LP Corrections

Alan uses:

$$LP\_Factor = \frac{1+\cos^2 2\theta \cos^2 2\theta_M}{\cos\theta \sin^2\theta} \quad (1)$$

This comes from the Lorentz factor:

$$L = \frac{1}{\sin\theta \sin 2\theta} = \frac{1}{\cos\theta \sin^2\theta} \quad (2)$$

and Polarisation with a monochromator:

$$P = \frac{1-K+K\cos^2 2\theta \cos^2 2\theta_M}{2} \quad (3)$$

where K is fractional polarisation of beam (the traditional expressions given in texts, e.g. Pecharsky).

For neutrons K = 0 and the LP expression becomes:

$$LP = \frac{1}{\cos\theta \sin^2\theta} \quad (4)$$

In Alan's expression (1) $2\theta_M = 90$ reduces to (4). This is the same as Lorentz_Factor.

With no monochromator and unpolarised source K = 0.5 and the LP expression becomes:

$$LP = \frac{0.5+0.5\cos^2 2\theta}{2\cos\theta \sin^2\theta} \quad (5)$$

Give or take a scale factor using $2\theta_M = 0$ in (1) reduces to (5).

Andy Fitch assumes radiation hitting sample is 100% plane polarised and that the analyser crystals have no effect on the vertical electric vector which I believe means K = 0 and one can therefore "pretend" you've got the neutron situation and use $2\theta_M = 90$ or expression (4). This is an approximation of a "real" situation where K is typically a small number.

The Madsen macro in topas.inc is:

$$LP = \frac{1}{2\cos\theta \sin^2\theta} \frac{1-pp+pp\cos^2 2\theta \cos^2 2\theta_M}{1+pp\cos^2 2\theta_M} \quad (6)$$

pp=0.5 for lab tubes with circularly polarised X-rays. The term on the bottom right is a constant and the equation reduces to:

$$LP = c\left(\frac{0.5+0.5\cos^2 2\theta \cos^2 2\theta_M}{2\cos\theta \sin^2\theta}\right) \quad (7)$$

which is the same as (1), give or take a scale factor.

Use pp = 0 for fully polarised synchrotron (ID31 is 100% plane polarised) which reduces to:

$$LP = \frac{1}{2\cos\theta \sin^2\theta} \quad (8)$$

which is again the same as $2\theta_M = 90$ in (1).

For a real synchrotron pp=0.05 and the expression becomes:

$$LP = c\left(\frac{0.95 + 0.05\cos^2 2\theta \cos^2 2\theta_M}{2\cos\theta \sin^2\theta}\right) \quad (9)$$

This is not going to be a million miles away from expression (4) in real situations.

GSAS

In gsas-speak there are three equations available:

IPOL = 0: $\dfrac{Ph + (1 - Ph)\cos^2 2\theta}{2\sin^2\theta\cos\theta}$ (10)

IPOL = 1: $\dfrac{1 + Ph\cos^2 2\theta}{\sin^2\theta\cos\theta}$ (11)

IPOL = 2: $\dfrac{1 + Ph\cos^2 2\theta}{(1 + \cos^2 2\theta)\sin^2\theta\cos\theta}$ (12)

For lab diffractometers with 26.6 mono angle people typically use IPOL = 0 and Ph = 0.555 or IPOL = 1 and Ph = 0.8. Putting $2\theta_M$ = 26.6 into Alan's expression gives:

$$LP\_Factor = \frac{1 + \cos^2 2\theta \times 0.8}{\cos\theta\sin^2\theta} = \frac{0.5 + \cos^2 2\theta \times 0.4}{2\cos\theta\sin^2\theta} = c\left(\frac{0.555 + 0.444 \times \cos^2 2\theta}{2\cos\theta\sin^2\theta}\right)$$

i.e. you have the gsas IPOL = 0 equation with Ph of 0.555. Or if we take the last equation and divide through by 0.555 we get:

$$c\left(\frac{0.555 + 0.444 \times \cos^2 2\theta}{2\cos\theta\sin^2\theta}\right) = \frac{c}{0.555}\left(\frac{1 + 0.8 \times \cos^2 2\theta}{\cos\theta\sin^2\theta}\right) \quad (14)$$

which is the gsas IPOL = 1 equation.

Fullprof

Fullprof uses:

$$P = \frac{1 - K + K\cos^2 2\theta\cos^2 2\theta_M}{2\sin^2\theta\cos\theta} \quad (15)$$

For neutrons manual says "K is ignored" but K = 0 is effectively used.

For characteristic X-rays (unpolarized beam) formula is:

$$P = \frac{1 + \cos^2 2\theta\cos^2 2\theta_M}{2\sin^2\theta\cos\theta}$$

i.e. K = 0.5 in the general formula multiplied by 2.

For synchrotrons K must be given and is ~ 0.1.

Summary

Synchrotron use: LP_Factor(90)

Neutron use: LP_Factor(90)

No monochromator use: LP_Factor(0)