{q}\times(\boldsymbol{s}_i\times\boldsymbol{q})\}e^{i\boldsymbol{q}\cdot(\boldsymbol{r}'-\boldsymbol{r}_i)}\langle\boldsymbol{r}'|\boldsymbol{r}''\rangle\langle\boldsymbol{r}''|\boldsymbol{k}\rangle$$

$$=\frac{1}{2\pi^2\hbar}\int d\boldsymbol{r}'\int d\boldsymbol{r}''e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}\int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}d\boldsymbol{q}\frac{1}{q^2}\boldsymbol{\sigma}\cdot\{\boldsymbol{q}\times(\boldsymbol{s}_i\times\boldsymbol{q})\}e^{i\boldsymbol{q}\cdot\boldsymbol{r}'}\delta(\boldsymbol{r}'-\boldsymbol{r}'')e^{i\boldsymbol{k}\cdot\boldsymbol{r}''}$$

$$=\frac{1}{2\pi^2\hbar}\int d\boldsymbol{r}'e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}\int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}d\boldsymbol{q}\frac{1}{q^2}\boldsymbol{\sigma}\cdot\{\boldsymbol{q}\times(\boldsymbol{s}_i\times\boldsymbol{q})\}e^{i(\boldsymbol{q}+\boldsymbol{k})\cdot\boldsymbol{r}'}$$

$$=\frac{1}{2\pi^2\hbar}\int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}d\boldsymbol{q}\frac{1}{q^2}\boldsymbol{\sigma}\cdot\{\boldsymbol{q}\times(\boldsymbol{s}_i\times\boldsymbol{q})\}\int d\boldsymbol{r}'e^{i(\boldsymbol{q}+\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}'}$$

$$=\frac{1}{2\pi^2\hbar}(2\pi)^3\int d\boldsymbol{q}\delta(\boldsymbol{q}+\boldsymbol{\kappa})e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}\frac{1}{q^2}\boldsymbol{\sigma}\cdot\{\boldsymbol{q}\times(\boldsymbol{s}_i\times\boldsymbol{q})\}$$

$$=4\pi e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\boldsymbol{\sigma}\cdot\{\overline{\boldsymbol{\kappa}}\times(\frac{\boldsymbol{s}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})\}$$

where

$\overline{\boldsymbol{\kappa}}=\frac{\boldsymbol{\kappa}}{\kappa}$; unit vector

$\boldsymbol{r}=\boldsymbol{R}+\boldsymbol{r}_i$

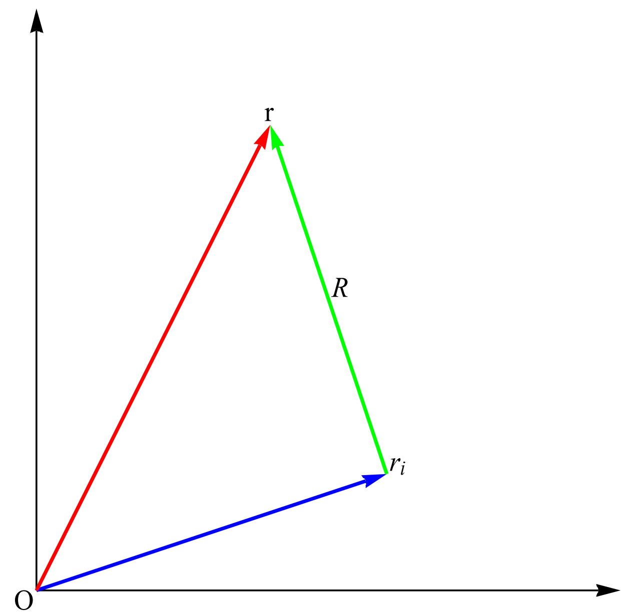


Fig. Neutron and electron position vectors. Neutron ($\boldsymbol{r}$). i-th electron ($\boldsymbol{r}_i$). $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}_i$.

$$\langle \boldsymbol{k} | \boldsymbol{r} \rangle = \langle \boldsymbol{r} | \boldsymbol{k} \rangle^* = \frac{1}{(2\pi)^{3/2}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$$

and

$$\boldsymbol{\kappa} = \boldsymbol{k} - \boldsymbol{k}'$$

$$\langle \boldsymbol{r}' | \boldsymbol{r}'' \rangle = \delta(\boldsymbol{r}' - \boldsymbol{r}'')$$

$$\int d\boldsymbol{r}' e^{i(\boldsymbol{q}+\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}'} = (2\pi)^3 \delta(\boldsymbol{q} + \boldsymbol{k} - \boldsymbol{k}') = (2\pi)^3 \delta(\boldsymbol{q} + \boldsymbol{\kappa})$$

6. Matrix calculation (II)

Next we calculate another matrix element,

$$
\begin{aligned}
\boldsymbol{p}_i \cdot \frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3} &= -\boldsymbol{p}_i \cdot \boldsymbol{\sigma}\times\nabla(\frac{1}{R}) \\
&= -\frac{1}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{\boldsymbol{p}_i \cdot \boldsymbol{\sigma}\times\nabla)\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R}) \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{\boldsymbol{p}_i \cdot(\boldsymbol{\sigma}\times\boldsymbol{q})\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R}) \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\cdot\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R})
\end{aligned}
$$

$$
\begin{aligned}
(2\pi)^3\langle\boldsymbol{k}'|\boldsymbol{p}_i\cdot\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}|\boldsymbol{k}\rangle &= (2\pi)^3\int d\boldsymbol{r}''\int d\boldsymbol{r}'\langle\boldsymbol{k}'|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\cdot\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\}e^{i\boldsymbol{q}\cdot\boldsymbol{R}}|\boldsymbol{r}''\rangle\langle\boldsymbol{r}''|\boldsymbol{k}\rangle \\
&= \frac{-i}{2\pi^2}(2\pi)^3\int d\boldsymbol{r}''\int d\boldsymbol{r}'\langle\boldsymbol{k}'|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\int d\boldsymbol{q}\frac{1}{q^2}\cdot\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\}e^{i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}_i)}|\boldsymbol{r}''\rangle\langle\boldsymbol{r}''|\boldsymbol{k}\rangle \\
&= \frac{-i}{2\pi^2}(2\pi)^3\int d\boldsymbol{r}''\int d\boldsymbol{r}'\langle\boldsymbol{k}'|\boldsymbol{r}'\rangle\int d\boldsymbol{q}\frac{1}{q^2}\cdot\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\}e^{i\boldsymbol{q}\cdot(\boldsymbol{r}'-\boldsymbol{r}_i)}\langle\boldsymbol{r}'|\boldsymbol{r}''\rangle\langle\boldsymbol{r}''|\boldsymbol{k}\rangle \\
&= \frac{-i}{2\pi^2}\int e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}d\boldsymbol{r}'\int d\boldsymbol{r}''\int d\boldsymbol{q}\frac{1}{q^2}\cdot\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\}e^{i\boldsymbol{q}\cdot(\boldsymbol{r}'-\boldsymbol{r}_i)}\delta(\boldsymbol{r}'-\boldsymbol{r}'')e^{i\boldsymbol{k}\cdot\boldsymbol{r}''} \\
&= \frac{-i}{2\pi^2}\int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}d\boldsymbol{r}'e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}\int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}d\boldsymbol{q}\frac{1}{q^2}\cdot\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\}e^{i(\boldsymbol{q}+\boldsymbol{k})\cdot\boldsymbol{r}'} \\
&= \frac{-i}{2\pi^2}\int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}d\boldsymbol{q}\frac{1}{q^2}\cdot\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\}\int d\boldsymbol{r}'e^{i(\boldsymbol{q}+\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}'} \\
&= \frac{-i}{2\pi^2}(2\pi)^3\int e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}d\boldsymbol{q}\delta(\boldsymbol{q}+\boldsymbol{\kappa})\frac{1}{q^2}\cdot\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\} \\
&= \frac{i4\pi}{\kappa}e^{i\kappa\cdot\boldsymbol{r}_i}\{\boldsymbol{\sigma}\cdot(\overline{\boldsymbol{\kappa}}\times\boldsymbol{p}_i)\}
\end{aligned}
$$

7. Matrix calculation (III)

$$
\begin{aligned}
\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}\cdot\boldsymbol{p}_i\cdot &= -[\boldsymbol{\sigma}\times\nabla(\frac{1}{R})]\cdot\boldsymbol{p}_i \\
&= -\frac{1}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{\boldsymbol{\sigma}\times\nabla)\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R})\cdot\boldsymbol{p}_i \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{(\boldsymbol{\sigma}\times\boldsymbol{q})\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R})\cdot\boldsymbol{p}_i \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{(\boldsymbol{\sigma}\times\boldsymbol{q})\}\exp[i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}_i)]\cdot\boldsymbol{p}_i \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{(\boldsymbol{\sigma}\times\boldsymbol{q})\}\exp(i\boldsymbol{q}\cdot\boldsymbol{r})\cdot\exp(-i\boldsymbol{q}\cdot\boldsymbol{r}_i)\boldsymbol{p}_i \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{(\boldsymbol{\sigma}\times\boldsymbol{q})\}\exp(i\boldsymbol{q}\cdot\boldsymbol{r})\cdot\{\boldsymbol{p}_i\exp(-i\boldsymbol{q}\cdot\boldsymbol{r}_i)+\hbar\boldsymbol{q}\cdot\exp(-i\boldsymbol{q}\cdot\boldsymbol{r}_i)\} \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{(\boldsymbol{\sigma}\times\boldsymbol{q})\cdot\boldsymbol{p}_i\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R}) \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{\boldsymbol{p}_i\cdot(\boldsymbol{\sigma}\times\boldsymbol{q})\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R}) \\
&= \frac{-i}{2\pi^2}\int d\boldsymbol{q}\frac{1}{q^2}\{\boldsymbol{\sigma}\cdot(\boldsymbol{q}\times\boldsymbol{p}_i)\}\exp(i\boldsymbol{q}\cdot\boldsymbol{R})
\end{aligned}
$$

since we use the commutation relation

$$\{\boldsymbol{p}_i,\exp(-i\boldsymbol{q}\cdot\boldsymbol{r}_i)\} = -\hbar\boldsymbol{q}\cdot\exp(-i\boldsymbol{q}\cdot\boldsymbol{r}_i)$$

and the relation

$$(\boldsymbol{\sigma}\times\boldsymbol{q})\cdot\boldsymbol{q} = 0\,.$$

This expression is exactly the same as that of $\boldsymbol{p}_i\cdot\dfrac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}$. Then we have

$$(2\pi)^3\langle\boldsymbol{k}'|\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}\cdot\boldsymbol{p}_i|\boldsymbol{k}\rangle = \frac{4\pi i}{\kappa}e^{i\kappa\cdot\boldsymbol{r}_i}\{\boldsymbol{\sigma}\cdot(\overline{\boldsymbol{\kappa}}\times\boldsymbol{p}_i)\}$$

8. Definition of $Q_\perp$

Then we have

$$(2\pi)^3\langle \boldsymbol{k}'|[\frac{1}{\hbar}\boldsymbol{\sigma}\cdot\nabla\times\left(\frac{\boldsymbol{s}_i\times\boldsymbol{R}}{R^3}\right)-\frac{1}{2\hbar}\left(\boldsymbol{p}_i\cdot\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}+\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}\cdot\boldsymbol{p}_i\right)]|\boldsymbol{k}\sigma\rangle$$
$$=4\pi e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\boldsymbol{\sigma}\cdot[\overline{\boldsymbol{\kappa}}\times(\frac{\boldsymbol{s}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})-\frac{i}{\kappa\hbar}(\overline{\boldsymbol{\kappa}}\times\boldsymbol{p}_i)]$$
$$=4\pi\boldsymbol{\sigma}\cdot e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}[\overline{\boldsymbol{\kappa}}\times(\frac{\boldsymbol{s}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})+\frac{i}{\kappa}e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}(\frac{\boldsymbol{p}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})]$$

Here we define $\boldsymbol{Q}_\perp$ as

$$\boldsymbol{Q}_\perp=\sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}[\overline{\boldsymbol{\kappa}}\times(\frac{\boldsymbol{s}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})+\frac{i}{\kappa}(\frac{\boldsymbol{p}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})]$$
$$=\sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}[\overline{\boldsymbol{\kappa}}\times(\frac{\boldsymbol{s}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})-\frac{i}{\kappa}(\overline{\boldsymbol{\kappa}}\times\frac{\boldsymbol{p}_i}{\hbar})]$$
$$=\boldsymbol{Q}_{\perp\boldsymbol{S}}+\boldsymbol{Q}_{\perp\boldsymbol{L}}$$

Then we have

$$(2\pi)^3\sum_i\langle \boldsymbol{k}'|[\frac{1}{\hbar}\boldsymbol{\sigma}\cdot\nabla\times\left(\frac{\boldsymbol{s}_i\times\boldsymbol{R}}{R^3}\right)-\frac{1}{2\hbar}\left(\boldsymbol{p}_i\cdot\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}+\frac{\boldsymbol{\sigma}\times\boldsymbol{R}}{R^3}\cdot\boldsymbol{p}_i\right)]|\boldsymbol{k}\sigma\rangle$$
$$=4\pi\sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\boldsymbol{\sigma}\cdot[\overline{\boldsymbol{\kappa}}\times(\frac{\boldsymbol{s}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})-\frac{i}{\kappa\hbar}(\overline{\boldsymbol{\kappa}}\times\boldsymbol{p}_i)]$$
$$=4\pi\boldsymbol{\sigma}\cdot\boldsymbol{Q}_\perp$$

and the differential cross section is

$$\frac{d^2\sigma}{d\Omega d\varepsilon'}=\frac{k'}{k}\frac{(\gamma r_0)^2}{16\pi^2}16\pi^2\sum_{\lambda,\lambda',\sigma,\sigma'}P_\lambda P_\sigma\,|\langle\lambda'\sigma'|\boldsymbol{\sigma}\cdot\boldsymbol{Q}_\perp|\boldsymbol{k}\lambda\sigma\rangle|^2\ \delta(\hbar\omega+E_\lambda-E_{\lambda'})$$
$$=\frac{k'}{k}(\gamma r_0)^2\sum_{\lambda,\lambda',\sigma,\sigma'}P_\lambda P_\sigma\,|\langle\lambda'\sigma'|\boldsymbol{\sigma}\cdot\boldsymbol{Q}_\perp|\lambda\sigma\rangle|^2\ \delta(\hbar\omega+E_\lambda-E_{\lambda'})$$

9. Quenching of the orbital angular momentum

Here we consider the case when the orbital angular momentum is quenched. Therefoe we consider only the spin angular momentum.

$$\begin{aligned}\boldsymbol{Q}_\perp &= \sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}[\overline{\boldsymbol{\kappa}}\times(\frac{\boldsymbol{s}_i}{\hbar}\times\overline{\boldsymbol{\kappa}})] \\ &= \sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\frac{1}{\hbar}[(\overline{\boldsymbol{\kappa}}\cdot\overline{\boldsymbol{\kappa}})\boldsymbol{s}_i-(\boldsymbol{s}_i\cdot\overline{\boldsymbol{\kappa}}\cdot)\overline{\boldsymbol{\kappa}}] \\ &= \frac{1}{\hbar}\sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}[\boldsymbol{s}_i-(\boldsymbol{s}_i\cdot\overline{\boldsymbol{\kappa}}\cdot)\overline{\boldsymbol{\kappa}}]\end{aligned}$$

where we use the vector formula,

$$\boldsymbol{A}\times(\boldsymbol{B}\times\boldsymbol{C})=(\boldsymbol{A}\cdot\boldsymbol{C})\boldsymbol{B}-(\boldsymbol{A}\cdot\boldsymbol{B})\boldsymbol{C}$$

We define the spin density as

$$\sum_i \boldsymbol{s}_i\delta(\boldsymbol{r}-\boldsymbol{r}_i)\,.$$

and its Fourier transform as

$$\boldsymbol{Q}=\boldsymbol{S}(-\boldsymbol{\kappa})=\sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\boldsymbol{s}_i=\int e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}d\boldsymbol{r}\sum_i \boldsymbol{s}_i\delta(\boldsymbol{r}-\boldsymbol{r}_i)$$

The spin magnetization operator is given by

$$\boldsymbol{M}_S=-\frac{2\mu_B}{\hbar}\boldsymbol{Q}=-\frac{2\mu_B}{\hbar}S(-\boldsymbol{\kappa})=\sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}(-2\mu_B)\frac{\boldsymbol{s}_i}{\hbar}$$

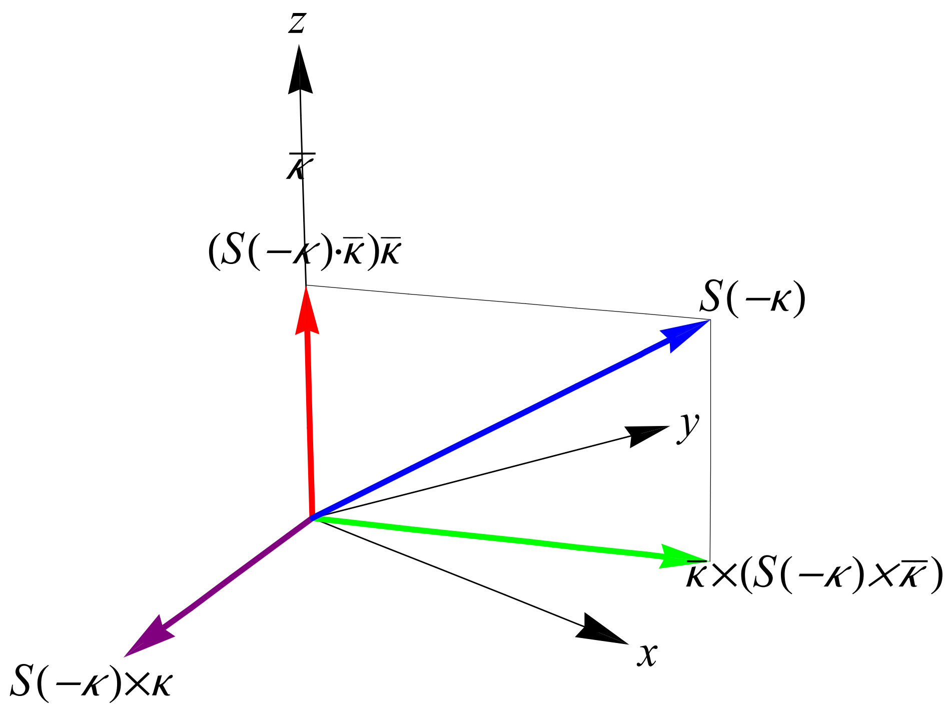
((Note)) We define the Fourier transform as

$$\boldsymbol{S}(\boldsymbol{\kappa})=\sum_i e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\boldsymbol{s}_i$$

Then we have

$$\boldsymbol{Q}_\perp=\boldsymbol{Q}-(\boldsymbol{Q}\cdot\overline{\boldsymbol{\kappa}})\overline{\boldsymbol{\kappa}}$$

We note



$$\boldsymbol{Q} = \boldsymbol{S}(-\boldsymbol{\kappa}) = \boldsymbol{Q}_\perp + \boldsymbol{Q}_{//}$$

$$\begin{aligned}\boldsymbol{Q}_\perp &= \overline{\boldsymbol{\kappa}} \times (\boldsymbol{Q} \times \overline{\boldsymbol{\kappa}}) \\ &= \boldsymbol{Q} - (\boldsymbol{Q} \cdot \overline{\boldsymbol{\kappa}})\overline{\boldsymbol{\kappa}}\end{aligned},$$

$$\boldsymbol{Q}_{//} = \overline{\boldsymbol{\kappa}}(\boldsymbol{Q} \cdot \overline{\boldsymbol{\kappa}})$$

Using these expressions, we get

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = (\gamma r_0)^2 \sum_{\lambda,\lambda',\sigma,\sigma'} P_\lambda P_\sigma \frac{k'}{k} |\langle \lambda'\sigma' | \boldsymbol{\sigma} \cdot \boldsymbol{Q}_\perp | \lambda\sigma \rangle|^2 \, \delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

Here we note that

$$
\begin{aligned}
K_1 &= \langle \lambda'\sigma' | \boldsymbol{\sigma}\cdot\boldsymbol{Q}_\perp | \lambda\sigma \rangle^* \langle \lambda'\sigma' | \boldsymbol{\sigma}\cdot\boldsymbol{Q}_\perp | \lambda\sigma \rangle \\
&= \langle \lambda\sigma | \boldsymbol{\sigma}\cdot\boldsymbol{Q}_\perp{}^+ | \lambda'\sigma' \rangle \langle \lambda'\sigma' | \boldsymbol{\sigma}\cdot\boldsymbol{Q}_\perp | \lambda\sigma \rangle \\
&= \sum_{\mu,\nu} \langle \lambda\sigma | \sigma_\mu Q_{\perp\mu}{}^+ | \lambda'\sigma' \rangle \langle \lambda'\sigma' | \sigma_\nu Q_{\perp\nu} | \lambda\sigma \rangle
\end{aligned}
$$

The energy of the system does not depend on the neutron polarization. We may sum over σ' to obtain

$$
\begin{aligned}
\frac{d^2\sigma}{d\Omega d\varepsilon'} &= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k} \\
&\quad \times \sum_{\mu,\nu} \langle \lambda | Q_{\perp\mu}{}^+ | \lambda' \rangle \langle \lambda' | Q_{\perp\nu} | \lambda \rangle \\
&\quad \times \sum_{\sigma,\sigma'} P_\sigma \langle \sigma | \sigma_\mu | \sigma' \rangle \langle \sigma' | \sigma_\nu | \sigma \rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'}) \\
&= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k} \\
&\quad \times \sum_{\mu,\nu} \langle \lambda | Q_{\perp\mu}{}^+ | \lambda' \rangle \langle \lambda' | Q_{\perp\nu}{}^+ | \lambda \rangle \\
&\quad \times \sum_{\sigma} P_\sigma \langle \sigma | \sigma_\mu \sigma_\nu | \sigma \rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'})
\end{aligned}
$$

where

$$
\sum_{\sigma'} \langle \sigma | \sigma_\mu | \sigma' \rangle \langle \sigma' | \sigma_\nu | \sigma \rangle = \langle \sigma | \sigma_\mu \sigma_\nu | \sigma \rangle
$$

Since

$$
\sum_{\sigma} P_\sigma \langle \sigma | \sigma_\mu \sigma_\nu | \sigma \rangle = \delta_{\mu\nu}
$$

with

$$
P_\sigma = \frac{1}{2}
$$

Then we have

$$\begin{aligned}
\frac{d^2\sigma}{d\Omega d\varepsilon'} &= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k} \sum_\mu \langle\lambda|Q_{\perp\mu}{}^+|\lambda'\rangle\langle\lambda'|Q_{\perp\mu}|\lambda\rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'}) \\
&= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k} \langle\lambda|\boldsymbol{Q}_\perp{}^+|\lambda'\rangle\cdot\langle\lambda'|\boldsymbol{Q}_\perp|\lambda\rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'}) \\
&= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k} \langle\lambda|\boldsymbol{Q}^+ - (\boldsymbol{Q}^+\cdot\bar{\boldsymbol{\kappa}})\bar{\boldsymbol{\kappa}}|\lambda'\rangle\cdot\langle\lambda'|\boldsymbol{Q} - (\boldsymbol{Q}\cdot\bar{\boldsymbol{\kappa}})\bar{\boldsymbol{\kappa}}|\lambda\rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'}) \\
&= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k} \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \bar{\kappa}_\alpha\bar{\kappa}_\beta)\langle\lambda|Q_\alpha{}^+|\lambda'\rangle\langle\lambda'|Q_\beta|\lambda\rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'})
\end{aligned}$$

Here we note that

$$\langle\lambda|\boldsymbol{Q}^+ - (\boldsymbol{Q}^+\cdot\bar{\boldsymbol{\kappa}})\bar{\boldsymbol{\kappa}}|\lambda'\rangle\cdot\langle\lambda'|\boldsymbol{Q} - (\boldsymbol{Q}\cdot\bar{\boldsymbol{\kappa}})\bar{\boldsymbol{\kappa}}|\lambda\rangle = \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \bar{\kappa}_\alpha\bar{\kappa}_\beta)\langle\lambda|Q_\alpha{}^+|\lambda'\rangle\langle\lambda'|Q_\beta|\lambda\rangle$$

where α and β stand for x, y, z, and $\delta_{\alpha\beta}$ is the Kronecker delta.

((Proof))

$$\begin{aligned}
\langle\lambda|\boldsymbol{Q}^+ - (\boldsymbol{Q}^+\cdot\bar{\boldsymbol{\kappa}})\bar{\boldsymbol{\kappa}}|\lambda'\rangle\cdot\langle\lambda'|\boldsymbol{Q} - (\boldsymbol{Q}\cdot\bar{\boldsymbol{\kappa}})\bar{\boldsymbol{\kappa}}|\lambda\rangle &= \sum_{\alpha,\beta} \{\langle\lambda|\boldsymbol{Q}^+|\lambda'\rangle - \bar{\kappa}_\alpha\langle\lambda|Q_\alpha{}^+|\lambda'\rangle\bar{\boldsymbol{\kappa}}\}\cdot\{\langle\lambda'|\boldsymbol{Q}|\lambda\rangle - \bar{\kappa}_\beta\langle\lambda|Q_\beta|\lambda'\rangle\bar{\boldsymbol{\kappa}}\} \\
&= \sum_{\alpha,\beta} \{\delta_{\alpha\beta}\langle\lambda|Q_\alpha{}^+|\lambda'\rangle\langle\lambda'|Q_\beta|\lambda\rangle - \bar{\kappa}_\alpha\bar{\kappa}_\beta\langle\lambda|Q_\alpha{}^+|\lambda'\rangle\langle\lambda|Q_\beta|\lambda'\rangle \\
&\quad - \bar{\kappa}_\alpha\bar{\kappa}_\beta\langle\lambda|Q_\alpha{}^+|\lambda'\rangle\langle\lambda'|Q_\beta|\lambda\rangle + \bar{\kappa}_\alpha\bar{\kappa}_\beta\langle\lambda|Q_\alpha{}^+|\lambda'\rangle\langle\lambda|Q_\beta|\lambda'\rangle\} \\
&= \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \bar{\kappa}_\alpha\bar{\kappa}_\beta)\langle\lambda|Q_\alpha{}^+|\lambda'\rangle\langle\lambda'|Q_\beta|\lambda\rangle
\end{aligned}$$

Then we have

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k} \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \bar{\kappa}_\alpha\bar{\kappa}_\beta)\langle\lambda|S_\alpha(\boldsymbol{\kappa})|\lambda'\rangle\langle\lambda'|S_\beta(-\boldsymbol{\kappa})|\lambda\rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

since

$$\boldsymbol{Q} = \boldsymbol{S}(-\boldsymbol{\kappa}) \qquad \text{and } \boldsymbol{Q}^+ = \boldsymbol{S}(\boldsymbol{\kappa})$$

10. Formulation

Using the formula for the Dirac function,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dt \exp[-i\left(\frac{\hbar\omega + E_\lambda - E_{\lambda'}}{\hbar}\right)t] = \delta(\frac{\hbar\omega + E_\lambda - E_{\lambda'}}{\hbar})$$
$$= \hbar\delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

or

$$\delta(\hbar\omega + E_\lambda - E_{\lambda'}) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} \exp[i(E_{\lambda'} - E_\lambda)\frac{t}{\hbar}]$$

we have

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \overline{\kappa}_\alpha\overline{\kappa}_\beta)\langle\lambda|S_\alpha(\boldsymbol{\kappa})|\lambda'\rangle\langle\lambda'|S_\beta(-\boldsymbol{\kappa})|\lambda\rangle\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt \exp[-i(\frac{\hbar\omega + E_\lambda - E_{\lambda'}}{\hbar})t]$$
$$= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \overline{\kappa}_\alpha\overline{\kappa}_\beta)\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t} \exp[i(\frac{-E_\lambda + E_{\lambda'}}{\hbar})t]\langle\lambda|S_\alpha(\boldsymbol{\kappa})|\lambda'\rangle\langle\lambda'|S_\beta(-\boldsymbol{\kappa})|\lambda\rangle$$
$$= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \overline{\kappa}_\alpha\overline{\kappa}_\beta)\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t}\langle\lambda|S_\alpha(\boldsymbol{\kappa})|\lambda'\rangle\langle\lambda'|(\frac{iHt}{\hbar})S_\beta(-\boldsymbol{\kappa})(-\frac{iHt}{\hbar})|\lambda\rangle$$
$$= (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \overline{\kappa}_\alpha\overline{\kappa}_\beta)\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t}\langle\lambda|S_\alpha(\boldsymbol{\kappa})|\lambda'\rangle\langle\lambda'|S_\beta(-\boldsymbol{\kappa},t)|\lambda\rangle$$

or

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \overline{\kappa}_\alpha\overline{\kappa}_\beta)\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt e^{-i\omega t}\langle\lambda|S_\alpha(\boldsymbol{\kappa})|\lambda'\rangle\langle\lambda'|S_\beta(-\boldsymbol{\kappa},t)|\lambda\rangle$$

where the Heisenberg operator is defined by

$$S_\alpha(-\boldsymbol{\kappa},t) = \exp(\frac{iHt}{\hbar})S_\alpha(-\boldsymbol{\kappa})\exp(-\frac{iHt}{\hbar})$$

and

$$H\left|\lambda\right\rangle = E_\lambda \left|\lambda\right\rangle,$$

where H is the Hamiltonian of the scattering system. We define the Fourier transform of the spin correlation function as

$$S^{\alpha\beta}(\kappa,\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dte^{-i\omega t}\left\langle\lambda\right|S_\alpha(\boldsymbol{\kappa})\left|\lambda'\right\rangle\left\langle\lambda'\right|S_\beta(-\boldsymbol{\kappa},t)\left|\lambda\right\rangle$$

Then we have

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \bar{\kappa}_\alpha\bar{\kappa}_\beta)S^{\alpha\beta}(\kappa,\omega)$$

---

11. Calculationof $\boldsymbol{Q}$

We now calculate $\boldsymbol{Q}$ defined by

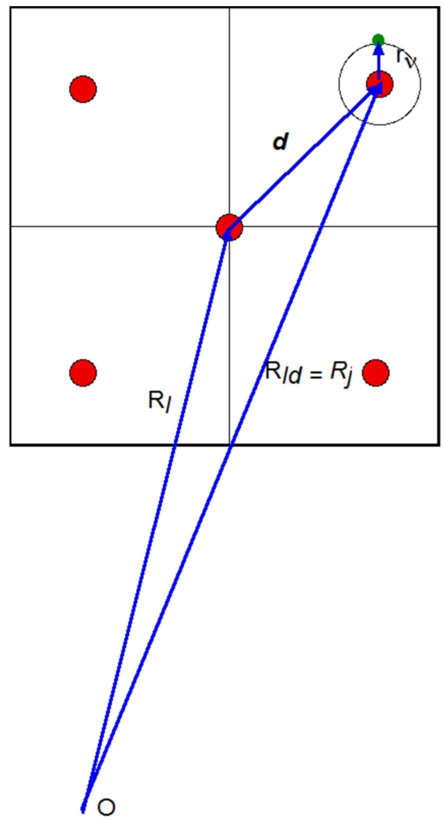
$$\boldsymbol{S}(-\boldsymbol{\kappa}) = \boldsymbol{Q} = \sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\boldsymbol{s}_i$$

with

$$\boldsymbol{r}_i = (\boldsymbol{R}_l + \boldsymbol{d}) + \boldsymbol{r}_\nu = \boldsymbol{R}_j + \boldsymbol{r}_\nu$$

The sum runs over all sites in the crystal.

$$\mathbf{Q} = \sum_i e^{i\boldsymbol{\kappa}\cdot\mathbf{r}_i}\mathbf{s}_i = \sum_{l,d} e^{i\boldsymbol{\kappa}\cdot(\mathbf{R}_l+\mathbf{d})}\sum_\nu e^{i\boldsymbol{\kappa}\cdot\mathbf{r}_\nu}\mathbf{s}_\nu$$



We show that

$$\left\langle \lambda' \middle| e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}} \sum_{\nu} e^{i\boldsymbol{\kappa}\cdot\mathbf{r}_{\nu}} \mathbf{s}_{\nu} \middle| \lambda \right\rangle = F_d(\boldsymbol{\kappa}) \left\langle \lambda' \middle| e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}} \mathbf{S}_{ld} \middle| \lambda \right\rangle \qquad (1)$$

where

$$\sum_{\nu} \hat{\boldsymbol{s}}_{\nu} = \hat{\boldsymbol{S}}_{ld}$$

12. Proof

A. Furrer, J. Mesort, and T. Strässle, Neutron scattering in condensed matter physics

The unpaired electrons on a given site will form a total spin $\boldsymbol{S}_{ld}$ according to the Hund's rule. The Wigner-Eckart theorem tells us that a matrix of the form $\langle \lambda' | \mathbf{s}_{\nu} | \lambda \rangle$ is proportional to $\langle \lambda' | \mathbf{S}_{ld} | \lambda \rangle$.

$$\langle \lambda' | \mathbf{S}(-\boldsymbol{\kappa}) | \lambda \rangle = \langle \lambda' | e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}} \sum_{\nu} e^{i\boldsymbol{\kappa}\cdot\mathbf{r}_{\nu}} \mathbf{s}_{\nu} | \lambda \rangle = \sum_{l,d} F_d(\boldsymbol{\kappa}) \langle \lambda' | e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}} \mathbf{S}_{ld} | \lambda \rangle$$

where $F_d(\boldsymbol{\kappa})$ is the Fourier transform of the normalized spin density nominated with the nth site and is referred to as the magnetic form factor.

Projection theorem (Wigner-Eckart theorem)

$$\langle \alpha'; j, m | \hat{\boldsymbol{V}}_q | \alpha; j, m' \rangle = \langle j, m | \hat{\boldsymbol{J}}_q | j, m' \rangle \frac{\langle \alpha'; j, m' | \hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{V}} | \alpha; j, m' \rangle}{\hbar^2 j(j+1)}$$

where $\hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{V}}$ is a scalar so its expectation value is independent of m.

$$\hat{\boldsymbol{V}} = \sum_{\nu} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_{\nu}} \hat{\boldsymbol{s}}_{\nu} \qquad \hat{\boldsymbol{J}} = \hat{\boldsymbol{S}}_j = \sum_{\nu} \hat{\boldsymbol{s}}_{\nu}$$

$$\hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{V}} = \sum_{\nu} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_{\nu}} \hat{\boldsymbol{s}}_{\nu} \cdot \boldsymbol{S}_j$$

$$\langle j, m | \sum_{\nu} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_{\nu}} \hat{\boldsymbol{s}}_{\nu} | j, m' \rangle = \langle j, m | \hat{\boldsymbol{S}}_j | j, m' \rangle \frac{\langle j, m' | \sum_{\nu} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_{\nu}} \hat{\boldsymbol{s}}_{\nu} \cdot \boldsymbol{S}_j | j, m' \rangle}{\hbar^2 j(j+1)}$$

The last term of this equation does not depend on the quantum number m. It does not depend on the direction of the spin and serves as a characteristic value for the magnetic scattering strength of the atom. This quantity is called the magnetic form factor $F_j(\boldsymbol{\kappa})$, which is obtained by the Fourier transform of the normalized spin density at the site j (or denoted by l, d)

$$\begin{aligned} \langle \lambda' | \boldsymbol{S}(-\boldsymbol{\kappa}) | \lambda \rangle = \langle \lambda' | \sum_{\nu} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_{\nu}} \hat{\boldsymbol{s}}_{\nu} | \lambda \rangle &= \langle \lambda' | \hat{\boldsymbol{S}}_{ld} | \lambda \rangle \frac{\langle \lambda | \sum_{\nu} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_{\nu}} \hat{\boldsymbol{s}}_{\nu} \cdot \boldsymbol{S}_{ld} | \lambda \rangle}{\hbar^2 S(S+1)} \\ &= F_d(\boldsymbol{\kappa}) \langle \lambda' | \hat{\boldsymbol{S}}_{ld} | \lambda \rangle \end{aligned}$$

where

$$F_d(\boldsymbol{\kappa}) = \frac{\langle \lambda | \sum_\nu e^{i\boldsymbol{\kappa}\cdot\mathbf{r}_\nu} \hat{\boldsymbol{s}}_\nu \cdot \boldsymbol{S}_{ld} | \lambda \rangle}{\hbar^2 S(S+1)}$$

13. Proof given by de Gennes

$$\overline{\boldsymbol{M}}_S = -\frac{2\mu_B}{\hbar}\overline{\boldsymbol{Q}} = -\frac{2\mu_B}{\hbar}\sum_i \overline{e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\boldsymbol{s}_i} = -\frac{2\mu_B}{\hbar}F(\boldsymbol{\kappa})\sum_i \boldsymbol{s}_i = -\frac{2\mu_B}{\hbar}F(\boldsymbol{\kappa})\boldsymbol{S}_j$$

with

$$\sum_i \overline{e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\boldsymbol{s}_i} = F(\boldsymbol{\kappa})\sum_i \boldsymbol{s}_i = F(\boldsymbol{\kappa})\boldsymbol{S}_j$$

14. Proof given by Squire

We put

$$f_\nu = e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_\nu}, \qquad g_{ld} = e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}}$$

Then the left-hand side of Eq.(1)

$$\langle \lambda' | e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}} \sum_\nu e^{i\boldsymbol{\kappa}\cdot\mathbf{r}_\nu} \mathbf{s}_\nu | \lambda \rangle = F_d(\boldsymbol{\kappa}) \langle \lambda' | e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}} \mathbf{S}_{ld} | \lambda \rangle \qquad (1)$$

is

$$\begin{aligned}
\langle \lambda' | g_{ld} \sum_\nu f_\nu \boldsymbol{s}_\nu | \lambda' \rangle &= \sum_\nu \langle \lambda' | f_\nu g_{ld} \boldsymbol{s}_\nu | \lambda' \rangle \\
&= \sum_{\nu,\lambda''} \langle \lambda' | f_\nu | \lambda'' \rangle \langle \lambda'' | g_{ld} \boldsymbol{s}_\nu | \lambda' \rangle \\
&= \sum_{\lambda''} \langle \lambda' | f_\nu | \lambda'' \rangle \langle \lambda'' | g_{ld} \sum_\nu \boldsymbol{s}_\nu | \lambda' \rangle
\end{aligned}$$

Note that the matrix element $\langle \lambda' | f_\nu | \lambda'' \rangle$ is independent of ν, since the electron space states are symmetric or anti-symmetric. f_ν depends only on the space variables of the electrons. Since the electron spin states and the nuclear position states are orthogonal, we have

$$\langle\lambda'|f_\nu|\lambda''\rangle = \langle\lambda'|f_\nu|\lambda''\rangle\delta_{\lambda',\lambda''}$$

$$\begin{aligned}
\langle\lambda'|g_{ld}\sum_\nu f_\nu \mathbf{s}_\nu|\lambda'\rangle &= \langle\lambda'|f_\nu|\lambda'\rangle\langle\lambda'|g_{ld}\sum_\nu \mathbf{s}_\nu|\lambda'\rangle \\
&= F_d(\boldsymbol{\kappa})\langle\lambda'|g_{ld}\sum_\nu \mathbf{s}_\nu|\lambda'\rangle \\
&= F_d(\boldsymbol{\kappa})\langle\lambda'|g_{ld}\mathbf{S}_{ld}|\lambda'\rangle \\
&= F_d(\boldsymbol{\kappa})\langle\lambda'|e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}}\mathbf{S}_{ld}|\lambda'\rangle
\end{aligned}$$

15. Magnetic form factor $F_d(\boldsymbol{\kappa})$

$F_d(\boldsymbol{\kappa})$ is the Fourier transform of the electron spin density around atom at $\boldsymbol{R}_j$,

$$F_d(\boldsymbol{\kappa}) = \frac{1}{Z}\int d\boldsymbol{r}\rho_m(\boldsymbol{r})e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}$$

where $\rho_m(\boldsymbol{r})/Z$ is the normalized spin density of the unpaired electrons and $\boldsymbol{r} = \boldsymbol{r}_\nu$.

16. Differential cross section (II)

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = (\gamma r_0)^2\sum_{\lambda,\lambda'}P_\lambda\frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta}-\overline{\kappa}_\alpha\overline{\kappa}_\beta)\langle\lambda|S_\alpha(\boldsymbol{\kappa})|\lambda'\rangle\langle\lambda'|S_\beta(-\boldsymbol{\kappa})|\lambda\rangle\delta(\hbar\omega+E_\lambda-E_{\lambda'})$$

Here we use

$$\langle\lambda'|\mathbf{S}_\beta(-\boldsymbol{\kappa})|\lambda\rangle = \sum_{l,d}F_d(\boldsymbol{\kappa})\langle\lambda'|e^{i\boldsymbol{\kappa}\cdot\mathbf{R}_{l,d}}\mathbf{S}_{ld}{}^\beta|\lambda\rangle$$

$$\langle\lambda|\mathbf{S}_\alpha(\boldsymbol{\kappa})|\lambda'\rangle = \langle\lambda'|\mathbf{S}_\alpha(-\boldsymbol{\kappa})|\lambda\rangle^* = \sum_{l,d}F_d(\boldsymbol{\kappa})^*\langle\lambda|e^{-i\boldsymbol{\kappa}\cdot\mathbf{R}_{ld}}\mathbf{S}_{l,d}{}^\alpha|\lambda'\rangle$$

Then we have the partial differential cross-section for the magnetic scattering by ions with only spin magnetic moment

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = (\gamma r_0)^2 \sum_{\lambda,\lambda'} P_\lambda \frac{k'}{k} \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \bar{\kappa}_\alpha \bar{\kappa}_\beta)$$
$$\times \sum_{ld} \sum_{l'd'} F_{d'}(\boldsymbol{\kappa})^* F_d(\boldsymbol{\kappa}) \langle \lambda | e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}} \boldsymbol{S}_{l'd'}{}^\alpha | \lambda' \rangle \langle \lambda' | e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}} \boldsymbol{S}_{ld}{}^\beta | \lambda \rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'})$$

Here we note that

$$\sum_{\lambda,\lambda'} P_\lambda \langle \lambda | e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}} \boldsymbol{S}_{l'd'}{}^\alpha | \lambda' \rangle \langle \lambda' | e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}} \boldsymbol{S}_{ld}{}^\beta | \lambda \rangle \delta(\hbar\omega + E_\lambda - E_{\lambda'})$$
$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \sum_{\lambda,\lambda'} P_\lambda \langle \lambda | e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}} \boldsymbol{S}_{l'd'}{}^\alpha | \lambda' \rangle \langle \lambda' | e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}} \boldsymbol{S}_{ld}{}^\beta | \lambda \rangle dt e^{-i\omega t} \exp[i(E_{\lambda'} - E_\lambda)\frac{t}{\hbar}]$$
$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \sum_{\lambda,\lambda'} P_\lambda \langle \lambda | e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}} \boldsymbol{S}_{l'd'}{}^\alpha | \lambda' \rangle \langle \lambda' | \exp(\frac{iHt}{\hbar}) e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}}$$
$$\exp(-\frac{iHt}{\hbar}) \exp(\frac{iHt}{\hbar}) \boldsymbol{S}_{ld}{}^\beta \exp(\frac{iHt}{\hbar}) | \lambda \rangle e^{-i\omega t} dt$$
$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \sum_{\lambda,\lambda'} P_\lambda \langle \lambda | e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}(0)} \boldsymbol{S}_{l'd'}{}^\alpha (0) | \lambda' \rangle \langle \lambda' | e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}(t)} \boldsymbol{S}_{ld}{}^\beta (t) | \lambda \rangle e^{-i\omega t} dt$$
$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \sum_{\lambda} P_\lambda \langle \lambda | e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}(0)} \boldsymbol{S}_{l'd'}{}^\alpha (0) e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}(t)} \boldsymbol{S}_{ld}{}^\beta (t) | \lambda \rangle e^{-i\omega t} dt$$
$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} < e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}(0)} \boldsymbol{S}_{l'd'}{}^\alpha (0) e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}(t)} \boldsymbol{S}_{ld}{}^\beta (t) > e^{-i\omega t} dt$$

Here we use the closure relation

$$\sum_{\lambda'} | \lambda' \rangle \langle \lambda' | = 1$$

The quantity < > in the last line is the thermal average of the operator enclosed at temperature *T*. The orientation of the electron spins have only a small effect on the interatomic force, and hence on the motion of the nuclei. Then we get

$$< e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}(0)} \boldsymbol{S}_{l'd'}{}^\alpha (0) e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}(t)} \boldsymbol{S}_{ld}{}^\beta (t) > = < e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}(0)} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}(t)} >< \boldsymbol{S}_{l'd'}{}^\alpha (0) \boldsymbol{S}_{ld}{}^\beta (t) >$$

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = \frac{(\gamma r_0)^2}{2\pi\hbar}\frac{k'}{k}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \overline{\kappa}_\alpha\overline{\kappa}_\beta)\sum_{ld}\sum_{l'd'}\frac{1}{4}g_{d'}dg_d F_{d'}(\boldsymbol{\kappa})^* F_d(\boldsymbol{\kappa})$$
$$\times \int_{-\infty}^{\infty} < e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{l'd'}(0)} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}_{ld}(t)} >< \boldsymbol{S}_{l'd'}{}^{\alpha}(0)\boldsymbol{S}_{ld}{}^{\beta}(t) > e^{-i\omega t}dt$$

17. Bravais lattice

For a Bravais crystal, we have

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = \frac{(\gamma r_0)^2}{2\pi\hbar}\frac{k'}{k}N\{\frac{1}{2}gF(\boldsymbol{\kappa})\}^2\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \overline{\kappa}_\alpha\overline{\kappa}_\beta)\sum_{l} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{l}}$$
$$\times$$
$$\int_{-\infty}^{\infty} < e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{u}_0(0)} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{u}_l(t)} >< \boldsymbol{S}_0{}^{\alpha}(0)\boldsymbol{S}_l{}^{\beta}(t) > e^{-i\omega t}dt$$

where $\boldsymbol{u}_l(t)$ is the displacement of nucleus l from its equilibrium position.

18. Elastic magnetic scattering

In the limit of $t\rightarrow\infty$,

$$< \boldsymbol{S}_0{}^{\alpha}(0)\boldsymbol{S}_l{}^{\beta}(t) >=< \boldsymbol{S}_0{}^{\alpha}\boldsymbol{S}_l{}^{\beta} >$$

$$\frac{d^2\sigma}{d\Omega d\varepsilon'} = \frac{(\gamma r_0)^2}{2\pi\hbar}\frac{k'}{k}N\{\frac{1}{2}gF(\boldsymbol{\kappa})\}^2 e^{-2W}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \overline{\kappa}_\alpha\overline{\kappa}_\beta)\sum_{l} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{l}} < \boldsymbol{S}_0{}^{\alpha}\boldsymbol{S}_l{}^{\beta} > 2\pi\delta(\omega)$$

where

$$\int_{-\infty}^{\infty} e^{-i\omega t}dt = 2\pi\delta(\omega)$$

$$< e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{u}_0(0)} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{u}_l(0)} >= \exp(-2W)$$

W is the Debye-Waller factor. Integrating of the differential cross section with respect to ε'.we get

$$\frac{d^2\sigma}{d\Omega} = (\gamma r_0)^2 N\{\frac{1}{2}gF(\boldsymbol{\kappa})\}^2 e^{-2W}\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \bar{\kappa}_\alpha\bar{\kappa}_\beta)\sum_l e^{i\boldsymbol{\kappa}\cdot\boldsymbol{l}} < \boldsymbol{S}_0{}^\alpha \boldsymbol{S}_l{}^\beta >$$

10 The limit of $\boldsymbol{\kappa} \to 0$

$$\begin{aligned}
\boldsymbol{Q}_\perp &= \sum_i e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}[\bar{\boldsymbol{\kappa}} \times (\frac{\boldsymbol{s}_i}{\hbar} \times \bar{\boldsymbol{\kappa}}) - \frac{i}{\kappa}(\bar{\boldsymbol{\kappa}} \times \frac{\boldsymbol{p}_i}{\hbar})] \\
&= \sum_i (\frac{2}{3}\frac{\boldsymbol{s}_i}{\hbar} + \frac{1}{3\hbar}\boldsymbol{l}_i) \\
&= \frac{1}{3\hbar}\sum_i (2\boldsymbol{s}_i + \boldsymbol{l}_i)
\end{aligned}$$

Note that

$\mu_B \sum_i \frac{(2\boldsymbol{s}_i + \boldsymbol{l}_i)}{\hbar}$ is the total magnetic moment of electrons.

where

$$e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}\frac{1}{\kappa}(\bar{\boldsymbol{\kappa}} \times \frac{\boldsymbol{p}_i}{\hbar}) \approx \frac{1}{3}i\frac{(\boldsymbol{r}_i \times \boldsymbol{p}_i)}{\hbar} = \frac{1}{3\hbar}i\boldsymbol{l}_i$$

This shows that the forward scattering cross section is proportional to the total magnetic moment of the electron.
((**Note**-1))

$$\begin{aligned}
\bar{\boldsymbol{\kappa}} \times (\frac{\boldsymbol{s}_i}{\hbar} \times \bar{\boldsymbol{\kappa}}) &= \frac{1}{\hbar}[\boldsymbol{s}_i - (\bar{\boldsymbol{\kappa}} \cdot \boldsymbol{s}_i)\bar{\boldsymbol{\kappa}}] \\
&= \frac{1}{\hbar}[\boldsymbol{s}_i - (\bar{\boldsymbol{\kappa}} \cdot \boldsymbol{s}_i)\bar{\boldsymbol{\kappa}}] \\
&\approx \frac{1}{\hbar}(\boldsymbol{s}_i - \frac{1}{3}\boldsymbol{s}_i) = \frac{2}{3\hbar}\boldsymbol{s}_i
\end{aligned}$$

Suppose that $\boldsymbol{s}_i = (0, 0, s_i)$ and $\bar{\boldsymbol{\kappa}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$.

$$(\bar{\boldsymbol{\kappa}} \cdot \boldsymbol{s}_i)\bar{\boldsymbol{\kappa}} = s_i\cos\theta(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

$$(\overline{\boldsymbol{\kappa}}\cdot\boldsymbol{s}_i)\overline{\boldsymbol{\kappa}}\to\frac{1}{3}s_i(0,0,1)=\frac{1}{3}\boldsymbol{s}_i$$

((**Note-2**))

$$e^{i\kappa\cdot r_i}\frac{1}{\kappa}(\overline{\boldsymbol{\kappa}}\times\boldsymbol{p}_i)\approx[1+i(\boldsymbol{\kappa}\cdot\boldsymbol{r}_i)+...]\frac{1}{\kappa^2}(\boldsymbol{\kappa}\times\boldsymbol{p}_i)$$
$$=\frac{1}{\kappa^2}(\boldsymbol{\kappa}\times\boldsymbol{p}_i)+i\frac{\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}{\kappa^2}(\boldsymbol{\kappa}\times\boldsymbol{p}_i)$$

We take the mean value of the limit as $\boldsymbol{\kappa}\to 0$. In this limit,

$$e^{i\kappa\cdot r_i}\frac{1}{\kappa}(\overline{\boldsymbol{\kappa}}\times\boldsymbol{p}_i)\approx\frac{1}{3}i(\boldsymbol{r}_i\times\boldsymbol{p}_i)=\frac{i\boldsymbol{L}_i}{3}$$

where $\boldsymbol{L}_i$ is the orbital angular momentum.

((**Note-3**))
Suppose that $\boldsymbol{r}_i=(0,0,r_i)$ and $\boldsymbol{\kappa}=\kappa(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$.
(i)

$$\frac{\boldsymbol{\kappa}}{\kappa^2}=\frac{1}{\kappa}(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$$

tends to

$$\frac{\boldsymbol{\kappa}}{\kappa^2}\to(0,0,0)$$

(ii)

$$\frac{\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}{\kappa^2}\boldsymbol{\kappa}=r_i\cos\theta(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$$
$$=r_i(\sin\theta\cos\theta\cos\phi,\sin\theta\cos\theta\sin\phi,\cos^2\theta),$$

tends to

$$\frac{\boldsymbol{\kappa}\cdot\boldsymbol{r}_i}{\kappa^2}\boldsymbol{\kappa}\rightarrow\frac{1}{3}r_i(0,0,1)=\frac{1}{3}\boldsymbol{r}_i$$

since

$$\frac{1}{4\pi}\int_0^{\pi}\sin^2\theta\cos\theta d\theta\int_0^{2\pi}\cos\phi d\phi=0,\qquad \frac{1}{4\pi}\int_0^{\pi}\sin^2\theta\cos\theta d\theta\int_0^{2\pi}\sin\phi d\phi=0$$

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

____\p.51

For N identical spins (un-polarized neutron), the cross section is given by

$$\frac{d^2\sigma}{d\Omega d\varepsilon'}=\frac{k'}{k}N(\gamma r_0)^2\{\frac{1}{2}gF(\boldsymbol{\kappa})\}^2\sum_{\alpha,\beta}(\delta_{\alpha\beta}-\hat{\kappa}_\alpha\hat{\kappa}_\beta)S^{\alpha\beta}(\boldsymbol{\kappa},\omega)$$

and $F(\boldsymbol{\kappa})$ is the magnetic form factor.

$$S^{\alpha\beta}(\kappa,\omega)=\frac{1}{2\pi N}\sum_{\boldsymbol{r},\boldsymbol{r}'}\int_{-\infty}^{\infty}d\tau e^{-i\omega\tau}e^{i\boldsymbol{\kappa}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\left\langle\hat{S}_{\boldsymbol{r}'}^{\alpha}(0)\hat{S}_{\boldsymbol{r}}^{\beta}(t)\right\rangle$$

Here we use the Heisenberg representation. We also introduce the Fourier transform,

$$\hat{S}_{\boldsymbol{r}}^{\alpha}(t)=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{q}}e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\hat{S}_{\boldsymbol{q}}^{\alpha}(t),$$

$$\hat{S}_{\boldsymbol{q}}^{\alpha}(t)=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{r}}e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\hat{S}_{\boldsymbol{r}}^{\alpha}(t).$$

Then we get

$$\begin{aligned}\sum_{\boldsymbol{r},\boldsymbol{r}'} e^{i\boldsymbol{\kappa}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\left\langle \hat{S}^{\alpha}_{\boldsymbol{r}'}(0)\hat{S}^{\beta}_{\boldsymbol{r}}(t)\right\rangle &= \frac{1}{N}\sum_{\boldsymbol{r},\boldsymbol{r}'} e^{i\boldsymbol{\kappa}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\sum_{\boldsymbol{q},\boldsymbol{q}'} e^{-i\boldsymbol{q}'\cdot\boldsymbol{r}'}e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\left\langle \hat{S}^{\alpha}_{\boldsymbol{q}'}(0)\hat{S}^{\beta}_{\boldsymbol{q}}(t)\right\rangle \\ &= \frac{1}{N}\sum_{\boldsymbol{q},\boldsymbol{q}'}\left\langle \hat{S}^{\alpha}_{\boldsymbol{q}'}(0)\hat{S}^{\beta}_{\boldsymbol{q}}(t)\right\rangle \sum_{\boldsymbol{r}'} e^{-i(\boldsymbol{\kappa}+\boldsymbol{q}')\cdot\boldsymbol{r}}\sum_{\boldsymbol{r}} e^{i(\boldsymbol{\kappa}-\boldsymbol{q})\cdot\boldsymbol{r}} \\ &= N\sum_{\boldsymbol{q},\boldsymbol{q}'}\left\langle \hat{S}^{\alpha}_{\boldsymbol{q}'}(0)\hat{S}^{\beta}_{\boldsymbol{q}}(t)\right\rangle \delta(\boldsymbol{\kappa}+\boldsymbol{q}')\delta(\boldsymbol{\kappa}-\boldsymbol{q}') \\ &= N\left\langle \hat{S}^{\alpha}_{-\boldsymbol{\kappa}}(0)\hat{S}^{\beta}_{\boldsymbol{\kappa}}(t)\right\rangle\end{aligned}.$$

Therefore we have

$$S^{\alpha\beta}(\kappa,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau e^{-i\omega\tau} d\tau\left\langle \hat{S}^{\alpha}_{-\boldsymbol{\kappa}}(0)\hat{S}^{\beta}_{\boldsymbol{\kappa}}(\tau)\right\rangle$$

It is clear from this equation that

$$\int_{-\infty}^{\infty} S^{\alpha\beta}(\boldsymbol{\kappa},\omega)d\omega = \left\langle \hat{S}^{\alpha}_{-\boldsymbol{\kappa}}(0)\hat{S}^{\beta}_{\boldsymbol{\kappa}}(0)\right\rangle. \qquad \text{(static correlation function)}$$

It is quite possible to measure the neutron scattering cross section as a function of ω keeping $\boldsymbol{\kappa}$ fixed, so we can derive the static correlation function by integrating over ω of the measured magnetic scattering function.

3. Measure of static correlation functions

The static approximation

There is a problem with this process, however, in that the measurements cannot in practice be taken over an infinite range of ω. So that we cannot evaluate the contribution to the integral for all values of ω.

(1) Accurate measurements can only be taken if there is a good signal-to-noise ratio and if the weight of the integral is concentrated over a relatively narrow range of ω. There is reason to hope that this latter condition might be reasonably satisfied near

the critical point, since the characteristic frequency ω_c tends to zero at the critical point.

(2) There is a second way in which we can attempt to extract the static correlation function from neutron-scattering measurements. This involves measuring the differential magnetic cross section rather than the partial differential magnetic cross section.

That is, we measure all the neutrons scattered into solid angle dΩ without regard to energy. This is easy to do in practice since it just involves using a detector with angular size dΩ.

$$\frac{d\sigma_s}{d\Omega} = \frac{N}{k}(\gamma r_0)^2 \int_0^\infty d\varepsilon' k' \{\frac{1}{2} gF(\boldsymbol{\kappa})\}^2 \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) S^{\alpha\beta}(\boldsymbol{\kappa}, \omega)$$

This integral involves k', k, and ω that vary with ε'.

$$\varepsilon' = \frac{\hbar^2 k'^2}{2M_n}, \qquad k' = \sqrt{\frac{2M_n \varepsilon'}{\hbar^2}}$$

$$\varepsilon' = \varepsilon - \hbar\omega, \qquad \hbar\omega = \varepsilon - \varepsilon'$$

$$\boldsymbol{\kappa} = \boldsymbol{k} - \boldsymbol{k}'$$

Clearly we cannot, in general, evaluate this integral unless we know the scattering function, and this is what we are trying to measure! There is one circumstance, however, in which matters simplify;

This is if all the weight of $S^{\alpha\beta}(\kappa, \omega)$ is at low frequencies such that

$$\hbar\omega << \varepsilon$$

If this is the case, it will be an excellent approximation to evaluate the integral with $\boldsymbol{k}$' and $\boldsymbol{k}$ held constant (such that $|\boldsymbol{k}'| = |\boldsymbol{k}|$),

$$\frac{d\sigma_s}{d\Omega} \approx N(\gamma r_0)^2 \{\frac{1}{2} gF(\boldsymbol{\kappa})\}^2 \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \left\langle \hat{S}^\alpha_{-\boldsymbol{\kappa}}(0) \hat{S}^\beta_{\boldsymbol{\kappa}}(0) \right\rangle$$

The approximation ($\hbar\omega << \varepsilon$) for all ω that contributes significantly to the scattering in the correlation function is known as the *static approximation*, because it gives the static correlation function. This approximation is equivalent to assuming that the spin vectors S have not have the time to change during the time it takes the neutron to cross an atom, so that the diffraction pattern corresponds to a “static set of spins.

((Advantage))

$\frac{d\sigma_s}{d\Omega}$ can be measured more easily and more accurately than $\frac{d^2\sigma}{d\Omega d\varepsilon'}$.

((Disadvantage))

We do not normally know how good the static approximation is.

To determine the spin correlation from

(1) $\frac{d^2\sigma_s}{d\Omega d\varepsilon'}$, $\hbar\omega = \varepsilon - \varepsilon'$ (quasi-elastic scattering)

(2)

$$\frac{d\sigma_s}{d\Omega} = \int_0^\infty \frac{d^2\sigma}{d\Omega d\varepsilon'} d\varepsilon' \approx N(\gamma r_0)^2 \{\frac{1}{2} gF(\kappa)\}^2 \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \left\langle \hat{S}_{-\kappa}^\alpha(0) \hat{S}_\kappa^\beta(0) \right\rangle$$

(static approximation)

6. Expression of $\frac{d\sigma_s}{d\Omega}$

$$\frac{d\sigma_s}{d\Omega} = N(\gamma r_0)^2 \{\frac{1}{2} gF(\boldsymbol{\kappa})\}^2 \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \left\langle \hat{S}_{-\boldsymbol{\kappa}}^\alpha(0) \hat{S}_{\boldsymbol{\kappa}}^\beta(0) \right\rangle$$

Note that

$$\hat{S}_{\boldsymbol{\kappa}}^\alpha(0) = \frac{1}{\sqrt{N}} \sum_j e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_j} \hat{S}_j^\alpha(0)$$

and

$$\left\langle \hat{S}_{-\boldsymbol{\kappa}}^{\alpha}(0)\hat{S}_{\boldsymbol{\kappa}}^{\beta}(0)\right\rangle = \frac{1}{N}\sum_{i,j} e^{-i\boldsymbol{\kappa}\cdot\boldsymbol{r}_i} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_j}\left\langle \hat{S}_i^{\alpha}(0)\hat{S}_j^{\alpha}(0)\right\rangle$$

$$= \frac{1}{N}\sum_{i,j} e^{-i\boldsymbol{\kappa}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}\left\langle \hat{S}_i^{\alpha}(0)\hat{S}_j^{\alpha}(0)\right\rangle$$

In this case, $\frac{d\sigma_s}{d\Omega}$ can be rewritten as

$$\frac{d\sigma_s}{d\Omega} = (\gamma r_0)^2\{\frac{1}{2}gf(\kappa)\}^2\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \hat{\kappa}_\alpha\hat{\kappa}_\beta)\sum_{i,j} e^{i\kappa\cdot(\mathbf{r}_j-\mathbf{r}_i)}\left\langle \hat{S}_i^{\alpha}(0)\hat{S}_j^{\beta}(0)\right\rangle$$

Here we put

$$F_\alpha(\kappa) = \gamma r_0\{\frac{1}{2}gf(\boldsymbol{\kappa})\}\sum_j e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_j}\hat{S}_j^{\alpha}(0)$$

which corresponds to the magnetic form factor. Then we have

$$\frac{d\sigma_s}{d\Omega} = \sum_{\alpha,\beta}(\delta_{\alpha\beta} - \hat{\kappa}_\alpha\hat{\kappa}_\beta)\left\langle F_\alpha^{\;*}(\boldsymbol{\kappa})F_\beta(\boldsymbol{\kappa})\right\rangle$$

(1) For $\hat{\kappa} \perp \hat{z}$

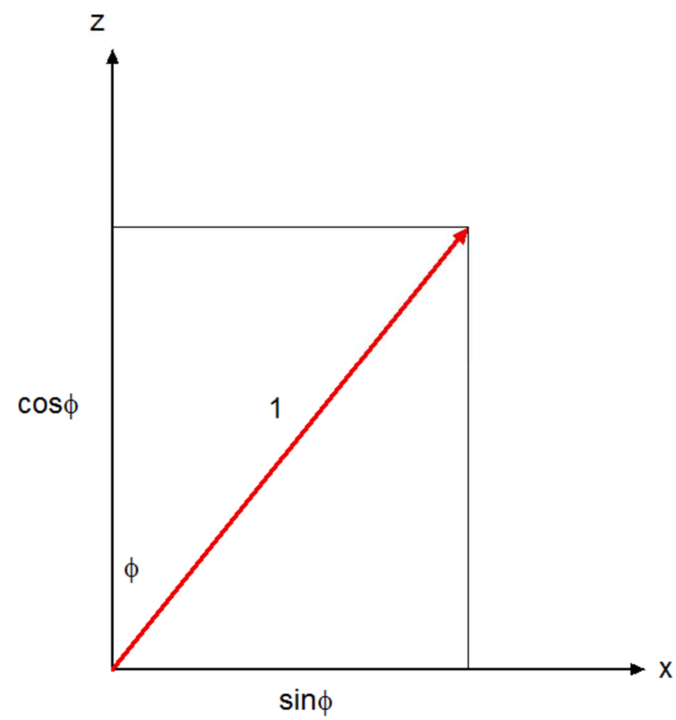
$$\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \hat{\kappa}_\alpha\hat{\kappa}_\beta)F_\alpha^{\;*}(\boldsymbol{\kappa})F_\beta(\boldsymbol{\kappa})$$
$$= \sum_\alpha F_\alpha^{\;*}(\boldsymbol{\kappa})F_\alpha(\boldsymbol{\kappa}) - F_z^{\;*}(\boldsymbol{\kappa})F_z(\boldsymbol{\kappa})$$
$$= F_x^{\;*}(\boldsymbol{\kappa})F_x(\boldsymbol{\kappa}) + F_y^{\;*}(\boldsymbol{\kappa})F_y(\boldsymbol{\kappa}) = 2\left|F_\perp(\boldsymbol{\kappa})\right|^2$$

(2) For $\hat{\kappa} \perp \hat{x}$

$$
\begin{aligned}
&\sum_{\alpha,\beta}(\delta_{\alpha\beta}-\hat{\kappa}_\alpha\hat{\kappa}_\beta)F_\alpha^*(\boldsymbol{\kappa})F_\beta(\boldsymbol{\kappa})\\
&=\sum_\alpha F_\alpha^*(\boldsymbol{\kappa})F_\alpha(\boldsymbol{\kappa})-F_x^*(\boldsymbol{\kappa})F_x(\boldsymbol{\kappa})\\
&=F_y^*(\boldsymbol{\kappa})F_y(\boldsymbol{\kappa})+F_z^*(\boldsymbol{\kappa})F_z(\boldsymbol{\kappa})^2
\end{aligned}
$$

(3)

$\hat{\kappa}_x=\sin\phi$, $\hat{\kappa}_z=\cos\phi$, $\hat{\kappa}_y=\cos\phi$



$$
\begin{aligned}
\sum_{\alpha,\beta}(\delta_{\alpha\beta}-\hat{\kappa}_\alpha\hat{\kappa}_\beta)F_\alpha^*(\boldsymbol{\kappa})F_\beta(\boldsymbol{\kappa}) &=\sum_\alpha|F_\alpha(\boldsymbol{\kappa})|^2-\sum_\alpha\hat{\kappa}_\alpha F_\alpha^*(\boldsymbol{\kappa})\sum_\beta\hat{\kappa}_\beta F_\beta(\boldsymbol{\kappa})\\
&=|F_x(\boldsymbol{\kappa})|^2+|F_y(\boldsymbol{\kappa})|^2+|F_z(\boldsymbol{\kappa})|^2\\
&-[\hat{\kappa}_xF_x^*(\boldsymbol{\kappa})+\hat{\kappa}_zF_z^*(\boldsymbol{\kappa})][\hat{\kappa}_xF_x(\boldsymbol{\kappa})+\hat{\kappa}_zF_z(\boldsymbol{\kappa})]\\
&=(1-\hat{\kappa}_x{}^2)|F_x(\boldsymbol{\kappa})|^2+(1-\hat{\kappa}_z{}^2)|F_z(\boldsymbol{\kappa})|^2+|F_y(\boldsymbol{\kappa})|^2
\end{aligned}
$$

where the cross terms are assumed to be equal to zero. Suppose that

$$\left|F_x(\boldsymbol{\kappa})\right|^2 = \left|F_y(\boldsymbol{\kappa})\right|^2 .$$

Then we have

$$\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \hat{\kappa}_\alpha\hat{\kappa}_\beta)F_\alpha^{\ *}(\boldsymbol{\kappa})F_\beta(\boldsymbol{\kappa}) = (2-\hat{\kappa}_x^{\ 2})\left|F_x(\boldsymbol{\kappa})\right|^2 + (1-\hat{\kappa}_z^{\ 2})\left|F_z(\boldsymbol{\kappa})\right|^2$$

$$= (2-\sin^2\phi)\left|F_x(\boldsymbol{\kappa})\right|^2 + (1-\cos^2\phi)\left|F_z(\boldsymbol{\kappa})\right|^2$$

$$= (1+\cos^2\phi)\left|F_x(\boldsymbol{\kappa})\right|^2 + \sin^2\phi)\left|F_z(\boldsymbol{\kappa})\right|^2$$

5. Bragg scattering and diffuse scattering

$$\frac{d\sigma_s}{d\Omega} = N(\gamma r_0)^2\{\frac{1}{2}gf(\boldsymbol{\kappa})\}^2\sum_{\alpha,\beta}(\delta_{\alpha\beta} - \hat{\kappa}_\alpha\hat{\kappa}_\beta)\sum_{\boldsymbol{r}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\left\langle \hat{S}_0^\alpha(0)\hat{S}_{\boldsymbol{r}}^\beta(0)\right\rangle$$

The spin correlation function

$$\left\langle \hat{S}_0^\alpha(0)\hat{S}_{\boldsymbol{r}}^\beta(0)\right\rangle = \left\langle \hat{S}_0^\alpha\hat{S}_{\boldsymbol{r}}^\beta\right\rangle$$

$$= \left\langle (\hat{S}_0^\alpha - \left\langle \hat{S}_0^\alpha\right\rangle)(\hat{S}_{\boldsymbol{r}}^\beta - \left\langle \hat{S}_{\boldsymbol{r}}^\beta\right\rangle)\right\rangle + \left\langle \hat{S}_0^\alpha\right\rangle\left\langle \hat{S}_{\boldsymbol{r}}^\beta\right\rangle$$

$$= \left\langle \Delta\hat{S}_0^\alpha\Delta\hat{S}_{\boldsymbol{r}}^\beta\right\rangle + \left\langle \hat{S}_0^\alpha\right\rangle\left\langle \hat{S}_{\boldsymbol{r}}^\beta\right\rangle$$

For convenience, we introduce the notation

$$C^{\alpha\beta}(\boldsymbol{r}) = \left\langle \Delta\hat{S}_0^\alpha\Delta\hat{S}_{\boldsymbol{r}}^\beta\right\rangle \qquad \text{(spin correlation function)}$$

Then we get

$$\sum_{\boldsymbol{r}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\left\langle \hat{S}_0^\alpha(0)\hat{S}_{\boldsymbol{r}}^\beta(0)\right\rangle = \sum_{\boldsymbol{r}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\left\langle \hat{S}_0^\alpha\right\rangle\left\langle \hat{S}_{\boldsymbol{r}}^\beta\right\rangle + \sum_{\boldsymbol{r}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}C^{\alpha\beta}(\boldsymbol{r})$$

which consists of the magnetic Bragg scattering and the magnetic diffuse scattering.

6. Expression of the diffuse scattering

What is the expression of the magnetic Bragg scattering in the reciprocal lattice?

$$I_1 = \sum_{\boldsymbol{r}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}} \left\langle \hat{S}_0^{\alpha} \right\rangle \left\langle \hat{S}_{\boldsymbol{r}}^{\beta} \right\rangle$$

Since

$$\hat{S}_{\boldsymbol{r}}^{\beta} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{q}'} e^{-i\boldsymbol{q}'\cdot\boldsymbol{r}} \hat{S}_{\boldsymbol{q}'}^{\beta} , \qquad \hat{S}_0^{\alpha} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{q}} \hat{S}_{\boldsymbol{q}}^{\alpha}$$

$$\begin{aligned} I_1 &= \frac{1}{N} \sum_{\boldsymbol{r}} \sum_{\boldsymbol{q},\boldsymbol{q}'} e^{i(\boldsymbol{\kappa}-\boldsymbol{q}')\cdot\boldsymbol{r}} \left\langle \hat{S}_{\boldsymbol{q}}^{\alpha} \right\rangle \left\langle \hat{S}_{\boldsymbol{q}'}^{\beta} \right\rangle \} \\ &= \sum_{\boldsymbol{q},\boldsymbol{q}'} \delta(\boldsymbol{\kappa}-\boldsymbol{q}') \left\langle \hat{S}_{\boldsymbol{q}}^{\alpha} \right\rangle \left\langle \hat{S}_{\boldsymbol{q}'}^{\beta} \right\rangle \} \\ &= \sum_{\boldsymbol{q}} \left\langle \hat{S}_{\boldsymbol{q}}^{\alpha} \right\rangle \left\langle \hat{S}_{\boldsymbol{\kappa}}^{\beta} \right\rangle \end{aligned}$$

What is the expression of the magnetic diffuse scattering in the reciprocal lattice?

$$\begin{aligned} I_2 &= \sum_{\boldsymbol{r}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}} C^{\alpha\beta}(\boldsymbol{r}) \\ &= \sum_{\boldsymbol{r}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}} \left\langle \Delta\hat{S}_0^{\alpha} \Delta\hat{S}_{\boldsymbol{r}}^{\beta} \right\rangle \\ &= \sum_{\boldsymbol{r}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}} \{ \left\langle \hat{S}_0^{\alpha} \hat{S}_{\boldsymbol{r}}^{\beta} \right\rangle - \left\langle \hat{S}_0^{\alpha} \right\rangle \left\langle \hat{S}_{\boldsymbol{r}}^{\beta} \right\rangle \} \end{aligned}$$

Since

$$\hat{S}_{\boldsymbol{r}}^{\beta} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{q}'} e^{-i\boldsymbol{q}'\cdot\boldsymbol{r}} \hat{S}_{\boldsymbol{q}'}^{\beta} , \qquad \hat{S}_0^{\alpha} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{q}} \hat{S}_{\boldsymbol{q}}^{\alpha}$$

$$
\begin{aligned}
I_2 &= \frac{1}{N}\sum_{\boldsymbol{r}}\sum_{\boldsymbol{q},\boldsymbol{q}'} e^{i(\boldsymbol{\kappa}-\boldsymbol{q}')\cdot\boldsymbol{r}}\{\left\langle \hat{S}^{\alpha}_{\boldsymbol{q}}\hat{S}^{\beta}_{\boldsymbol{q}'}\right\rangle - \left\langle \hat{S}^{\alpha}_{\boldsymbol{q}}\right\rangle\left\langle \hat{S}^{\beta}_{\boldsymbol{q}'}\right\rangle\} \\
&= \sum_{\boldsymbol{q},\boldsymbol{q}'}\delta(\boldsymbol{\kappa}-\boldsymbol{q}')\{\left\langle \hat{S}^{\alpha}_{\boldsymbol{q}}\hat{S}^{\beta}_{\boldsymbol{q}'}\right\rangle - \left\langle \hat{S}^{\alpha}_{\boldsymbol{q}}\right\rangle\left\langle \hat{S}^{\beta}_{\boldsymbol{q}'}\right\rangle\} \\
&= \sum_{\boldsymbol{q}}\{\left\langle \hat{S}^{\alpha}_{\boldsymbol{q}}\hat{S}^{\beta}_{\boldsymbol{\kappa}}\right\rangle - \left\langle \hat{S}^{\alpha}_{\boldsymbol{q}}\right\rangle\left\langle \hat{S}^{\beta}_{\boldsymbol{\kappa}}\right\rangle\} \\
&= \sum_{\boldsymbol{q}}\{\Delta\hat{S}^{\alpha}_{\boldsymbol{q}}\Delta\hat{S}^{\beta}_{\boldsymbol{\kappa}}\}
\end{aligned}
$$

7. $F_\alpha(\kappa)$ for the ferromagnet

For the ferromagnetic systes,

$$\hat{S}^{\alpha}_{j}(0) = \hat{S}^{\alpha}_{0}$$

Then we get

$$F_\alpha(\boldsymbol{\kappa}) = \gamma r_0\{\frac{1}{2}gf(\boldsymbol{\kappa})\}\hat{S}^{\alpha}_{0}\sum_j e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_j} = N\gamma r_0\{\frac{1}{2}gf(\boldsymbol{\kappa})\}\hat{S}^{\alpha}_{0}\sum_{\boldsymbol{G}}\delta(\boldsymbol{\kappa}-\boldsymbol{G}),$$

which means that the ferromagnetic reflections appear at

$$\boldsymbol{\kappa} = \boldsymbol{G}.$$

8. $F_\alpha(\kappa)$ for the antiferromagnet

For the antiferromagnetic systems,

$$\hat{S}^{\alpha}_{j}(0) = \hat{S}^{\alpha}_{0}e^{i\mathbf{q}\cdot\mathbf{r}_j}$$

Then we get

$$
\begin{aligned}
F_\alpha(\boldsymbol{\kappa}) &= \gamma r_0\{\frac{1}{2}gf(\boldsymbol{\kappa})\}\hat{S}^{\alpha}_{0}\sum_j e^{i(\boldsymbol{\kappa}+\boldsymbol{q})\cdot\boldsymbol{r}_j} \\
&= N\gamma r_0\{\frac{1}{2}gf(\boldsymbol{\kappa})\}\hat{S}^{\alpha}_{0}\sum_{\boldsymbol{G}}\delta(\boldsymbol{\kappa}+\boldsymbol{q}-\boldsymbol{G})
\end{aligned}
$$

which means that the antiferromagnetic reflections appear at

$$\boldsymbol{\kappa} = \boldsymbol{G} \pm \boldsymbol{q} \ .$$

9. Perfect paramagnet

$$\frac{d\sigma_s}{d\Omega} = (\gamma r_0)^2 \{\frac{1}{2} g f(\boldsymbol{\kappa})\}^2 \frac{2}{3} NS(S+1)$$

10. Elastic scattering

First we consider

$$S^{\alpha\beta}(\kappa,\omega) = \frac{1}{2\pi N} \sum_{i,j} \int_{-\infty}^{\infty} e^{-i\omega\tau} d\tau e^{i\kappa\cdot(j-i)} \left\langle \hat{S}_i^{\alpha}(0) \hat{S}_j^{\beta}(\tau) \right\rangle$$

This s cattering function is a Fourier transform in time and space of a spin correlation function $\left\langle \hat{S}_l^{\alpha}(0) \hat{S}_j^{\beta}(\tau) \right\rangle$ between spins at different times 0 and τ. Now, in the paramagnetic state all spin correlations will become zero after long times,

$$\lim_{\tau\to\infty} \left\langle \hat{S}_l^{\alpha}(0) \hat{S}_j^{\beta}(\tau) \right\rangle = 0$$

In the ordered magnetic state this will no longer be true. The ordered state remains ordered for all time, so that spin correlations remain finite as $\tau\to\infty$. There will be at least one value of α and β for any sites i and j where

$$\lim_{\tau\to\infty} \left\langle \hat{S}_l^{\alpha}(0) \hat{S}_j^{\beta}(\tau) \right\rangle = 0$$

How about antiferromagnet?

$$S_j^{\alpha} = Se^{i\mathbf{q}\cdot\mathbf{R}_j} + \delta S_j^{\alpha}$$

with $q_0 = \frac{1}{2}\mathbf{G}$.

We consider the second term

Elastic neutron scattering

Formulation

Note the identity

Then

$$\{\hat{A},\hat{B}\} = \int_0^{\beta} d\lambda \left\langle \hat{A}\hat{B}(i\hbar\lambda)\right\rangle - \beta\left\langle \hat{A}\right\rangle\left\langle \hat{B}\right\rangle]$$

The wave-length dependent susceptibility

$$\begin{aligned}\chi^{\alpha\beta}(\kappa) &= g^2\mu_B{}^2\{\hat{S}^{\alpha}_{-\kappa}(0),\hat{S}^{\beta}_{\kappa}(0)\}\\ &= g^2\mu_B{}^2[\int_0^{\beta} d\lambda\left\langle \hat{S}^{\alpha}_{-\kappa}(0),\hat{S}^{\beta}_{\kappa}(i\hbar\lambda)\right\rangle - \beta\left\langle \hat{S}^{\alpha}_{-\kappa}(0)\right\rangle\left\langle \hat{S}^{\beta}_{\kappa}(0)\right\rangle]\end{aligned}$$

In the limit $\boldsymbol{\kappa} = 0$ when the total spin is a constant of motion

$$\hat{S}_\kappa^\beta(i\hbar\lambda) = \hat{S}_0^\beta(0) .$$

$$\chi^{\alpha\beta}(\kappa = 0) = \beta g^2 {\mu_B}^2 \left\langle \hat{S}_{\kappa=0}^\alpha(0)\hat{S}_{\kappa=0}^\beta(0)\right\rangle - \left\langle \hat{S}_{\kappa=0}^\alpha(0)\right\rangle\left\langle \hat{S}_{\kappa=0}^\beta(0)\right\rangle$$

Since

$$\hat{S}_{\kappa=0}^\alpha(0) = \frac{1}{\sqrt{N}}\sum_r \hat{S}_r^\alpha(0) = \frac{1}{\sqrt{N}} S_{tot}^\alpha$$

we get

$$\chi^{\alpha\beta}(\kappa = 0) = \frac{g^2 {\mu_B}^2}{Nk_B T}\left\langle S_{tot}^\alpha S_{tot}^\beta\right\rangle - \left\langle S_{tot}^\alpha\right\rangle\left\langle S_{tot}^\alpha\right\rangle) .$$

When $\alpha = z$ (easy axis) and

$$M_T = g\mu_B S_{tot}^z$$

we have

$$\chi^{zz}(\kappa = 0) = \frac{1}{Nk_B T}[\left\langle {M_T}^2\right\rangle - \left\langle M_T\right\rangle^2]$$

We see the classical susceptibility of an assemblage of a large number of N of spins is proportional to the mean square fluctuation of the magnetization per atom.

2. The power spectrum in terms of the relaxation function (Marshall and Lowde)

$$S^{\alpha\beta}(\kappa,\omega) - S_{Bragg}^{\alpha\beta}(\kappa,\omega) = \frac{\hbar\omega}{1 - e^{-\hbar\omega\beta}}\frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau e^{-i\omega\tau}\{\hat{S}_{-\kappa}^\alpha(\tau = 0), \hat{S}_\kappa^\beta(\tau)\}$$

where

$$S_{Bragg}^{\alpha\beta}(\kappa,\omega) = \delta(\omega)\left\langle \hat{S}_{-\kappa}^{\alpha}(t=0)\right\rangle \left\langle \hat{S}_{\kappa}^{\beta}(t=0)\right\rangle .$$

$$\begin{aligned}
\int_{-\infty}^{\infty} d\omega \frac{1-e^{-\hbar\omega\beta}}{\hbar\omega}[S^{\alpha\beta}(\kappa,\omega) - S_{Bragg}^{\alpha\beta}(\kappa,\omega)] &= \int_{-\infty}^{\infty} d\omega \frac{1}{2\pi\beta}\int_{-\infty}^{\infty} d\tau e^{-i\omega\tau}\{\hat{S}_{-\kappa}^{\alpha}(\tau=0),\hat{S}_{\kappa}^{\beta}(\tau)\} \\
&= \frac{1}{\beta}\{\hat{S}_{-\kappa}^{\alpha}(0),\hat{S}_{\kappa}^{\beta}(0)\} \\
&= \frac{k_B T}{g^2 {\mu_B}^2}\chi^{\alpha\beta}(\kappa) \\
&= \frac{1}{3}S(S+1)\frac{\chi^{\alpha\beta}(\kappa)}{\chi_0}
\end{aligned}$$

where

$$\chi_0 = \frac{g^2 {\mu_B}^2}{3k_B}S(S+1)$$

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Y. Ishikawa

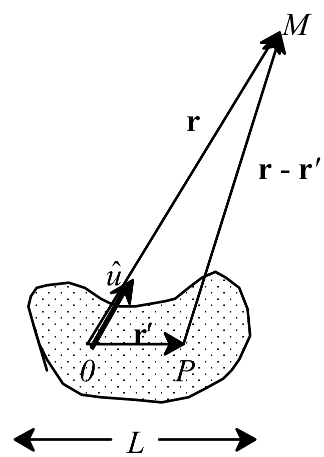
APPENDIX

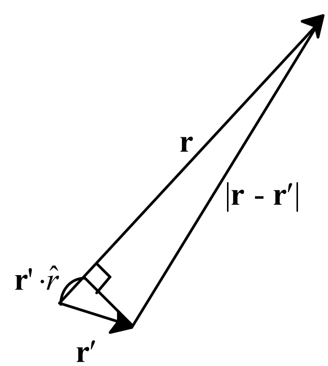
A1. Born approximation

$$\langle \mathbf{r} | \psi^{(\pm)} \rangle = \langle \mathbf{r} | \mathbf{k} \rangle - \frac{2m}{\hbar^2} \int d\mathbf{r}' \frac{e^{\pm ik|\mathbf{r}-\mathbf{r}'|}}{4\pi |\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') \langle \mathbf{r}' | \psi^{(\pm)} \rangle$$

where

$$\langle \mathbf{r} | \mathbf{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}}$$





Here we consider the case of $\langle \mathbf{r} | \psi^{(+)} \rangle$.

$$|\mathbf{r} - \mathbf{r}'| = r - \mathbf{r}' \cdot \mathbf{e}_r$$

$$\mathbf{k}' = k\mathbf{e}_r$$

$$e^{ik|\mathbf{r}-\mathbf{r}'|} \approx e^{ik(r-\mathbf{r}'\cdot\mathbf{e}_r)} = e^{ikr}e^{-i\mathbf{k}'\cdot\mathbf{r}'} \qquad \text{for large } r.$$

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \approx \frac{1}{r}$$

Then we have

$$\langle \boldsymbol{r}|\psi^{(+)}\rangle = \langle \boldsymbol{r}|\boldsymbol{k}\rangle - \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{e^{ikr}}{r}\int d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}V(\boldsymbol{r}')\langle \boldsymbol{r}'|\psi^{(+)}\rangle$$

or

$$\langle \boldsymbol{r}|\psi^{(+)}\rangle = \frac{1}{(2\pi)^{3/2}}[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + -\frac{e^{ikr}}{r}f(\boldsymbol{k}',\boldsymbol{k})]$$

The first term: original plane wave in propagation direction $\boldsymbol{k}$. The second term: outgoing spherical wave with amplitude $f(\boldsymbol{k}',\boldsymbol{k})$.

$$f(\mathbf{k}',\mathbf{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\int d\mathbf{r}'\frac{e^{-i\mathbf{k}'\cdot\mathbf{r}'}}{(2\pi)^{3/2}}V(\mathbf{r}')\langle \mathbf{r}'|\psi^{(\pm)}\rangle = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\langle \mathbf{k}'|\hat{V}|\psi^{(+)}\rangle$$

differential cross section

$$\frac{d\sigma}{d\Omega} = |f(\boldsymbol{k}',\boldsymbol{k})|^2$$

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\langle \boldsymbol{k}'|\hat{V}|\psi^{(+)}\rangle = -\frac{m}{2\pi\hbar^2}(2\pi)^3\langle \boldsymbol{k}'|\hat{V}|\psi^{(+)}\rangle$$

where

$\boldsymbol{q} = \boldsymbol{k}-\boldsymbol{k}'$: scattering wave vector.

A.2 magnetic moment of neutron, electron, and proton

(a) Neutron

$$\boldsymbol{\mu}_n = -2\gamma \frac{e\hbar}{2m_p c} \frac{\mathbf{s}_n}{\hbar} = -2\gamma\mu_N \frac{\mathbf{s}_n}{\hbar} = -\gamma\mu_N \boldsymbol{\sigma}$$

where γ = 1.913 (gyromagnetic ratio). $s_n = \frac{\hbar}{2}$

$\mu_N = 5.05078324 \times 10^{-27}$ J/T (SI units)

or

$\mu_N = 5.05078324 \times 10^{-24}$ emu (cgs units)

(b) Electron

$$\boldsymbol{\mu}_e = -2\left(\frac{e\hbar}{2m_e c}\right)\frac{\mathbf{s}_e}{\hbar} = -2\mu_B \frac{\mathbf{s}_e}{\hbar}$$

where $s_e = \frac{\hbar}{2}$

μ_B=9.27400915 x 10^{-21} emu

(c) Proton

$$\boldsymbol{\mu}_p = 2(2.79)\mu_N \frac{\mathbf{s}_p}{\hbar} = -2.79\mu_N \sigma_p$$

((**Mathematica**))

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

rule1 = {μB → 9.27400915 × 10^-21, kB → 1.3806504 × 10^-16,
    NA → 6.02214179 × 10^23, c → 2.99792 × 10^10,
    ℏ → 1.054571628 10^-27, me → 9.10938215 10^-28,
    mp → 1.672621637 × 10^-24, mn → 1.674927211 × 10^-24,
    qe → 4.8032068 × 10^-10, eV → 1.602176487 × 10^-12,
    meV → 1.602176487 × 10^-15, keV → 1.602176487 × 10^-9,
    MeV → 1.602176487 × 10^-6};
```

$$\mu el = \frac{qe\,\hbar}{2\,me\,c} \; \text{//. rule1}$$

9.27403×10^{-21}

$$\mu p = \frac{qe\,\hbar}{2\,mp\,c} \; \text{//. rule1}$$

5.05079×10^{-24}

$$r0 = \frac{qe^2}{me\,c^2} \; \text{//. rule1}$$

2.81795×10^{-13}