International Tables for Crystallography (2006). Vol. C, Table 6.1.1.10, p. 586.

Table 6.1.1.9. $f_{nl}(\alpha, S) = \int_0^\infty r^n \exp(-\alpha r) j_l(Sr)\, dr$

n \ l	1	2	3	4
0	$\frac{1}{(S^2+\alpha^2)}$	$\frac{2\alpha}{(S^2+\alpha^2)^2}$	$\frac{2(3\alpha^2-S^2)}{(S^2+\alpha^2)^3}$	$\frac{24\alpha(\alpha^2-S^2)}{(S^2+\alpha^2)^4}$
1		$\frac{2S}{(S^2+\alpha^2)^2}$	$\frac{8S\alpha}{(S^2+\alpha^2)^3}$	$\frac{8S(5\alpha^2-S^2)}{(S^2+\alpha^2)^4}$
2			$\frac{8S^2}{(S^2+\alpha^2)^3}$	$\frac{48S^2\alpha}{(S^2+\alpha^2)^4}$
3				$\frac{48S^3}{(S^2+\alpha^2)^4}$

6.1.1.6.1. *Gram–Charlier series*

In the Gram–Charlier series expansion (Kuznetsov, Stratonovich & Tikhonov, 1960), the general p.d.f. $\rho(\mathbf{u})$ is approximated by

$$\left[1 - c^j D_j + \frac{c^{jk}}{2!} D_j D_k - \ldots + (-)^p \frac{c^{jk\ldots\zeta}}{p!} D_\alpha D_\beta \ldots D_\zeta\right] \rho_o(\mathbf{u}). \qquad (6.1.1.43)$$

The operator $D_\alpha D_\beta \ldots D_\zeta$ is the pth partial (covariant) derivative $\partial^p/\partial u_\alpha \partial u_\beta \ldots \partial u_\zeta$, and $c^{jk\ldots\zeta}$ is a contravariant component of the coefficient tensor. The quasi-moment coefficient tensors are symmetric for all permutations of indices. The first four have three, six, ten, and fifteen unique components for site symmetry 1. The third- and fourth-order terms describe the skewness and the kurtosis of the p.d.f., respectively.

The Gram–Charlier series may be rewritten using general multidimensional Hermite polynomial tensors, defined by

$$H_{\alpha\beta\ldots\zeta}(\mathbf{u}) = (-)^p \exp(\tfrac{1}{2}\sigma_{jk}^{-1} u^j u^k) \times D_\alpha D_\beta \ldots D_\zeta \exp(-\tfrac{1}{2}\sigma_{jk}^{-1} u^j u^k). \qquad (6.1.1.44)$$

For $w_j = \sigma_{jk}^{-1} u^k$, and with $\sigma_{jk}^{-1} = \sigma_{kj}^{-1}$ and $w_j w_k = w_k w_j$, the first few general Hermite polynomials may be expressed as

$$\begin{aligned} {}^0H(\mathbf{u}) &= 1 \\ {}^1H_j(\mathbf{u}) &= w_j \\ {}^2H_{jk}(\mathbf{u}) &= w_j w_k - \sigma_{jk}^{-1} \\ {}^3H_{jk}(\mathbf{u}) &= w_j w_k w_l - w_j \sigma_{kl}^{-1} - w_k \sigma_{lj}^{-1} - w_l \sigma_{jk}^{-1} \\ &= w_j w_k w_l - 3 w_{(j} \sigma_{kl)}^{-1} \\ {}^4H_{jklm}(\mathbf{u}) &= w_j w_k w_l w_m - 6 w_{(j} w_k \sigma_{lm)}^{-1} + 3\sigma_{j(k}^{-1} \sigma_{lm)}^{-1}. \end{aligned} \qquad (6.1.1.45)$$

Indices in parentheses indicate terms to be averaged over all unique permutations of those indices.

The Gram–Charlier series is then

$$\rho_o(\mathbf{u}) \left[1 + \frac{1}{3!} c^{jkl} H_{jkl}(\mathbf{u}) + \frac{1}{4!} c^{jklm} H_{jklm}(\mathbf{u}) + \ldots\right], \qquad (6.1.1.46)$$

in which the mean and the dispersion of $\rho_o(\mathbf{u})$ have been chosen to make c^j and c^{jk} vanish.

The Fourier transform, after truncating at the quartic term, gives an approximation to the generalized temperature factor:

$$T(\mathbf{S}) = T_o(\mathbf{S}) \left[1 + \frac{i^3}{3!} c^{jkl} S_j S_k S_l + \frac{i^4}{4!} c^{jklm} S_j S_k S_l S_m\right], \qquad (6.1.1.47)$$

i.e. the Fourier transform of the Hermite polynomial expansion about the Gaussian p.d.f. is a power-series expansion about the Gaussian temperature factor with even-order terms real and odd-order terms imaginary.

Because of the symmetry of the relationship between the Fourier transform of a real function and its inverse, the functional form of the p.d.f. and that of the temperature factor can be interchanged. Exchanging the role of the Hermite polynomials and the power series from the Gram–Charlier expansion has been studied by Scheringer (1985), with the objective of obtaining the one-particle potentials more directly.

Table 6.1.1.10. *Indices nmp allowed by the site symmetry for the functions $H_n(z)\Phi_{mp}(\varphi)$; μ, ν and j are integers such that $m, n \geq 0$; $(-)^n$ implies $p = -$ for n odd and $p = +$ for n even*

Site symmetry	Coordinate axes	Indices
1	Any	All (n, m, p)
$\bar{1}$	Any	$(n, n+2j, p)$
2	$2 \parallel x$	$(n, m, (-)^n)$
	$2 \parallel y$	$(n, m, (-)^{n-m})$
	$2 \parallel z$	$(n, 2\nu, p)$
m	$m \perp x$	$(n, m, (-)^m)$
	$m \perp y$	$(n, m, +)$
	$m \perp z$	$(2\mu, m, p)$
$2/m$	$2 \parallel x, m \perp x$	$(m+2j, m, (-)^m)$
	$2 \parallel y, m \perp y$	$(m+2j, m, +)$
	$2 \parallel z, m \perp z$	$(2\mu, 2\nu, p)$
222	$2 \parallel z, 2 \parallel y$	$(n, 2\nu, (-)^n)$
$mm2$	$2 \parallel x, m \perp z$	$(2\mu, m+)$
	$2 \parallel y, m \perp z$	$(2\mu, m, (-)^m)$
	$2 \parallel z, m \perp y$	$(n, 2\nu, +)$
mmm	$m \perp z, m \perp y, m \perp z$	$(2\mu, 2\nu, +)$
4	$4 \parallel z$	$(n, 4\nu, p)$
$\bar{4}$	$\bar{4} \parallel z$	$(n, 2n+4j, p)$
$4/m$	$4 \parallel z, m \perp z$	$(2\mu, 4\nu, p)$
422	$4 \parallel z, 2 \parallel y$	$(n, 4\nu, (-)^n)$
$4mm$	$4 \parallel z, m \perp y$	$(n, 4\nu, +)$
$\bar{4}2m$	$\bar{4} \parallel z, 2 \parallel x$	$(n, 2n+4j, (-)^n)$
	$\bar{4} \parallel z, m \perp y$	$(n, 2n+4j, +)$
$4/mmm$	$4 \parallel z, m \perp z, m \perp x$	$(2\mu, 4\nu, +)$
3	$3 \parallel z$	$(n, 3\nu, p)$
$\bar{3}$	$\bar{3} \parallel z$	$(m+2j, 3\nu, p)$
32	$3 \parallel z, 2 \parallel y$	$(n, 3\nu, (-)^{n-m})$
	$3 \parallel z, 2 \parallel x$	$(n, 3\nu, (-)^n)$
$3m$	$3 \parallel z, m \perp y$	$(n, 3\nu, +)$
	$3 \parallel z, m \perp x$	$(n, 3\nu, (-)^m)$
$\bar{3}m$	$\bar{3} \parallel z, m \perp y$	$(m+2j, 3\nu, +)$
	$\bar{3} \parallel z, m \perp x$	$(m+2j, 3\nu, (-)^m)$
6	$6 \parallel z$	$(n, 6\nu, p)$
$\bar{6}$	$\bar{6} \parallel z$	$(2\mu, 3\nu, p)$
$6/m$	$6 \parallel z, m \perp z$	$(2\mu, 6\nu, p)$
622	$6 \parallel z, 2 \parallel y$	$(n, 6\nu, (-)^n)$
$6mm$	$6 \parallel z, m \perp y$	$(n, 6\nu, +)$
$\bar{6}m2$	$\bar{6} \parallel z, m \perp y$	$(2\mu, 3\nu, +)$
	$\bar{6} \parallel z, m \perp x$	$(2\mu, 3\nu, (-)^m)$
$6/mmm$	$6 \parallel z, m \perp z, m \perp y$	$(2\mu, 6\nu, +)$

6.1.1.6.2. *Fourier-invariant expansions*

When truncated, an expression for a multipole expansion, p.d.f. or temperature factor must retain those terms essential to the accuracy required of the expansion. Some authors (*e.g.*

references