Derivation of likelihood functions and posterior moments used in STARANISO.

by Ian J. Tickle, Global Phasing Ltd.

Version of 11th Mar 2018.

This derivation has many features is common with that of French & Wilson's (henceforth 'FW') 'TRUNCATE' algorithm used to obtain the Bayesian posterior half-order moment (expectation of half power) of the intensity (*i.e.* the expected amplitude), given the prior expectation of the X-ray intensity, its experimentally measured value and its standard uncertainty. The expressions for the relevant probability density functions and other relevant equations are repeated here for easy reference.

Popov & Bourenkov (henceforth 'PB') proposed a likelihood function based on the acentric Wilson distribution (centric reflexions were excluded in their algorithm). They used this in an optimisation of the absolute scale and the unconstrained components of the anisotropy tensor of the observed intensities. The derivation of the 'PB' likelihood function is reproduced below (with minor changes in notation). Then a new likelihood function 'FW' based on the FW posterior likelihood is derived. The major difference between the PB and FW functions is that the former is error-free, i.e. it takes no account of experimental errors, whereas the latter assumes a Gaussian model for the experimental errors in the observed intensities, exactly as in the FW TRUNCATE treatment. This implies that for observed negative intensities, which can arise only through measurement error, the PB likelihood is undefined and hence all negative intensities must either be excluded from the optimisation of the PB likelihood functions or set to zero. This is likely to have a significant impact on the results in those cases where the true intensity is small relative to the mean intensity, since such intensities do carry information. Hence the PB functions are only of theoretical interest and are not used in practice.

Note that in the case of twinning two implicit assumptions are made, first that all the twin domains have the same anisotropy of diffraction and second that that anisotropy obeys the twin symmetry. In the case of the first assumption, diffraction anisotropy arises from a number of factors, for example the variability in the strengths and the directionality of intermolecular interactions (which is likely to be same for all twin domains), but also from radiation damage (which may well differ between twin domains). In the case of the second assumption, twinning is largely a geometrical effect due to shape symmetry of the twin domain and to symmetry in the interactions at its boundaries (so twinned domains are able to pack together during crystal growth as easily as untwinned ones), but this does not necessarily imply that the diffraction anisotropy obeys that shape symmetry. There is therefore no *a priori* reason why either of these two assumptions should hold in any particular case. In the case that the anisotropy does not obey the twin symmetry knowledge of the twin operators is required.

Sections:

1. PB likelihood function: untwinned acentric & centric perfect hemihedral twin cases.

For an untwinned acentric or perfect hemihedrally twinned centric reflexion the prior probability density function (PDF) $\mathrm{P}_{\mathrm{a}\,\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}})$ of the true intensity $J_{\boldsymbol{h}}$ (conditional on its prior expectation $S_{\boldsymbol{h}}$) is assumed to be the acentric Wilson PDF:	
$$\mathrm{P}_{\mathrm{a}\,\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}) \quad = \quad S_{\boldsymbol{h}}^{-1} \exp(-J_{\boldsymbol{h}}/S_{\boldsymbol{h}})$$	(1)
The prior expectation $S_{\boldsymbol{h}}$ of $J_{\boldsymbol{h}}$ can be expressed in terms of the zone-enhancement factor $\varepsilon_{\boldsymbol{h}}$, a spherically-symmetric standard 'profile' function $\hat{S}(\lvert\mathbf{s}_{\boldsymbol{h}}\rvert)$, the absolute scale factor g, and the overall anisotropic displacement tensor $\mathbf{U}$ on F:	
$$S_{\boldsymbol{h}}(g, \mathbf{U}) \quad = \quad \epsilon_{\boldsymbol{h}} \hat{S}(\lvert\mathbf{s}_{\boldsymbol{h}}\rvert)\, g \exp(-4\pi^2 \tilde{\mathbf{s}}_{\boldsymbol{h}} \mathbf{U} \mathbf{s}_{\boldsymbol{h}})$$	(2)
Taking the negative log of (1), the contribution to the negative log-likelihood gain is then given by (omitting terms that are independent of the parameters):	
$$-\mathrm{LLG}_{\mathrm{a}\,\boldsymbol{h}}(g, \mathbf{U}) \quad = \quad \ln(S_{\boldsymbol{h}}) + J_{\boldsymbol{h}}/S_{\boldsymbol{h}}$$	(3)

2. PB likelihood function: untwinned centric case.

For untwinned centric reflexions we use the centric Wilson PDF as the prior $\mathrm{P}_{\mathrm{c}\,\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}})$:	
$$\mathrm{P}_{\mathrm{c}\,\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}) \quad = \quad (2\pi S_{\boldsymbol{h}} J_{\boldsymbol{h}})^{-½} \exp(-J_{\boldsymbol{h}}/2 S_{\boldsymbol{h}})$$	(4)
Again, taking the negative log of (4), the contribution to the negative log-likelihood gain is given by:	
$$-\mathrm{LLG}_{\mathrm{c}\,\boldsymbol{h}}(g, \mathbf{U}) \quad = \quad ½(\ln(2\pi S_{\boldsymbol{h}} J_{\boldsymbol{h}}) + J_{\boldsymbol{h}}/S_{\boldsymbol{h}})$$	(5)
PB appear not to have included centric reflexions in their treatment, though it is not clear why, given that it's such a simple modification.	

3. PB likelihood function: acentric perfect general and hemihedral twin cases.

In the perfect general twin case (N equal twin domains; usually N = 2: hemihedry, 4: tetartohedry or 8: ogdohedry), the PDF for acentric reflexions is:	
$$\mathrm{P}_{\mathrm{at}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}) \;=\; \frac{N^N J_{\boldsymbol{h}}^{N-1}}{(N-1)!\,S_{\boldsymbol{h}}^N}\exp(-N J_{\boldsymbol{h}}/S_{\boldsymbol{h}})$$	(6)
Again, taking the log of (6), the contribution to the negative log-likelihood gain is:	
$$-\mathrm{LLG}_{\mathrm{at}\,\boldsymbol{h}}(g,\mathbf{U}) \;=\; N(\ln(S_{\boldsymbol{h}}) + J_{\boldsymbol{h}}/S_{\boldsymbol{h}})$$	(7)
In the perfect hemihedral twin case (N = 2) the PDF and -LLG for acentric reflexions are therefore:	
$$\mathrm{P}_{\mathrm{at}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}) \;=\; 4S_{\boldsymbol{h}}^{-2}J_{\boldsymbol{h}}\exp(-2J_{\boldsymbol{h}}/S_{\boldsymbol{h}})$$ $$-\mathrm{LLG}_{\mathrm{at}\,\boldsymbol{h}}(g,\mathbf{U}) \;=\; \ln(S_{\boldsymbol{h}}^2/4J_{\boldsymbol{h}}) + 2J_{\boldsymbol{h}}/S_{\boldsymbol{h}}$$	(8) (9)

4. PB likelihood function: centric perfect general twin case.

In the perfect general twin case (N equal twin domains) the PDF for centric reflexions is:	
$$\mathrm{P}_{\mathrm{ct}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}) \;=\; \frac{(N/2)^{N/2} J_{\boldsymbol{h}}^{N/2-1}}{\Gamma(N/2)\,S_{\boldsymbol{h}}^{N/2}}\exp(-N J_{\boldsymbol{h}}/2S_{\boldsymbol{h}})$$ $$-\mathrm{LLG}_{\mathrm{ct}\boldsymbol{h}}(g,\mathbf{U},\alpha) \;=\; (N/2)\,(\ln(S_{\boldsymbol{h}})+J_{\boldsymbol{h}}/S_{\boldsymbol{h}})$$	(10) (11)
For N = 2 this reduces to the acentric untwinned case (3).	

5. PB likelihood function: acentric imperfect general and hemihedral twin cases.

In the imperfect general twin case (*N* unequal twin domains) the PDF for acentric reflexions is:	
$\mathrm{P}_{\mathrm{at}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}) \;=\; S_{\boldsymbol{h}}^{-1}\,\Sigma_i^N\,\alpha_i^{-1}\,(\Pi_{j=1,\,j\neq i}^N\,\frac{\alpha_i}{\alpha_i-\alpha_j})\,\exp(-J_{\boldsymbol{h}}/\alpha_i S_{\boldsymbol{h}})$	(12)
In the imperfect hemihedral twin case (*N* = 2) this reduces to:	
$\mathrm{P}_{\mathrm{at}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}) \;=\; ((1-2\alpha)S_{\boldsymbol{h}})^{-1}\,(\exp(-J_{\boldsymbol{h}}/(1-\alpha)S_{\boldsymbol{h}}) - \exp(-J_{\boldsymbol{h}}/\alpha S_{\boldsymbol{h}}))$ $-\mathrm{LLG}_{\mathrm{at}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}) \;=\; -\ln(\mathrm{P}_{\mathrm{at}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}))$	(13) (14)

6. PB likelihood function: centric imperfect hemihedral twin case.

In the imperfect hemihedral twin case the PDF for centric reflexions is:	
$\mathrm{P}_{\mathrm{ct}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}) \;=\; (2\sqrt{\alpha(1-\alpha)}S_{\boldsymbol{h}})^{-1}\,\exp(-J_{\boldsymbol{h}}/2\alpha S_{\boldsymbol{h}})\;{}_1\mathrm{F}_1(½;1;(1-2\alpha)J_{\boldsymbol{h}}/2\alpha(1-\alpha)S_{\boldsymbol{h}})$ $= (2\sqrt{\alpha(1-\alpha)}S_{\boldsymbol{h}})^{-1}\,\exp(-J_{\boldsymbol{h}}/4\alpha(1-\alpha)S_{\boldsymbol{h}})\;\mathrm{I}_0((1-2\alpha)J_{\boldsymbol{h}}/4\alpha(1-\alpha)S_{\boldsymbol{h}})$ $= (2\sqrt{\alpha(1-\alpha)}S_{\boldsymbol{h}})^{-1}\,\exp(-J_{\boldsymbol{h}}/2(1-\alpha)S_{\boldsymbol{h}})\;\mathrm{I'}_0((1-2\alpha)J_{\boldsymbol{h}}/4\alpha(1-\alpha)S_{\boldsymbol{h}})$ $-\mathrm{LLG}_{\mathrm{ct}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}) \;=\; -\ln(\mathrm{P}_{\mathrm{ct}\,\boldsymbol{h}}(J_{\boldsymbol{h}}\,\vert\,S_{\boldsymbol{h}}))$	 (15) (16)

where ${}_1\mathrm{F}_1(a; b; z)$ is Kummer’s confluent hypergeometric function, $\mathrm{I}_0(z)$ is the zero-order modified Bessel function and $\mathrm{I}_0'(x)$ is the scaled zero-order modified Bessel function: $\mathrm{I}_0'(x)=\exp(-x)\,\mathrm{I}_0(x)$. This avoids the division by *α* for *α* near to zero. In (15) it is not necessary to deal specifically with the edge cases where *α* is near 0 or 0.5 since unlike (13) there is no cancellation of large terms.

7. FW likelihood function: untwinned acentric case.

Since the prior distribution $P_h(J_h \mid S_h)$ of the true intensity J_h (conditional on the prior expectation S_h of J_h) is independent of the error distribution $P_h(I_h \mid J_h, \sigma_h)$ of the measured intensity I_h, then the joint distribution of I_h and J_h is simply the product of their respective densities:	
$$P_h(I_h, J_h \mid S_h, \sigma_h) = P_h(I_h \mid J_h, \sigma_h)\; P_h(J_h \mid S_h)$$	(17)
The PDF of I_h conditional on S_h and the standard deviation σ_h of I_h is therefore given by marginalising out the unknown J_h from the joint distribution:	
$$\begin{aligned} P_h(I_h \mid S_h, \sigma_h) &= \int_0^\infty P_h(I_h, J_h \mid S_h, \sigma_h)\, dJ_h \\ &= \int_0^\infty P_h(I_h \mid J_h, \sigma_h)\, P_h(J_h \mid S_h)\, dJ_h \end{aligned}$$	(18)
We assume that $P_h(I_h \mid J_h, \sigma_h)$ is the normal error distribution of I_h :	
$$P_h(I_h \mid J_h, \sigma_h) = (\sigma_h \sqrt{2\pi})^{-1} \exp(-(I_h - J_h)^2/2\sigma_h{}^2)$$	(20)
In the untwinned acentric case:	
$$P_h(J_h \mid S_h) = S_h^{-1} \exp(-J_h/S_h)$$	
so in this case:	
$$P_h(I_h \mid S_h, \sigma_h) = (\sigma_h \sqrt{2\pi}\, S_h)^{-1} \int_0^\infty \exp(-(I_h - J_h)^2/2\sigma_h{}^2) \exp(-J_h/S_h)\, dJ_h$$	(21)

8. FW integral: case of small integer powers of J_h.

The prior distribution $\mathrm{P}_{\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}})$ of J_h takes different forms depending on the centricity of ***h*** and the twin fraction(s). Also, very similar integrals will be required later for the evaluation in the various specific cases of the posterior moments $\langle J_{\boldsymbol{h}}^m \rangle$ of J_h, so it is convenient to generalise the form of the required integral $\mathrm{Q}_{\boldsymbol{h}}(\mu, \nu, \xi)$ here, incorporating the order *m* of the moment:	
$$\begin{aligned} \mathrm{Q}_{\boldsymbol{h}}(\mu,\nu,\xi) &= (\sigma_{\boldsymbol{h}}\sqrt{2\pi}\,S_{\boldsymbol{h}}^{\mu})^{-1}\int_0^\infty J_{\boldsymbol{h}}^{\nu}\exp(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\,2})\exp(-\xi J_{\boldsymbol{h}}/S_{\boldsymbol{h}})\,dJ_{\boldsymbol{h}} \\ &= (\sigma_{\boldsymbol{h}}\sqrt{2\pi}\,S_{\boldsymbol{h}}^{\mu})^{-1}\int_0^\infty J_{\boldsymbol{h}}^{\nu}\exp(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\,2}-\xi J_{\boldsymbol{h}}/S_{\boldsymbol{h}})\,dJ_{\boldsymbol{h}} \\ &= (\sigma_{\boldsymbol{h}}\sqrt{2\pi}\,S_{\boldsymbol{h}}^{\mu})^{-1}\int_0^\infty J_{\boldsymbol{h}}^{\nu}\exp(-I_{\boldsymbol{h}}^{\,2}/2\sigma_{\boldsymbol{h}}^{\,2}+I_{\boldsymbol{h}}J_{\boldsymbol{h}}/\sigma_{\boldsymbol{h}}^{\,2}-J_{\boldsymbol{h}}^{\,2}/2\sigma_{\boldsymbol{h}}^{\,2}-\xi J_{\boldsymbol{h}}/S_{\boldsymbol{h}})\,dJ_{\boldsymbol{h}} \\ &= (\sigma_{\boldsymbol{h}}\sqrt{2\pi}\,S_{\boldsymbol{h}}^{\mu})^{-1}\exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2-\xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}}) \\ &\qquad \int_0^\infty J_{\boldsymbol{h}}^{\nu}\exp(-(J_{\boldsymbol{h}}/\sigma_{\boldsymbol{h}}-(I_{\boldsymbol{h}}/\sigma_{\boldsymbol{h}}-\xi\sigma_{\boldsymbol{h}}/S_{\boldsymbol{h}}))^2/2)\,dJ_{\boldsymbol{h}} \\ &= \sigma_{\boldsymbol{h}}^{\nu}(\sqrt{2\pi}\,S_{\boldsymbol{h}}^{\mu})^{-1}\exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2-\xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}})\int_0^\infty u_{\boldsymbol{h}}^{\nu}\exp(-(u_{\boldsymbol{h}}-t_{\boldsymbol{h}}(\xi))^2/2)\,du_{\boldsymbol{h}} \end{aligned}$$	(22)
where $u_{\boldsymbol{h}}=J_{\boldsymbol{h}}/\sigma_{\boldsymbol{h}}$ and $t_{\boldsymbol{h}}(\xi)=I_{\boldsymbol{h}}/\sigma_{\boldsymbol{h}}-\xi\sigma_{\boldsymbol{h}}/S_{\boldsymbol{h}}$. For small positive integer values (0, 1 or 2) of ν the integral in (22) can be expressed in terms of the normal probability function φ and its integral Φ:	
$$\begin{aligned} \mathrm{Q}_{\boldsymbol{h}}(\mu,0,\xi) &= (\sqrt{2\pi}\,S_{\boldsymbol{h}}^{\mu})^{-1}\exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2-\xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}})\int_0^\infty \exp(-(u_{\boldsymbol{h}}-t_{\boldsymbol{h}}(\xi))^2/2)\,du_{\boldsymbol{h}} \\ &= S_{\boldsymbol{h}}^{-\mu}\exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2-\xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}})\,\Phi(t_{\boldsymbol{h}}(\xi)) \end{aligned}$$	(23)
$$\begin{aligned} \mathrm{Q}_{\boldsymbol{h}}(\mu,1,\xi) &= \sigma_{\boldsymbol{h}}(\sqrt{2\pi}\,S_{\boldsymbol{h}}^{\mu})^{-1}\exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2-\xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}})\int_0^\infty u_{\boldsymbol{h}}\exp(-(u_{\boldsymbol{h}}-t_{\boldsymbol{h}}(\xi))^2/2)\,du_{\boldsymbol{h}} \\ &= \sigma_{\boldsymbol{h}}S_{\boldsymbol{h}}^{-\mu}\exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2-\xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}})\,(t_{\boldsymbol{h}}(\xi)\,\Phi(t_{\boldsymbol{h}}(\xi))+\phi(t_{\boldsymbol{h}}(\xi))) \end{aligned}$$	(24)
$$\begin{aligned} \mathrm{Q}_{\boldsymbol{h}}(\mu,2,\xi) &= \sigma_{\boldsymbol{h}}^2(\sqrt{2\pi}\,S_{\boldsymbol{h}}^{\mu})^{-1}\exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2-\xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}})\int_0^\infty u_{\boldsymbol{h}}^2\exp(-(u_{\boldsymbol{h}}-t_{\boldsymbol{h}}(\xi))^2/2)\,du_{\boldsymbol{h}} \\ &= \sigma_{\boldsymbol{h}}^2S_{\boldsymbol{h}}^{-\mu}\exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2-\xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}})\,((t_{\boldsymbol{h}}^2(\xi)+1)\,\Phi(t_{\boldsymbol{h}}(\xi))+t_{\boldsymbol{h}}(\xi)\,\phi(t_{\boldsymbol{h}}(\xi))) \end{aligned}$$	(25)

9. FW integral: case of non-integer and large integer powers of J_h.

For other values of ν the integral in (22) can be expressed in terms of the parabolic cylinder functions D, or alternatively U and V [http://mathworld.wolfram.com/ParabolicCylinderFunction.html]. Factoring out the constant term in the integral:	
$$\int_0^\infty u^\nu \exp(-(u-t)^2/2)\, du \quad = \quad \exp(-t^2/2) \int_0^\infty u^\nu \exp(-u^2/2+t\,u)\, du$$	(26)
Using the formula in Gradshteyn & Ryzhik, 7th Ed., p.365, eqn. 3.462(1) for $\nu > 0$ and $\beta > 0$:	
$$\int_0^\infty x^{\nu-1} \exp(-\beta x^2 - \gamma x)\, dx \quad = \quad (2\beta)^{-\nu/2} \Gamma(\nu) \exp(\gamma^2/8\beta)\, \mathrm{D}_{-\nu}(\gamma/\sqrt{2\beta})$$	(27)
Making the necessary substitutions:	
$$\exp(-t^2/2) \int_0^\infty u^\nu \exp(-u^2/2+t\,u)\, du \quad = \quad \Gamma(\nu+1) \exp(-t^2/4)\, \mathrm{D}_{-\nu-1}(-t)$$	(28)
An alternative definition of the PCFs (see above MathWorld site) is:	
$$\mathrm{U}(a, x) \quad = \quad \mathrm{D}_{-a-½}(x)$$	(29)
Therefore for $a = \nu + ½$:	
$$\int_0^\infty u^\nu \exp(-(u-t)^2/2)\, du \quad = \quad \Gamma(\nu+1) \exp(-t^2/4)\, \mathrm{U}(\nu+½, -t)$$	(30)
Therefore from (22) the required integral in the general case is:	
$$\mathrm{Q}_{\boldsymbol{h}}(\mu, \nu, \xi) \quad = \quad \sigma_{\boldsymbol{h}}^\nu (\sqrt{2\pi} S_{\boldsymbol{h}}^\mu)^{-1} \exp((\xi\sigma_{\boldsymbol{h}})^2/2S_{\boldsymbol{h}}^2 - \xi I_{\boldsymbol{h}}/S_{\boldsymbol{h}}) \; \Gamma(\nu+1) \exp(-t_{\boldsymbol{h}}^2(\xi)/4)\, \mathrm{U}(\nu+½, -t_{\boldsymbol{h}}(\xi))$$	(31)

10. FW integral: implementation of parabolic cylinder functions in Fortran 90.

A Fortran 90 subroutine is available to calculate the PCFs U(a,x) and V(a,x) for $x \geq 0$ by numerical methods [Netlib software repository: algorithm toms/850; see also http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.100.6920&rep=rep1&type=pdf].

To avoid floating-point underflows and overflows in the exponential terms and to improve the relative accuracy of the result, the algorithm returns scaled PCFs:

$$\tilde{\mathrm{U}}(a,x) = \mathrm{F}(a,x)\,\mathrm{U}(a,x) \tag{32}$$

$$\tilde{\mathrm{V}}(a,x) = \mathrm{V}(a,x)\,/\,\mathrm{F}(a,x) \tag{33}$$

$$\mathrm{V}(a,x) = (\Gamma(\tfrac{1}{2}+a)/\pi)\,(\sin(\pi a)\,\mathrm{D}_{-a-\frac{1}{2}}(x) + \mathrm{D}_{-a-\frac{1}{2}}(-x)) \tag{34}$$

where the scaling factor F(a,x) is:

$$\mathrm{F}(a,x) = (x/2+\sqrt{x^2/4+a})^{a}\,\exp((x/2)\,\sqrt{x^2/4+a}-a/2) \tag{35}$$

Therefore now writing (30) in terms of the scaled PCFs:

$$\begin{aligned}\int_0^\infty u^{\nu}\exp(-(u-t)^2/2)\,du &= \Gamma(\tfrac{1}{2}+a)\,\exp(-t^2/4)\,\mathrm{U}(a,-t)\\ &= \Gamma(\tfrac{1}{2}+a)\,\exp(-t^2/4)\,\tilde{\mathrm{U}}(a,-t)\,/\,\mathrm{F}(a,-t)\\ &= \Gamma(\tfrac{1}{2}+a)\,(-t/2+\sqrt{t^2/4+a})^{-a}\\ &\quad\ \exp(-t^2/4+(t/2)\sqrt{t^2/4+a}+a/2)\,\tilde{\mathrm{U}}(a,-t)\end{aligned} \tag{36}$$

Since the PCF algorithm used cannot return function values for $x < 0$, the following transformation must be used:

$$\begin{aligned}\mathrm{U}(a,x) &= \pi\,\mathrm{V}(a,-x)\,/\,\Gamma(\tfrac{1}{2}+a) - \sin(\pi a)\,\mathrm{U}(a,-x)\\ &= \mathrm{F}(a,-x)\,(\pi\,\tilde{\mathrm{V}}(a,-x)\,/\,\Gamma(\tfrac{1}{2}+a) - \sin(\pi a)\,\tilde{\mathrm{U}}(a,-x)\,/\,\mathrm{F}^2(a,-x))\end{aligned} \tag{37}$$

or in terms of t for $t > 0$:

$$\mathrm{U}(a,-t) = \mathrm{F}(a,t)\,(\pi\,\tilde{\mathrm{V}}(a,t)\,/\,\Gamma(\tfrac{1}{2}+a) - \sin(\pi a)\,\tilde{\mathrm{U}}(a,t)\,/\,\mathrm{F}^2(a,t)) \tag{38}$$

Substitution of (38) in (36) and again combining exponential terms as before to avoid floating-point overflows then gives the required value of the integral for $t > 0$:

$$\begin{aligned}\int_0^\infty u^{\nu}\exp(-(u-t)^2/2)\,du &= \Gamma(\tfrac{1}{2}+a)\,(t/2+\sqrt{t^2/4+a})^{a}\,\exp(-t^2/4+(t/2)\sqrt{t^2/4+a}-a/2)\\ &\quad\ (\pi\,\tilde{\mathrm{V}}(a,t)\,/\,\Gamma(\tfrac{1}{2}+a) - \sin(\pi a)\,\tilde{\mathrm{U}}(a,t)\,/\,\mathrm{F}^2(a,t))\end{aligned} \tag{39}$$

11. FW likelihood function & posterior moments: untwinned acentric & centric perfect hemihedral twin cases.

In the untwinned acentric & centric perfect hemihedral twin cases, the required form of the Q integral is:

$$\begin{aligned} \mathrm{P}_{\boldsymbol{h}}(I_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}) &= \left(\sigma_{\boldsymbol{h}} \sqrt{2\pi} S_{\boldsymbol{h}}\right)^{-1} \int_0^{\infty} \exp\left(-(I_{\boldsymbol{h}} - J_{\boldsymbol{h}})^2 / 2\sigma_{\boldsymbol{h}}^{\,2}\right) \exp\left(-J_{\boldsymbol{h}} / S_{\boldsymbol{h}}\right) dJ_{\boldsymbol{h}} \\ &= Q_{\boldsymbol{h}}(1,\, 0,\, 1) \\ &= S_{\boldsymbol{h}}^{-1} \exp\left(\sigma_{\boldsymbol{h}}^2 / 2 S_{\boldsymbol{h}}^2 - I_{\boldsymbol{h}} / S_{\boldsymbol{h}}\right) \Phi\left(t_{\boldsymbol{h}}(1)\right) \end{aligned} \tag{40}$$

where $t_{\boldsymbol{h}}(1) = I_{\boldsymbol{h}}/\sigma_{\boldsymbol{h}} - \sigma_{\boldsymbol{h}}/S_{\boldsymbol{h}}$. Hence the contribution to the negative log-likelihood gain is:

$$-\mathrm{LLG}_{\mathrm{a}\boldsymbol{h}}(g, \mathbf{U}) = \ln\left(S_{\boldsymbol{h}} / \Phi\left(t_{\boldsymbol{h}}(1)\right)\right) - \sigma_{\boldsymbol{h}}^{\,2} / 2 S_{\boldsymbol{h}}^2 + I_{\boldsymbol{h}} / S_{\boldsymbol{h}} \tag{41}$$

In the general untwinned case the posterior density of $J_{\boldsymbol{h}}$ from Bayes' theorem is the normalised joint probability density (14) $\mathrm{P}_{\boldsymbol{h}}(I_{\boldsymbol{h}}, J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}})$:

$$\begin{aligned} \mathrm{P}_{\boldsymbol{h}}(J_{\boldsymbol{h}} \mid I_{\boldsymbol{h}}, S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}) &= \mathrm{P}_{\boldsymbol{h}}(I_{\boldsymbol{h}}, J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}) \;/\; \int_0^{\infty} \mathrm{P}_{\boldsymbol{h}}(I_{\boldsymbol{h}}, J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}})\, dJ_{\boldsymbol{h}} \\ &= \mathrm{P}_{\boldsymbol{h}}(I_{\boldsymbol{h}} \mid J_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}})\, \mathrm{P}_{\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}) \;/\; \int_0^{\infty} \mathrm{P}_{\boldsymbol{h}}(I_{\boldsymbol{h}} \mid J_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}})\, \mathrm{P}_{\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}})\, dJ_{\boldsymbol{h}} \end{aligned} \tag{42}$$

The *m*'th posterior moment (expectation of *m*'th power) of $J_{\boldsymbol{h}}$ is then:

$$\langle J_{\boldsymbol{h}}^m \rangle = \int_0^{\infty} J_{\boldsymbol{h}}^m\, \mathrm{P}_{\boldsymbol{h}}(J_{\boldsymbol{h}} \mid I_{\boldsymbol{h}}, S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}})\, dJ_{\boldsymbol{h}} \tag{43}$$

In the untwinned acentric and centric perfect hemihedral twin cases this is:

$$\begin{aligned} \langle J_{\boldsymbol{h}}^m \rangle &= \int_0^{\infty} J_{\boldsymbol{h}}^m\, \mathrm{P}_{\boldsymbol{h}}(I_{\boldsymbol{h}} \mid J_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}})\, \mathrm{P}_{\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}})\, dJ_{\boldsymbol{h}} \;/\; \int_0^{\infty} \mathrm{P}_{\boldsymbol{h}}(I_{\boldsymbol{h}} \mid J_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}})\, \mathrm{P}_{\boldsymbol{h}}(J_{\boldsymbol{h}} \mid S_{\boldsymbol{h}})\, dJ_{\boldsymbol{h}} \\ &= Q_{\boldsymbol{h}}(0,\, m,\, 1) \;/\; Q_{\boldsymbol{h}}(0,\, 0,\, 1) \end{aligned} \tag{44}$$

Note that for all the moments the value of μ is irrelevant since it cancels out.

In this case the posterior half- (m = ½) and first-order (m = 1) moments (*i.e.* the estimates of the true amplitude and intensity) are:

$$\langle F_{\boldsymbol{h}} \rangle = \langle J_{\boldsymbol{h}}^{½} \rangle = \left(\sigma_{\boldsymbol{h}} / 2\pi\right)^{½}\, \Gamma\left(\tfrac{3}{2}\right) \exp\left(-t_{\boldsymbol{h}}^{\,2}(1)/4\right) \mathrm{U}\left(1, -t_{\boldsymbol{h}}(1)\right) / \Phi\left(t_{\boldsymbol{h}}(1)\right) \tag{45}$$

$$\begin{aligned} \langle J_{\boldsymbol{h}} \rangle &= \left(t_{\boldsymbol{h}}(1)\, \Phi\left(t_{\boldsymbol{h}}(1)\right) + \phi\left(t_{\boldsymbol{h}}(1)\right)\right) / \Phi\left(t_{\boldsymbol{h}}(1)\right) \\ &= t_{\boldsymbol{h}}(1) + \phi\left(t_{\boldsymbol{h}}(1)\right) / \Phi\left(t_{\boldsymbol{h}}(1)\right) \end{aligned} \tag{46}$$

The standard deviation of *F* is the square root of the second moment of the deviation *F* from the mean:

$$\begin{aligned} \sigma(F_{\boldsymbol{h}}) &= \left\langle \left(F_{\boldsymbol{h}} - \langle F_{\boldsymbol{h}} \rangle\right)^2 \right\rangle^{½} \\ &= \left(\langle F_{\boldsymbol{h}}^2 \rangle - \langle F_{\boldsymbol{h}} \rangle^2\right)^{½} \\ &= \left(\langle J_{\boldsymbol{h}} \rangle - \langle J_{\boldsymbol{h}}^{½} \rangle^2\right)^{½} \end{aligned} \tag{47}$$

12. FW likelihood function & posterior moments: untwinned centric case.

For untwinned centric reflexions we have similarly:

$$\begin{aligned} \mathrm{P}_{c\boldsymbol{h}}(I_{\boldsymbol{h}}\,|\,S_{\boldsymbol{h}},\sigma_{\boldsymbol{h}}) &= (2\pi\,\sigma_{\boldsymbol{h}}S_{\boldsymbol{h}}^{½})^{-1}\int_0^\infty J_{\boldsymbol{h}}^{-½}\exp(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^2)\exp(-J_{\boldsymbol{h}}/2S_{\boldsymbol{h}})\,dJ_{\boldsymbol{h}} \\ &= (2\pi)^{-½}\mathrm{Q}_{\mathbf{h}}(½,\,-½,\,½) \\ &= (2\pi(\sigma_{\boldsymbol{h}}S_{\boldsymbol{h}})^{½})^{-1}\exp(\sigma_{\boldsymbol{h}}^2/8\,S_{\boldsymbol{h}}^2-I_{\boldsymbol{h}}/2S_{\boldsymbol{h}})\,\Gamma(½)\exp(-t_{\boldsymbol{h}}^2(½)/4)\,\mathrm{U}(0,-t_{\boldsymbol{h}}(½)) \end{aligned} \tag{48}$$

where $t_{\boldsymbol{h}}(½)=I_{\boldsymbol{h}}/\sigma_{\boldsymbol{h}}-\sigma_{\boldsymbol{h}}/2S_{\boldsymbol{h}}$. Hence the contribution to the negative log-likelihood gain in the centric case is:

$$-\mathrm{LLG}_{c\boldsymbol{h}}(g,\mathbf{U}) = \ln(2\pi(\sigma_{\boldsymbol{h}}S_{\boldsymbol{h}})^{½}\,/\,\Gamma(½)\exp(-t_{\boldsymbol{h}}^2(½)/4))\,\mathrm{U}(0,-t_{\boldsymbol{h}}(½)) - \sigma_{\boldsymbol{h}}^2/8\,S_{\boldsymbol{h}}^2 + I_{\boldsymbol{h}}/2S_{\boldsymbol{h}} \tag{49}$$

Note that the centric contribution to the FW function is not simply related to the acentric one, as it was for the PB function.

The *m*'th posterior moment of $J_{\boldsymbol{h}}$ in this case is then:

$$\begin{aligned} \langle J_{\boldsymbol{h}}^m\rangle &= \mathrm{Q}_{\mathbf{h}}(0,\,m-½,\,½)\,/\,\mathrm{Q}_{\mathbf{h}}(0,\,-½,\,½) \\ &= \mathrm{U}(m,-t_{\boldsymbol{h}}(½))\,/\,\mathrm{U}(0,-t_{\boldsymbol{h}}(½)) \end{aligned} \tag{50}$$

The half- and first-order posterior moments of $J_{\boldsymbol{h}}$ are then:

$$\begin{aligned} \langle J_{\boldsymbol{h}}^{½}\rangle &= \mathrm{Q}_{\mathbf{h}}(0,\,0,\,½)\,/\,\mathrm{Q}_{\mathbf{h}}(0,\,-½,\,½) \\ &= (2\pi\,\sigma_{\boldsymbol{h}})^{½}\,\Phi(t_{\boldsymbol{h}}(½))\,/\,\Gamma(½)\exp(-t_{\boldsymbol{h}}^2(½)/4)\,\mathrm{U}(0,-t_{\boldsymbol{h}}(½)) \\ \langle J_{\boldsymbol{h}}\rangle &= \mathrm{Q}_{\mathbf{h}}(0,\,½,\,½)\,/\,\mathrm{Q}_{\mathbf{h}}(0,\,-½,\,½) \\ &= \sigma_{\boldsymbol{h}}\,\Gamma(\tfrac{3}{2})\,\mathrm{U}(1,-t_{\boldsymbol{h}}(½))\,/\,\Gamma(½)\,\mathrm{U}(0,-t_{\boldsymbol{h}}(½)) \end{aligned} \tag{51}$$

13. FW likelihood function & posterior moments: acentric perfect hemihedral twin case.

For perfect hemihedrally twinned acentric reflexions, substituting (8) and (20) in (18) and again discarding factors that are independent of the parameters g and $\mathbf{U}$:	
$$\begin{aligned} \mathrm{P}_{\mathrm{at}\boldsymbol{h}}(I_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}) &= 4\,(\sigma_{\boldsymbol{h}}\sqrt{(2\pi)}S_{\boldsymbol{h}}^2)^{-1}\int_0^\infty J_{\boldsymbol{h}} \exp(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\,2}) \exp(-2J_{\boldsymbol{h}}/S_{\boldsymbol{h}})\, dJ_{\boldsymbol{h}} \\ &= 4\,Q_{\boldsymbol{h}}(2, 1, 2) \\ &= 4\,\sigma_{\boldsymbol{h}} S_{\boldsymbol{h}}^{-2} \exp(2\,\sigma_{\boldsymbol{h}}^2/S_{\boldsymbol{h}}^2 - 2\,I_{\boldsymbol{h}}/S_{\boldsymbol{h}})\,(t_{\boldsymbol{h}}(2)\,\Phi(t_{\boldsymbol{h}}(2)) + \phi(t_{\boldsymbol{h}}(2))) \end{aligned}$$	(52)
where $t_{\boldsymbol{h}}(2)=I_{\boldsymbol{h}}/\sigma_{\boldsymbol{h}}-2\sigma_{\boldsymbol{h}}/S_{\boldsymbol{h}}$. Hence the contribution to the negative log-likelihood gain in the acentric perfect hemihedral twin case is:	
$$-\mathrm{LLG}_{\mathrm{at}\boldsymbol{h}}(g, \mathbf{U}) = \ln(S_{\boldsymbol{h}}^2 / 4\,\sigma_{\boldsymbol{h}}\,(t_{\boldsymbol{h}}(2)\,\Phi(t_{\boldsymbol{h}}(2)) + \phi(t_{\boldsymbol{h}}(2)))) - 2\,\sigma_{\boldsymbol{h}}^2/S_{\boldsymbol{h}}^2 + 2\,I_{\boldsymbol{h}}/S_{\boldsymbol{h}}$$	(53)
The m'th posterior moment of $J_{\boldsymbol{h}}$ in this case is then:	
$$\langle J_{\boldsymbol{h}}^m \rangle = Q_{\boldsymbol{h}}(0, m+1, 2) / Q_{\boldsymbol{h}}(0, 1, 2)$$	(54)
The half- and first-order posterior moments of $J_{\boldsymbol{h}}$ are:	
$$\begin{aligned} \langle J_{\boldsymbol{h}}^{½} \rangle &= Q_{\boldsymbol{h}}(0, \tfrac{3}{2}, 2) / Q_{\boldsymbol{h}}(0, 1, 2) \\ &= (\sigma_{\boldsymbol{h}}/2\pi)^{½}\,\Gamma(\tfrac{5}{2}) \exp(-t_{\boldsymbol{h}}^2(2)/4)\,\mathrm{U}(2, -t_{\boldsymbol{h}}(2)) / (t_{\boldsymbol{h}}(2)\,\Phi(t_{\boldsymbol{h}}(2)) + \phi(t_{\boldsymbol{h}}(2))) \\ \langle J_{\boldsymbol{h}} \rangle &= Q_{\boldsymbol{h}}(0, 2, 2) / Q_{\boldsymbol{h}}(0, 1, 2) \\ &= \sigma_{\boldsymbol{h}}\,((t_{\boldsymbol{h}}^2(2)+1)\,\Phi(t_{\boldsymbol{h}}(2)) + t_{\boldsymbol{h}}(2)\,\phi(t_{\boldsymbol{h}}(2))) / (t_{\boldsymbol{h}}(2)\,\Phi(t_{\boldsymbol{h}}(2)) + \phi(t_{\boldsymbol{h}}(2))) \\ &= \sigma_{\boldsymbol{h}}\,(t_{\boldsymbol{h}}^2(2) + 1 + t_{\boldsymbol{h}}(2)\,\phi(t_{\boldsymbol{h}}(2)) / \Phi(t_{\boldsymbol{h}}(2))) / (t_{\boldsymbol{h}}(2) + \phi(t_{\boldsymbol{h}}(2)) / \Phi(t_{\boldsymbol{h}}(2))) \end{aligned}$$	(55)

14. FW likelihood function & posterior moments: acentric imperfect hemihedral twin case.

The PDF and -LLG in the acentric imperfect hemihedral twin case is:

$$\mathrm{P}_{\mathrm{at}\boldsymbol{h}}(I_{\boldsymbol{h}} \,|\, S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}, \alpha) \;=\; \mathrm{f}(1-\alpha) + \mathrm{f}(\alpha) \tag{56}$$

where:

$$\begin{aligned}
\mathrm{f}(x) &= \left(\sigma_{\boldsymbol{h}}\sqrt{2\pi}(2x-1)S_{\boldsymbol{h}}\right)^{-1}\int_0^\infty \exp\left(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\,2}\right)\,\exp\left(-J_{\boldsymbol{h}}/x\,S_{\boldsymbol{h}}\right)\,dJ_{\boldsymbol{h}} \\
&= (2x-1)^{-1}\,Q_{\boldsymbol{h}}(1,\,0,\,x^{-1}) && (57) \\
\mathrm{P}_{\mathrm{at}\boldsymbol{h}}(I_{\boldsymbol{h}} \,|\, S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}, \alpha) &= (1-2\alpha)^{-1}\left(Q_{\boldsymbol{h}}(1,\,0,\,(1-\alpha)^{-1}) - Q_{\boldsymbol{h}}(1,\,0,\,\alpha^{-1})\right) && (58) \\
-\mathrm{LLG}_{\mathrm{at}\boldsymbol{h}}(g, \mathbf{U}, \alpha) &= -\ln\left(\mathrm{P}_{\mathrm{at}\boldsymbol{h}}(I_{\boldsymbol{h}} \,|\, S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}, \alpha)\right) && (59)
\end{aligned}$$

In (58) & (59) care must be taken to deal with values of the twin fraction *α* near zero causing ill-conditioning which can occur during optimisation of *α*. We use the scaled cumulative normal density, factoring out the exponentially increasing component of the function: $\Phi'(t_{\boldsymbol{h}}(\alpha^{-1})) = \exp(t_{\boldsymbol{h}}^2(\alpha^{-1})/2)\,\Phi(t_{\boldsymbol{h}}(\alpha^{-1}))$ whenever $t_{\boldsymbol{h}}(\alpha^{-1}) \le 0$ in the calculation of $Q_{\boldsymbol{h}}(1,\,0,\,\alpha^{-1})$ using (23). It is not necessary to deal similarly with values of *α* near 1 in the first term of (58) since we can always replace 1-*α* by *α* (*i.e.* by definition *α* can always be moved to the range $0 \le \alpha \le 0.5$). By using a first-order Taylor expansion in 1-2*α* we can deal with ill-conditioning due to *α* near the perfect twin case 0.5 (since then both numerator and denominator in (58) are near zero).

The *m*'th posterior moment of $J_{\boldsymbol{h}}$ in this case is then:

$$\langle J_{\boldsymbol{h}}^m \rangle = \left(Q_{\boldsymbol{h}}(0,\,m,\,(1-\alpha)^{-1}) - Q_{\boldsymbol{h}}(0,\,m,\,\alpha^{-1})\right) \,/\, \left(Q_{\boldsymbol{h}}(0,\,0,\,(1-\alpha)^{-1}) - Q_{\boldsymbol{h}}(0,\,0,\,\alpha^{-1})\right) \tag{60}$$

The half- and first-order posterior moments of $J_{\boldsymbol{h}}$ are:

$$\begin{aligned}
\langle J_{\boldsymbol{h}}^{½} \rangle &= \left(Q_{\boldsymbol{h}}(0,\,½,\,(1-\alpha)^{-1}) - Q_{\boldsymbol{h}}(0,\,½,\,\alpha^{-1})\right) \,/\, \left(Q_{\boldsymbol{h}}(0,\,0,\,(1-\alpha)^{-1}) - Q_{\boldsymbol{h}}(0,\,0,\,\alpha^{-1})\right) \\
&= (\sigma_{\boldsymbol{h}}/2\pi)^{½}\,\Gamma\left(\tfrac{3}{2}\right)\left(\exp\left(-t_{\boldsymbol{h}}^2((1-\alpha)^{-1})/4\right)\mathrm{U}\left(1,-t_{\boldsymbol{h}}((1-\alpha)^{-1})\right)\right) - \\
&\quad \exp\left(-t_{\boldsymbol{h}}^2(\alpha^{-1})/4\right)\mathrm{U}\left(1,-t_{\boldsymbol{h}}(\alpha^{-1})\right)) \,/\, \left(\Phi(t_{\boldsymbol{h}}((1-\alpha)^{-1})) - \Phi(t_{\boldsymbol{h}}(\alpha^{-1}))\right) && (61) \\
\langle J_{\boldsymbol{h}} \rangle &= \left(Q_{\boldsymbol{h}}(0,\,1,\,(1-\alpha)^{-1}) - Q_{\boldsymbol{h}}(0,\,1,\,\alpha^{-1})\right) \,/\, \left(Q_{\boldsymbol{h}}(0,\,0,\,(1-\alpha)^{-1}) - Q_{\boldsymbol{h}}(0,\,0,\,\alpha^{-1})\right) \\
&= \sigma_{\boldsymbol{h}}\left(t_{\boldsymbol{h}}((1-\alpha)^{-1})\,\Phi(t_{\boldsymbol{h}}((1-\alpha)^{-1})) + \phi(t_{\boldsymbol{h}}((1-\alpha)^{-1})) - \right. \\
&\quad \left. t_{\boldsymbol{h}}(\alpha^{-1})\,\Phi(t_{\boldsymbol{h}}(\alpha^{-1})) - \phi(t_{\boldsymbol{h}}(\alpha^{-1}))\right) \,/\, \left(\Phi(t_{\boldsymbol{h}}((1-\alpha)^{-1})) - \Phi(t_{\boldsymbol{h}}(\alpha^{-1}))\right) && (62)
\end{aligned}$$

15. FW likelihood function & posterior moments: centric imperfect hemihedral twin case.

The PDF in the centric imperfect hemihedral twin case is:	
$$\begin{aligned}\mathrm{P}_{\mathrm{ct}\boldsymbol{h}}(I_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}, \alpha) &= \left(2\,\sigma_{\boldsymbol{h}}\sqrt{2\pi\,\alpha(1-\alpha)}\,S_{\boldsymbol{h}}\right)^{-1}\int_0^\infty \exp\left(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\;2} - J_{\boldsymbol{h}}/2\,\alpha S_{\boldsymbol{h}}\right) \\ &\qquad {}_1\mathrm{F}_1(½;\ 1;\ (1-2\,\alpha)\,J_{\boldsymbol{h}}\,/\,2\,\alpha(1-\alpha)S_{\boldsymbol{h}})\ dJ_{\boldsymbol{h}} \\ &= \left(2\,\sigma_{\boldsymbol{h}}\sqrt{2\pi\,\alpha(1-\alpha)}\,S_{\boldsymbol{h}}\right)^{-1}\int_0^\infty \exp\left(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\;2} - J_{\boldsymbol{h}}/4\,\alpha(1-\alpha)S_{\boldsymbol{h}}\right) \\ &\qquad \mathrm{I}_0((1-2\,\alpha)\,J_{\boldsymbol{h}}\,/\,4\,\alpha(1-\alpha)\,S_{\boldsymbol{h}})\ dJ_{\boldsymbol{h}} \\ &= \left(2\,\sigma_{\boldsymbol{h}}\sqrt{2\pi\,\alpha(1-\alpha)}\,S_{\boldsymbol{h}}\right)^{-1}\int_0^\infty \exp\left(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\;2} - J_{\boldsymbol{h}}/2(1-\alpha)S_{\boldsymbol{h}}\right) \\ &\qquad \mathrm{I}'_0((1-2\,\alpha)\,J_{\boldsymbol{h}}\,/\,4\,\alpha(1-\alpha)\,S_{\boldsymbol{h}})\ dJ_{\boldsymbol{h}}\end{aligned}$$	(63)
$$-\mathrm{LLG}_{\mathrm{ct}\boldsymbol{h}}(g, \mathbf{U}, \alpha) = -\ln\left(\mathrm{P}_{\mathrm{ct}\boldsymbol{h}}(I_{\boldsymbol{h}} \mid S_{\boldsymbol{h}}, \sigma_{\boldsymbol{h}}, \alpha)\right)$$	(64)
In (63) we again use a scaled function, in this case the scaled modified Bessel function I'_0 in order to factor out the exponentially increasing component of the function and thus avoid floating-point overflow. Note that in this case there are no ill-conditioning issues from the division by *α* for values of *α* near to zero. The general *m*'th order posterior moment of $J_{\boldsymbol{h}}$ in this case is then:	
$$\langle J_{\boldsymbol{h}}^m \rangle = \int_0^\infty J_{\boldsymbol{h}}^m \exp\left(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\;2} - J_{\boldsymbol{h}}/2(1-\alpha)S_{\boldsymbol{h}}\right) \mathrm{I}'_0((1-2\,\alpha)\,J_{\boldsymbol{h}}\,/\,4\,\alpha(1-\alpha)\,S_{\boldsymbol{h}})\ dJ_{\boldsymbol{h}}\ \Big/ \int_0^\infty \exp\left(-(I_{\boldsymbol{h}}-J_{\boldsymbol{h}})^2/2\sigma_{\boldsymbol{h}}^{\;2} - J_{\boldsymbol{h}}/2(1-\alpha)S_{\boldsymbol{h}}\right) \mathrm{I}'_0((1-2\,\alpha)\,J_{\boldsymbol{h}}\,/\,4\,\alpha(1-\alpha)\,S_{\boldsymbol{h}})\ dJ_{\boldsymbol{h}}$$	(65)
This expression cannot be further simplified, so the integrals must be evaluated numerically.	

16. REFERENCE

Rees, D.C. (1982) "A General Theory of X-ray Intensity Statistics for Twins by Merohedry". *Acta Cryst.* A**38**, 201-7.