by V. Pomjakushin (2014)
Maple script for calculations related to the practicum (http://sinq.web.psi.ch/sinq/instr/hrpt/praktikum.html). Also includes dot-product and cross-product functions in anybasis.

> $with(LinearAlgebra):$

Metric tensor G1_{ij}

Scalar product should be defined throught the metric tensor G.

> $G := \langle a[1], a[2], a[3] \rangle . `<|>`(a[1], a[2], a[3]);$

$$G := \begin{bmatrix} a_1^2 & a_1 a_2 & a_1 a_3 \\ a_1 a_2 & a_2^2 & a_2 a_3 \\ a_1 a_3 & a_2 a_3 & a_3^2 \end{bmatrix} \quad (1.1$$

> $m_{1,1} := a_1 a_1 :$
$m_{2,1} := a_1 a_2 \cos(\alpha_3) :$
$m_{3,1} := a_1 a_3 \cos(\alpha_2) :$
$m_{2,2} := a_2 a_2 :$
$m_{3,2} := a_3 a_2 \cos(\alpha_1) :$
$m_{3,3} := a_3 a_3 :$
$G1 := Matrix(3, 3, \{(1, 1) = m_{1,1}, (1, 2) = m_{2,1}, (1, 3) = m_{3,1}, (2, 1) = m_{2,1}, (2, 2) = m_{2,2}, (2, 3) = m_{3,2}, (3, 1) = m_{3,1}, (3, 2) = m_{3,2}, (3, 3) = m_{3,3}\});$

(1.2

$$G1 := \begin{bmatrix} a_1^2 & a_1 a_2 \cos(\alpha_3) & a_1 a_3 \cos(\alpha_2) \\ a_1 a_2 \cos(\alpha_3) & a_2^2 & a_3 a_2 \cos(\alpha_1) \\ a_1 a_3 \cos(\alpha_2) & a_3 a_2 \cos(\alpha_1) & a_3^2 \end{bmatrix} \quad (1.2)$$

Volume^2 is det(G1).

> $Vol := RealDomain\text{:-}simplify\left(Determinant(G1)^{\frac{1}{2}}\right);$

$$Vol := \sqrt{1 + 2\cos(\alpha_1)\cos(\alpha_3)\cos(\alpha_2) - \cos(\alpha_1)^2 - \cos(\alpha_3)^2 - \cos(\alpha_2)^2}\; |a_1 a_2 a_3| \quad (1.3)$$

We define the dual basis metric tensor

```
> G2 := MatrixInverse(G1) :
  unassign('i'); unassign('j', k);
  d2 := add(add((G2[i, j]·h[i]·h[j]), j = 1 ..3), i = 1 ..3) :
  simplify(d2);
```

$$\Big(\cos(\alpha_2)^2 a_1^2 a_3^2 h_2^2 - 2\cos(\alpha_2)\cos(\alpha_3) a_1^2 a_2 a_3 h_2 h_3 - 2\cos(\alpha_2)\cos(\alpha_1) a_1 a_2 a_3^2 h_1 h_2 + \cos(\alpha_3)^2 a_1^2 a_2^2 h_3^2 - 2\cos(\alpha_3)\cos(\alpha_1) a_1 a_2^2 a_3 h_1 h_3 + \cos(\alpha_1)^2 a_2^2 a_3^2 h_1^2 + 2\cos(\alpha_2) a_1 a_2^2 a_3 h_1 h_3 + 2\cos(\alpha_3) a_1 a_2 a_3^2 h_1 h_2 + 2\cos(\alpha_1) a_1^2 a_2 a_3 h_2 h_3 - h_3^2 a_1^2 a_2^2 - h_2^2 a_1^2 a_3^2 - h_1^2 a_2^2 a_3^2\Big) \Big/ \Big(a_1^2 a_2^2 a_3^2 \big(-2\cos(\alpha_1)\cos(\alpha_3)\cos(\alpha_2) + \cos(\alpha_2)^2 + \cos(\alpha_3)^2 + \cos(\alpha_1)^2 - 1\big)\Big) \quad (1.4)$$

Intro

Praktikum for neutron diffraction. Determination of long range antiferromagnetic order by powder neutron diffraction.

From the analysis of the nuclear and magnetic Bragg peak intensities and positions we will verify the crystal and magnetic structures of manganese sulfide and determine the size of the magnetic moment on manganese.

Integral intensity for powder Bragg scattering.
1. Lorentz factor

> $L := \theta \mapsto \frac{1}{\sin(\theta)\,\sin(2\,\theta)}$

$$L := \theta \mapsto \frac{1}{\sin(\theta)\,\sin(2\,\theta)} \quad \textbf{(2.1}$$

2. Lattice sum over Bravias lattice. It is important for calculations only if one uses different elementary cell for magnetic and nuclear structure factor calculations.

> $LS := \frac{N\,(2\,\pi)^3}{v0}$

$$LS := \frac{8\,N\,\pi^3}{v0} \quad \textbf{(2.2}$$

Define zeroth cell with centering translations & the lattice

Define F-centering translations

```
> #q:= `<|>`(h, k, l);
  cf[1] := `<|>`(0, 0, 0);
  cf[2] := `<|>`(1/2, 1/2, 0);
  cf[3] := `<|>`(1/2, 0, 1/2);
```

$cf[4] := \text{`<|>`}\left(0, \frac{1}{2}, \frac{1}{2}\right);$

$$cf_1 := \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}$$

$$cf_2 := \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}$$

$$cf_3 := \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix}$$

$$cf_4 := \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \quad \textbf{(3.1}$$

2theta from H

> $G1cube := RealDomain{:-}simplify\left(subs\left(\left[a_1 = c, \alpha_1 = \frac{\pi}{2}\right], \left[a_2 = c, \alpha_2 = \frac{\pi}{2}\right], \left[a_3 = c, \alpha_3 = \frac{\pi}{2}\right], G1\right)\right);$

$d2cube := RealDomain{:-}simplify\left(subs\left(\left[a_1 = c, \alpha_1 = \frac{\pi}{2}\right], \left[a_2 = c, \alpha_2 = \frac{\pi}{2}\right], \left[a_3 = c, \alpha_3 = \frac{\pi}{2}\right], d2^{\frac{1}{2}}\right) \text{ assuming } c > 0\right);$

$$G1cube := \begin{bmatrix} c^2 & 0 & 0 \\ 0 & c^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix}$$

$$d2cube := \frac{\sqrt{h_1^2 + h_2^2 + h_3^2}}{|c|} \quad \textbf{(3.2}$$

> $qvec := 2 \cdot \mathrm{Pi} \cdot d2cube;$

$$evalf\left(\frac{2\cdot \mathrm{Pi}}{5.209}\right);$$

$$qvec := \frac{2\,\pi\,\sqrt{h_1^2+h_2^2+h_3^2}}{|c|}$$

$$1.206217183 \qquad (3.3$$

Bragg law

> $Bragg := 2\cdot\sin(\theta) = \lambda\cdot d2cube;$

$$Bragg := 2\sin(\theta) = \frac{\lambda\,\sqrt{h_1^2+h_2^2+h_3^2}}{|c|} \qquad (3.4$$

theta as a function of **H.**

> $t2 := solve(\mathrm{Bragg}, \theta);$

$t2 := (subs([\lambda = 1.886,\ c = 5.209],\ solve(\mathrm{Bragg}, \theta)));$

$$t2 := \arcsin\left(\frac{\lambda\,\sqrt{h_1^2+h_2^2+h_3^2}}{2\,|c|}\right)$$

$$t2 := \arcsin\left(\frac{0.9430000000\,\sqrt{h_1^2+h_2^2+h_3^2}}{|5.209|}\right) \qquad (3.5$$

qvec as a ...

> $qvec := evalf\left(subs\left([\lambda = 1.886],\ \frac{4\cdot\pi\cdot\sin(t2)}{\mathrm{lambda}}\right)\right);$

$$qvec := 1.206217183\,\sqrt{h_1^2+h_2^2+h_3^2} \qquad (3.6$$

Set the atoms

Set up Mn atoms, both positions and spins

```
> for j from 1 to 4 do
    b[j] := b_Mn :
    r[j] := `&lt;|&gt;`(0, 0, 0) + cf[j];
    s[j] := `&lt;|&gt;`(s0, -s0, 0)·exp(2·Pi·I·&lt;1/2|1/2|1/2&gt;.r[j]);
  end do; unassign('j');
```

$$b_1 := b_{Mn}$$

$$r_1 := \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}$$

$$s_1 := \begin{bmatrix} s0 & -s0 & 0 \end{bmatrix}$$

$$b_2 := b_{Mn}$$

$$r_2 := \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}$$

$$s_2 := \begin{bmatrix} -s0 & s0 & 0 \end{bmatrix}$$

$$b_3 := b_{Mn}$$

$$r_3 := \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix}$$

$$s_3 := \begin{bmatrix} -s0 & s0 & 0 \end{bmatrix}$$

$$b_4 := b_{Mn}$$

$$r_4 := \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

(4.1

$$s_4 := \begin{bmatrix} -s0 & s0 & 0 \end{bmatrix}$$ (4.1

=> Magnetic form-factor coeff. (A,a,B,b,C,c,D)
MMN3 0.4198 14.2829 0.6054 5.4689 0.9241 -0.0088 -0.9498

> $MMN3 := \langle 0.4198,\ 14.2829,\ 0.6054,\ 5.4689,\ 0.9241,\ -0.0088,\ -0.9498,\ 0 \rangle$:

From international tables mMn(q) ff of Mn3+ of q= $\frac{4\,\pi\,\sin(\theta)}{\lambda}$

> $\# j0 := (s) \rightarrow A\cdot\exp(-a\cdot s^2) + B\cdot\exp(-b\cdot s^2) + C\cdot\exp(-c\cdot s^2) + \mathrm{D};$

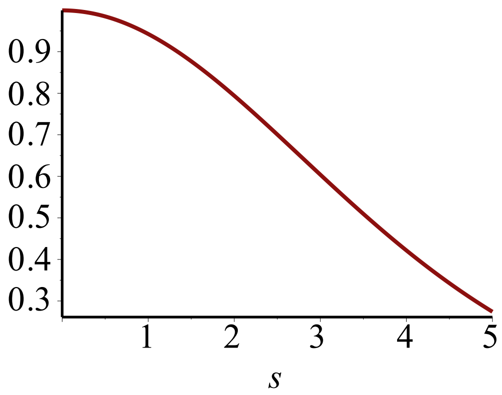
$j0 := (s, A :: Vector) \rightarrow add(A[i]\cdot\exp(-A[i+1]\cdot s^2), i = \mathrm{seq}(1\,..\,7, 2));$

$mMn := (s) \rightarrow j0\left(\frac{s}{4\cdot\mathrm{Pi}}, MMN3\right);$

$$j0 := (s, A::Vector) \mapsto add\left(A_i\, \mathrm{e}^{-A_{i+1}\, s^2}, i = seq(1\,..7, 2)\right)$$

$$mMn := s \mapsto j0\left(\frac{s}{4\,\pi}, MMN3\right)$$ (4.2

> $plot(mMn(s), s = 0\,..5);$



Set up S-atoms

> **for** j **from** 1 **to** 4 **do**
  $b[j+4] := b_S$:
  $r[j+4] := \text{`<|>`}\left(\frac{1}{2}, 0, 0\right) + cf[j]$;
 end do: $unassign('j')$;
 $eval(r)$;

$$\text{table}\left(\left[1 = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}, 2 = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}, 3 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix}, 4 = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}, 5 = \begin{bmatrix} \frac{1}{2} & 0 & 0 \end{bmatrix}, 6 = \begin{bmatrix} 1 & \frac{1}{2} & 0 \end{bmatrix}, 7 = \begin{bmatrix} 1 & 0 & \frac{1}{2} \end{bmatrix}, 8 = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix}\right]\right) \quad \textbf{(4.3}$$

Nuclear intensity and peak positions

First calculate numerically, in 10^{-12} [cm]

$\#q := (\,`<,>`(h, k, l)\,)^{\%T}$

Nuclear structure factor

> $F := (q) \rightarrow add(b[j] \cdot \exp(2 \cdot \mathrm{Pi} \cdot I \cdot (r[j].q)), j = 1..8);$
$eval(F(\langle h, k, l \rangle));$
$factor(\%);$

$$F := q \mapsto add\left(b_j\, \mathrm{e}^{2\,\mathrm{I}\,\pi\,\left(Typesetting:-delayDotProduct\left(r_j,\, q\right)\right)}, j = 1..8\right)$$

$$b_{Mn} + b_{Mn}\,\mathrm{e}^{2\,\mathrm{I}\,\pi\left(\frac{h}{2} + \frac{k}{2}\right)} + b_{Mn}\,\mathrm{e}^{2\,\mathrm{I}\,\pi\left(\frac{h}{2} + \frac{l}{2}\right)} + b_{Mn}\,\mathrm{e}^{2\,\mathrm{I}\,\pi\left(\frac{k}{2} + \frac{l}{2}\right)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,h} + b_S\,\mathrm{e}^{2\,\mathrm{I}\,\pi\left(h + \frac{k}{2}\right)} + b_S\,\mathrm{e}^{2\,\mathrm{I}\,\pi\left(h + \frac{l}{2}\right)} + b_S\,\mathrm{e}^{2\,\mathrm{I}\,\pi\left(\frac{h}{2} + \frac{k}{2} + \frac{l}{2}\right)}$$

$$b_{Mn} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+k)} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+l)} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(k+l)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,h} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(2h+k)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(2h+l)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+k+l)} \quad \textbf{(5.1.1)}$$

$$b_{Mn} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+k)} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+l)} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(k+l)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,h} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(2h+k)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(2h+l)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+k+l)} \quad \textbf{(5.1.2)}$$

$$b_{Mn} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+k)} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+l)} + b_{Mn}\,\mathrm{e}^{\mathrm{I}\,\pi\,(k+l)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,h} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(2h+k)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(2h+l)} + b_S\,\mathrm{e}^{\mathrm{I}\,\pi\,(h+k+l)} \quad \textbf{(5.1.2)}$$

Extinction rules

The sum is either 4b_Mn +/- 4b_S or 0.

$assume(h, even);\ F(\langle h, 0, 0 \rangle);\ simplify(\%)$

$$4\,b_{Mn} + 4\,b_S$$

$$4\,b_{Mn} + 4\,b_S \quad \textbf{(5.1.1.1)}$$

$assume(h, even, k, even);\ F(\langle h, k, 0 \rangle);\ simplify(\%)$

$$4\,b_{Mn} + 4\,b_S$$

$$4\,b_{Mn} + 4\,b_S \quad \textbf{(5.1.1.2)}$$

$assume(h, even, k, odd); F(\langle h, k, 0\rangle); simplify(\%)$

$$b_S + b_S (-1)^{2 h\sim + k\sim}$$

$$0 \quad \textbf{(5.1.1.3)}$$

$assume(h, even, k, even, l, even); F(\langle h, k, l\rangle); simplify(\%)$

$$4 b_{Mn} + 4 b_S$$

$$4 b_{Mn} + 4 b_S \quad \textbf{(5.1.1.4)}$$

$assume(h, even, k, even, l, odd); F(\langle h, k, l\rangle); simplify(\%)$

$$b_S + b_S (-1)^{2 h\sim + l\sim}$$

$$0 \quad \textbf{(5.1.1.5)}$$

$assume(h, odd, k, odd, l, even); F(\langle h, k, l\rangle); simplify(\%)$

$$b_S + b_S (-1)^{2 h\sim + k\sim}$$

$$0 \quad \textbf{(5.1.1.6)}$$

$assume(h, odd, k, odd, l, odd); F(\langle h, k, l\rangle) ; simplify(\%)$

$$4 b_{Mn} - 2 b_S + b_S (-1)^{2 h\sim + k\sim} + b_S (-1)^{2 h\sim + l\sim}$$

$$4 b_{Mn} - 4 b_S \quad \textbf{(5.1.1.7)}$$

$F(\langle 1, 1, 1\rangle); F(\langle 2, 0, 0\rangle)$

$$4 b_{Mn} - 4 b_S$$

$$4 b_{Mn} + 4 b_S \quad \textbf{(5.1.1.8)}$$

$lh := [\langle 1, 1, 1\rangle, \langle 2, 0, 0\rangle, \langle 2, 2, 0\rangle, \langle 3, 1, 1\rangle];$

$$lh := \left[\begin{bmatrix}1\\1\\1\end{bmatrix}, \begin{bmatrix}2\\0\\0\end{bmatrix}, \begin{bmatrix}2\\2\\0\end{bmatrix}, \begin{bmatrix}3\\1\\1\end{bmatrix}\right] \quad \textbf{(5.1.3)}$$

Numerical F(h) in 10^{-12} [cm]

$bnum := [b_{Mn} = -0.373,\ b_S = +0.2847];$

$$bnum := [b_{Mn} = -0.373, b_S = 0.2847] \quad \textbf{(5.1.4)}$$

the scattering lengths are in 10^{-12} [cm]

$subs(bnum, eval(F(\langle 1, 1, 1\rangle)));$
$subs(bnum, eval(F(\langle 2, 0, 0\rangle)));$
$subs(bnum, eval(F(\langle 2, 2, 0\rangle)));$
$subs(bnum, eval(F(\langle 3, 1, 1\rangle)));$

$$-2.6308$$
$$-0.3532$$
$$-0.3532$$
$$-2.6308 \quad \textbf{(5.1.5)}$$

Calculate the peak positions for the hkl-list. First nuclear.

> $lh := [\langle 1, 1, 1\rangle, \langle 2, 0, 0\rangle, \langle 2, 2, 0\rangle, \langle 3, 1, 1\rangle]:$
> $mult := [8, 6, 12, 24];$
> $seq\left(\left[HKL = h, evalf\left(2 \cdot \frac{t2 \cdot 180}{\pi}\right)\right], h \in lh\right);$

$$mult := [8, 6, 12, 24]$$

$$\left[HKL = \begin{bmatrix}1\\1\\1\end{bmatrix}, 36.54757372\right], \left[HKL = \begin{bmatrix}2\\0\\0\end{bmatrix}, 42.45421864\right], \left[HKL = \begin{bmatrix}2\\2\\0\end{bmatrix}, 61.59937241\right], \left[HKL = \begin{bmatrix}3\\1\\1\end{bmatrix}, 73.79967604\right] \quad \textbf{(5.1.6)}$$

Then magnetic peak positions.

> $lh := \left[\left\langle \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle, \left\langle \frac{3}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle, \left\langle \frac{3}{2}, \frac{3}{2}, \frac{1}{2}\right\rangle, \left\langle \frac{5}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle\right]:$

$seq\left(\left[HKL = h, evalf\left(\frac{t2 \cdot 2 \cdot 180}{\mathrm{Pi}}\right)\right], h \in lh\right)$

$$\left[HKL = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, 18.03997726\right], \left[HKL = \begin{bmatrix} \frac{3}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, 34.94031101\right], \left[HKL = \begin{bmatrix} \frac{3}{2} \\ \frac{3}{2} \\ \frac{1}{2} \end{bmatrix}, 46.47606041\right], \left[HKL = \begin{bmatrix} \frac{5}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, 56.11235915\right] \quad (5.1.7)$$

#seq(h[i] = $h \| i$, i = 1 ..3);

Intensity. We set the rtable ma[].

> $lh := [\langle 1, 1, 1\rangle, \langle 2, 0, 0\rangle, \langle 2, 2, 0\rangle, \langle 3, 1, 1\rangle]:$
$mult := [8, 6, 12, 24];$

> **for** i **from** 1 **to** 4 **do**
$ma[lh[i]] := mult[i]$
end do:

$$mult := [8, 6, 12, 24] \quad (5.1.8)$$

Lorenz factor

> $seq([HKL = h, evalf(L(t2))], h \in lh);$

$$\left[HKL = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, 5.355592645\right], \left[HKL = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}, 4.091742821\right], \left[HKL = \begin{bmatrix} 2 \\ 2 \\ 0 \end{bmatrix}, 2.220194594\right], \left[HKL = \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix}, 1.734374830\right] \quad (5.1.9)$$

Structure factor

> $seq([HKL = h, evalf(F(h))], h \in lh);$

$$\left[HKL = \begin{bmatrix}1\\1\\1\end{bmatrix}, 4.\, b_{Mn} - 4.\, b_S\right], \left[HKL = \begin{bmatrix}2\\0\\0\end{bmatrix}, 4.\, b_{Mn} + 4.\, b_S\right], \left[HKL = \begin{bmatrix}2\\2\\0\end{bmatrix}, 4.\, b_{Mn} + 4.\, b_S\right], \left[HKL = \begin{bmatrix}3\\1\\1\end{bmatrix}, 4.\, b_{Mn} - 4.\, b_S\right] \quad \textbf{(5.1.10)}$$

Numeric square of structure factor

> $seq\left(\left[HKL = h, evalf\left(\left(subs(bnum, F(h))\right)^2\right)\right], h \in lh\right);$

$$\left[HKL = \begin{bmatrix}1\\1\\1\end{bmatrix}, 6.92110864\right], \left[HKL = \begin{bmatrix}2\\0\\0\end{bmatrix}, 0.12475024\right], \left[HKL = \begin{bmatrix}2\\2\\0\end{bmatrix}, 0.12475024\right], \left[HKL = \begin{bmatrix}3\\1\\1\end{bmatrix}, 6.92110864\right] \quad \textbf{(5.1.11)}$$

Intensity without multiplicity

> $seq\left(\left[HKL = h, evalf\left(L(t2) \cdot \left(subs(bnum, F(h))\right)^2\right)\right], h \in lh\right);$

$$\left[HKL = \begin{bmatrix}1\\1\\1\end{bmatrix}, 37.06663854\right], \left[HKL = \begin{bmatrix}2\\0\\0\end{bmatrix}, 0.5104458990\right], \left[HKL = \begin{bmatrix}2\\2\\0\end{bmatrix}, 0.2769698085\right], \left[HKL = \begin{bmatrix}3\\1\\1\end{bmatrix}, 12.00379662\right] \quad \textbf{(5.1.12)}$$

Total Intensity

> $seq\left(\left[HKL = h, evalf\left(L(t2) \cdot \left(subs(bnum, F(h))\right)^2 \cdot ma[h]\right)\right], h \in lh\right);$

$$\left[HKL = \begin{bmatrix}1\\1\\1\end{bmatrix}, 296.5331083\right], \left[HKL = \begin{bmatrix}2\\0\\0\end{bmatrix}, 3.062675394\right], \left[HKL = \begin{bmatrix}2\\2\\0\end{bmatrix}, 3.323637701\right], \left[HKL = \begin{bmatrix}3\\1\\1\end{bmatrix}, 288.0911189\right] \quad \textbf{(5.1.13)}$$

Analytical version

Magnetic intensity

First: close to numerical calculation way. In units 10^{-12} [cm]

List of Q-vectors of the first magnetic Bragg peaks

> $lh := \left[\left\langle \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle, \left\langle \frac{3}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle, \left\langle \frac{3}{2}, \frac{3}{2}, \frac{1}{2}\right\rangle, \left\langle \frac{5}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle\right]$

$$lh := \left[\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, \begin{bmatrix} \frac{3}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, \begin{bmatrix} \frac{3}{2} \\ \frac{3}{2} \\ \frac{1}{2} \end{bmatrix}, \begin{bmatrix} \frac{5}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}\right] \quad (6.1.1)$$

Double cross product.

eval vs. subs.

subs does just "syntactic substitution"

one should use delayed substitution! with '...'

```
> #S:=⟨s[1], s[2], s[3]⟩;
  #S:=⟨s,-s, 0⟩;
  #Q:=lh[4];
```

```
> s[1]
```

$$\begin{bmatrix} s0 & -s0 & 0 \end{bmatrix} \quad (6.1.2)$$

Double cross product Qp perpendiqular $Q_{\perp}$ = [Q x S x Q]/(Q·Q)

> $Qp := (S :: Vector, Q :: Vector) \rightarrow \frac{\text{'\&x'}(Q, (\text{'\&x'}(S, Q)))}{\text{'.'}(Q, Q)};$

$\#Qp := (S :: Vector, Q :: Vector) \rightarrow \frac{S\cdot(Q.Q) - Q\cdot(Q.S)}{(Q.Q)};$

$$Qp := (S::Vector, Q::Vector) \mapsto \frac{\text{'LinearAlgebra:-\&x'}(Q, \text{'LinearAlgebra:-\&x'}(S, Q))}{\text{'`.`'}(Q, Q)} \quad (6.1.3)$$

```
> (eval('.'(q, q), q = lh[1]));
```

$$\frac{3}{4} \tag{6.1.4}$$

```
> eval(Qp(s[1], <q_1, q_2, q_3>)) assuming real;
  eval(Qp(s[1], lh[2])) assuming real;
```

$$\left[\begin{array}{c} \frac{q_2 \left(q_1 s0 + q_2 s0\right) + q_3^2 s0}{q_1^2 + q_2^2 + q_3^2} \\ \frac{-q_1 \left(q_1 s0 + q_2 s0\right) - q_3^2 s0}{q_1^2 + q_2^2 + q_3^2} \\ \frac{-q_1 q_3 s0 + q_2 q_3 s0}{q_1^2 + q_2^2 + q_3^2} \end{array}\right]$$

$$\left[\begin{array}{c} \frac{5 s0}{11} \\ -\frac{13 s0}{11} \\ -\frac{2 s0}{11} \end{array}\right] \tag{6.1.5}$$

```
> (subs(q = lh[1],'DotProduct'(q, q)));
  eval(subs(q = lh[1],'DotProduct'(q, q)));
  eval(subs(q = lh[1],'.'(q, q)));

  eval(subs(q = lh[1],'&x'(q, q)));
```

$$DotProduct\left(\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix},\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}\right)$$

$$\frac{3}{4}$$

$$\frac{3}{4}$$

$$\begin{bmatrix}0\\0\\0\end{bmatrix} \quad (6.1.6)$$

sum and add are principally different. The sum is intended to evaluate summations and must be able to operate on expression generated outside the sum function. The summation index is not local to the sum. http://www.mapleprimes.com/questions/43498-Sum-Versus-Add

> $Fm := (Q :: Vector) \rightarrow add(\mathrm{r0}\cdot \mathrm{Qp}(s[j], Q)\cdot \exp(2\cdot \mathrm{Pi}\cdot I\cdot (r[j].Q)), j=1..4);$
$Phase := (Q :: Vector, r :: Vector) \rightarrow \exp(2\cdot \mathrm{Pi}\cdot I\cdot (r.Q));$

$$Fm := Q{::}Vector \mapsto add\left(r0\ Qp\left(s_j, Q\right)\ e^{2\,I\,\pi\,\left(Typesetting{:}-delayDotProduct\left(r_j, Q\right)\right)}, j=1..4\right)$$

$$Phase := (Q{::}Vector, r{::}Vector) \mapsto e^{2\,I\,\pi\,(Typesetting{:}-delayDotProduct(r, Q))} \quad (6.1.7)$$

r0 is $\frac{1}{2}\,r_e\,\gamma$ in 10^{-12}cm, same units as for nuclear.

> $r0num := [r0=0.2695];$

$$r0num := [r0=0.2695] \quad (6.1.8)$$

> $seq(eval(Qp(s[i], lh[2])), i=1..4);$

$seq(eval(Phase(lh[2], r[i])), i=1..4);$

$$\left[\begin{matrix}\frac{5\,s0}{11}\\ -\frac{13\,s0}{11}\\ -\frac{2\,s0}{11}\end{matrix}\right], \left[\begin{matrix}-\frac{5\,s0}{11}\\ \frac{13\,s0}{11}\\ \frac{2\,s0}{11}\end{matrix}\right], \left[\begin{matrix}-\frac{5\,s0}{11}\\ \frac{13\,s0}{11}\\ \frac{2\,s0}{11}\end{matrix}\right], \left[\begin{matrix}-\frac{5\,s0}{11}\\ \frac{13\,s0}{11}\\ \frac{2\,s0}{11}\end{matrix}\right]$$

$$1, 1, 1, -1 \tag{6.1.9}$$

$> lh := \left[\left\langle\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right\rangle, \left\langle-\frac{1}{2}, -\frac{1}{2}, \frac{3}{2}\right\rangle, \left\langle\frac{3}{2}, -\frac{1}{2}, -\frac{1}{2}\right\rangle, \left\langle\frac{1}{2}, -\frac{3}{2}, \frac{1}{2}\right\rangle\right]$

$$lh := \left[\left[\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\\ \frac{1}{2}\end{matrix}\right], \left[\begin{matrix}-\frac{1}{2}\\ -\frac{1}{2}\\ \frac{3}{2}\end{matrix}\right], \left[\begin{matrix}\frac{3}{2}\\ -\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right], \left[\begin{matrix}\frac{1}{2}\\ -\frac{3}{2}\\ \frac{1}{2}\end{matrix}\right]\right] \tag{6.1.10}$$

$> seq\left(\left[HKL = h, evalf\left(j0\left(\frac{qvec}{4\cdot \mathrm{Pi}}, MMN3\right)\right)\right], h \in lh\right);$

$$\left[HKL = \left[\begin{matrix}\frac{1}{2}\\ \frac{1}{2}\\ \frac{1}{2}\end{matrix}\right], 0.9376498075\right], \left[HKL = \left[\begin{matrix}-\frac{1}{2}\\ -\frac{1}{2}\\ \frac{3}{2}\end{matrix}\right], 0.7939001556\right], \left[HKL = \left[\begin{matrix}\frac{3}{2}\\ -\frac{1}{2}\\ -\frac{1}{2}\end{matrix}\right], 0.7939001556\right], \left[HKL = \left[\begin{matrix}\frac{1}{2}\\ -\frac{3}{2}\\ \frac{1}{2}\end{matrix}\right], \right. \tag{6.1.11}$$

$$0.7939001556$$

>

> $seq([HKL = h, eval(Fm(h))], h \in lh);$

$$\left[HKL = \begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\\ \frac{1}{2}\end{bmatrix}, \begin{bmatrix}4\,r0\,s0\\ -4\,r0\,s0\\ 0\end{bmatrix}\right], \left[HKL = \begin{bmatrix}-\frac{1}{2}\\ -\frac{1}{2}\\ \frac{3}{2}\end{bmatrix}, \begin{bmatrix}4\,r0\,s0\\ -4\,r0\,s0\\ 0\end{bmatrix}\right], \left[HKL = \begin{bmatrix}\frac{3}{2}\\ -\frac{1}{2}\\ -\frac{1}{2}\end{bmatrix}, \begin{bmatrix}-\frac{4\,r0\,s0}{11}\\ -\frac{28\,r0\,s0}{11}\\ \frac{16\,r0\,s0}{11}\end{bmatrix}\right], \left[HKL = \begin{bmatrix}\frac{1}{2}\\ -\frac{3}{2}\\ \frac{1}{2}\end{bmatrix}, \begin{bmatrix}\frac{28\,r0\,s0}{11}\\ \frac{4\,r0\,s0}{11}\\ -\frac{16\,r0\,s0}{11}\end{bmatrix}\right] \tag{6.1.12}$$

> $eval(Fm(lh[1]), \{r0 = 0.2695, s0 = 3\});$
$evalf(\%); evalf(Norm(\%, Euclidean) \cdot 0.93);$

$$\frac{\begin{bmatrix}0.606375\\-0.606375\\0.0\end{bmatrix}}{\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}\cdot\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}} - \frac{\begin{bmatrix}-0.606375\\0.606375\\0.0\end{bmatrix}}{\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}\cdot\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}} - \frac{\begin{bmatrix}-0.606375\\0.606375\\0.0\end{bmatrix}}{\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}\cdot\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}} - \frac{\begin{bmatrix}-0.606375\\0.606375\\0.0\end{bmatrix}}{\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}\cdot\begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}}$$

$$\begin{bmatrix}3.23400000000000\\-3.23400000000000\\0.\end{bmatrix}$$

$$4.253416995 \qquad \textbf{(6.1.13)}$$

Absolute values of Fmag: to be compared with fullprof

> $seq([HKL = h, evalf(mMn(qvec) \cdot Norm(eval(Fm(h), \{r0 = 0.2695, s0 = 3\}), Euclidean))], h \in lh);$

$$\left[HKL = \begin{bmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{bmatrix}, 4.288403896\right], \left[HKL = \begin{bmatrix}-\frac{1}{2}\\-\frac{1}{2}\\\frac{3}{2}\end{bmatrix}, 3.630955283\right], \left[HKL = \begin{bmatrix}\frac{3}{2}\\-\frac{1}{2}\\-\frac{1}{2}\end{bmatrix}, 1.896204555\right], \left[HKL = \begin{bmatrix}\frac{1}{2}\\-\frac{3}{2}\\\frac{1}{2}\end{bmatrix}, 1.896204555\right] \qquad \textbf{(6.1.14)}$$

> $seq\left(\left[HKL = h, evalf\left((mMn(qvec) \cdot Norm(eval(Fm(h), \{r0 = 0.2695, s0 = 3\}), Euclidean))^2\right)\right], h \in lh\right);$

$$\left[HKL = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, 18.39040798\right], \left[HKL = \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{2} \\ \frac{3}{2} \end{bmatrix}, 13.18383627\right], \left[HKL = \begin{bmatrix} \frac{3}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{bmatrix}, 3.595591711\right], \left[HKL = \begin{bmatrix} \frac{1}{2} \\ -\frac{3}{2} \\ \frac{1}{2} \end{bmatrix}, 3.595591711\right] \quad \textbf{(6.1.15)}$$

Total magnetic intensities

> $seq\left(\left[HKL = h, evalf\left(2 \cdot L(t2) \cdot (mMn(qvec) \cdot Norm(eval(Fm(h), \{r0 = 0.2695, s0 = 3\}), Euclidean))^2\right)\right], h \in lh\right);$

$$\left[HKL = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, 757.5643460\right], \left[HKL = \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{2} \\ \frac{3}{2} \end{bmatrix}, 153.3570245\right], \left[HKL = \begin{bmatrix} \frac{3}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{bmatrix}, 41.82464306\right], \left[HKL = \begin{bmatrix} \frac{1}{2} \\ -\frac{3}{2} \\ \frac{1}{2} \end{bmatrix}, 41.82464306\right] \quad \textbf{(6.1.16)}$$

Lorentz factor

> $seq([HKL = h, evalf(\, L(t2))], h \in lh);$

$$\left[HKL = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, 20.59672484\right], \left[HKL = \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{2} \\ \frac{3}{2} \end{bmatrix}, 5.816100162\right], \left[HKL = \begin{bmatrix} \frac{3}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{bmatrix}, 5.816100162\right], \left[HKL = \begin{bmatrix} \frac{1}{2} \\ -\frac{3}{2} \\ \frac{1}{2} \end{bmatrix}, 5.816100162\right] \quad \textbf{(6.1.17)}$$

> $\#assume(s0, real);$
$\# \, seq\left(\left[HKL = h, evalf\left(2 \cdot L(t2) \cdot (mMn(qvec) \cdot Norm(eval(Fm(h), \{r0 = 0.2695\}), Euclidean))^2\right)\right], h \in lh\right);$

> $h := lh[1];$

$$h := \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \quad \textbf{(6.1.18)}$$

```
> simplify(eval(L(t2)), assume = real);
```

$$20.59672484 \quad \textbf{(6.1.19)}$$

```
> 2·L(t2)·(mMn(qvec))^2·eval(Fm(h).Fm(h), {r0 = 0.2695}) :
> simplify(%, 'assume=real' );
```

$$84.17381632\, s0^2 \quad \textbf{(6.1.20)}$$

Experimental magnetic/nuclear (Im/In) intensities for 1/2,1/2,1/2 and 1,1,1 is 5174/2095
In=C*2.6.53
Im=C*89.8*s0^2
So mag mom in muB

```
> evalf((296.53/84.18*5174/2095·2)^(1/2)); unassign('h');
```

$$4.171248414 \quad \textbf{(6.1.21)}$$

```
> #evalf(2·L(t2)·(mMn(qvec)·Norm(eval(Fm(h), {r0 = 0.2695}), Euclidean))^2 )
> V := ⟨v[1], v[2], v[3]⟩;
  Norm(V);
  (Norm(V, Euclidean))^2;
  V . V;
```

▶ Playing. Alternative way to create the list of inensities using inert form of Fm. All analytical!

- **Calculate moment analitically**
- **Scalar product in anybasis**
- **Conversions between basis and dual basis (reciprocal)**
- **Calculating cross product in anybasis**
- **Own Levi-Civita**
- **some useful stuff About sum and add in maple**