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THE DEBYE SCATTERING FORMULA IN n DIMENSIONS

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Abstract. An integral for the Debye scattering formula is given which is valid for any dimension $n \geq 2$. Explicit formulas for $n = 2, \ldots, 8$ are provided, too.

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1. The Debye scattering formula in $n = 3$ dimensions

The Debye scattering formula (also called Debye scattering function) is of fundamental importance for X-ray diffraction in disordered materials and can be found in many textbooks on diffraction [1, 2]. It is based on the assumption that the distance vector $\mathbf{r}_{i,j}$ between two atoms i and j takes on any orientation in space for an amorphous material. The tip of $\mathbf{r}_{i,j}$ lies on the surface of a sphere of radius $\|\mathbf{r}_{i,j}\| = r_{i,j}$. In the totally disordered case the surface density $f(\mathbf{r}_{i,j})$ of the tip is constant along the surface, that is $f(\mathbf{r}_{i,j}) = 1$. The contribution of $\mathbf{r}_{i,j}$ to the diffraction pattern is obtained from integrating $f(\mathbf{r}_{i,j})$ over the entire surface of the n-sphere. If $f(\mathbf{r}_{i,j}) = 1$ and the sphere is of dimension $n = 3$, then the classical Debye scattering function results (see the entry for $n = 3$ in table 1).

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If the material is not totally disordered, then $f(\mathbf{r}_{i,j})$ will not be constant any more. This case had been examined in previous papers [3, 4]. In the present paper we assume that $f(\mathbf{r}_{i,j}) = 1$ but n can take on arbitrary integer values $n = 2, 3, 4, \ldots$. We will give an integral from which the explicit form of the Debye scattering formula for given n can be calculated.

2. An one-dimensional integral over the surface of the n-sphere

We consider an n-dimensional euclidian coordinate system E_n. Within E_n let $f(\mathbf{a})$ be a continuous real-valued function where $\mathbf{a}$ is a n-dimensional vector in E_n. Blumenson [5] gave a simple formula for the integral F($\mathbf{a}$,n) of $f(\mathbf{a})$ over the surface of the n-dimensional sphere of radius r with the origin as center. With $\|\mathbf{a}\| = a$ as the length of $\mathbf{a}$ and with ϕ as the angle between the vectors $\mathbf{a}$ and $\mathbf{r}$ we have

$$(1) \qquad F(\mathbf{a}, n) = \int_{\phi=0}^{\pi} \frac{2r^{n-1}\pi^{(n-1)/2}}{\Gamma\left(\frac{n-1}{2}\right)} f(a\, r\, \cos(\phi), r^2) \sin(\phi)^{n-2} d\phi.$$

For $f(a\, r \cos(\phi), r^2) = 1$ one gets from (1) the surface area of the n-sphere, that is $(2\pi^{n/2}/\Gamma(n/2))r^{n-1}$. We have to choose the suitable function $f(k, n)$ in order to derive the n-dimensional Debye scattering formula $F(k, n)$ where $\mathbf{k}$ is the scattering vector. The contribution of $\mathbf{r}_{i,j}$ to the diffracted intensity $I(k, n)$ depends on the scalar product $\mathbf{k} \cdot \mathbf{r}_{i,j} = k\, r_{i,j} \cos\phi = f(\phi)$. Furthermore, we have to normalize the integral by the volume of the n-sphere. We therefore have for the n-dimensional Debye scattering function $F(k, n)$

$$(2) \qquad F(k, n) = \int_{\phi=0}^{\pi} \frac{\Gamma\left(\frac{n}{2}\right)}{\sqrt{\pi}\Gamma\left(\frac{n-1}{2}\right)} \cos(k\, r_{i,j}\, \cos(\phi)) \sin(\phi)^{n-2} d\phi.$$

The integral (2) can be solved using a computer algebra program. Care must be taken for the case n=even, in which one sets the upper integration limit equal to $\pi/2$ and subsequently multiplies the resulting integral by the factor 2. The solution of (2) is the n-dimensional Debye Scattering formula (3). With $J(i, x)$ as the i-th Bessel function of the first kind $F(k, n)$ is

$$(3) \qquad F(k, n) = 2^{\left(\frac{n}{2}-1\right)} \Gamma\left(\frac{n}{2}\right) (k\, r_{i,j})^{\left(-\frac{n}{2}\right)} \left(J\left(\frac{n}{2}, k\, r_{i,j}\right) n - J\left(\frac{n}{2}+1, k\, r_{i,j}\right) k\, r_{i,j}\right)$$

One can insert concrete values for n into 3. The resulting formulas for $n = 2, \ldots, 8$ are compiled in table 1. One observes that the well known formula for $n = 3$ is recovered. Just as an aside: The factors 1, 1, 2, 3, 8, 15, 48,... in the numerators are equal to the double factorials, see the integer sequence http://oeis.org/A006882 in the Online Encyclopedia of Integer Sequences [6].

3. Examples: Scattering functions for some simplexes

The intensity $I(k, n)$ scattered by an atomic assembly in n dimensions depends on its atoms $m = 1, 2, \ldots$ with their atomic scattering factors $f(k)_i$ and their mutually distance vectors $\mathbf{r}_{i,j}$. (The $f(k)_m$ should not be confused with the function f in the preceding section.) Then the total intensity $I(k, n)$ scattered from such an assembly of M atoms is equal to

$$I(k,n) = \sum_{i=1}^{M} \sum_{j=1}^{M} f(k)_i f^*(k)_j F(k,n). \tag{4}$$

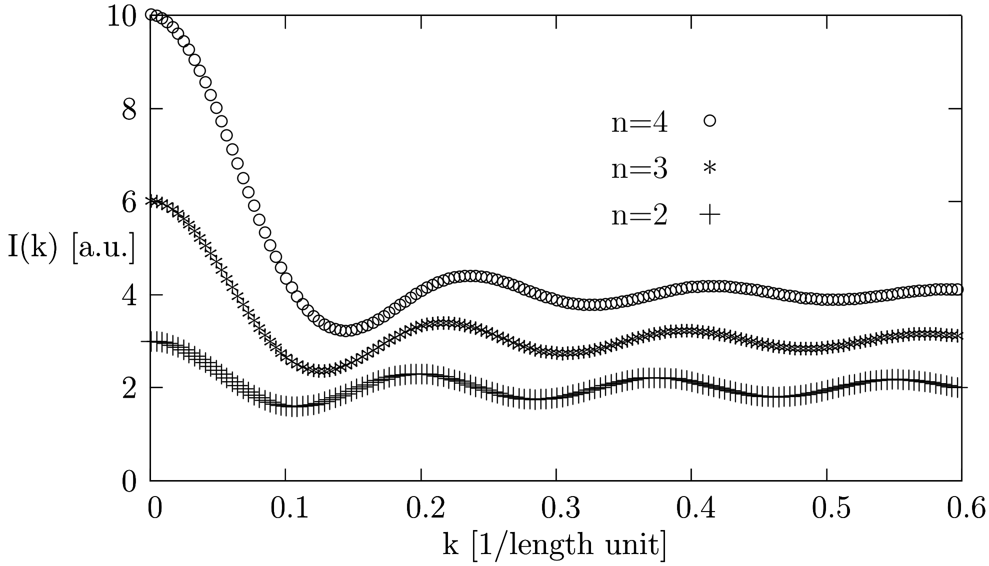
As a first simple application of (2) we give in figure 1 the scattering functions for the n-simplexes in the dimensions $n = 2, 3, 4$, that is the scattering functions of the triangle, the tetrahedron and the pentachoron. The $n+1$ vertices of the n-simplex have the $n+1$-dimensional position vectors $(1, 0, \ldots, 0)$, $(0, 1, \ldots, 0)$, $\ldots$, $(0, 0, \ldots, 1)$. From them one gets immediately the required distance vectors $\mathbf{r}_{i,j}$. For simplicity we set $f(k)_m = 1$ for all m and we use arbitrary units.

Figure 1 displays the curves $I(k, n)$ for $n = 2, 3, 4$. One observes that for $k = 0$ the scattering curve $I(k, n)$ starts at $n(n + 1)/2$ which is exactly the number of edges of the n-simplex, as expected. Furthermore, for higher k the scattering approaches $n - 1$ which corresponds to the average number of neighbours for atom m, again as expected.

4. Conclusion

The n-dimensional Debye scattering formula has been derived from a simple one-dimensional integral. Admittedly, applications for the cases $n > 3$ are not known yet, but

FIGURE 1. Scattering functions for the simplexes in the dimensions $n = 2, 3, 4$.



we do not want to rule them out. Higher-dimensional X-ray crystallography is common for the description of scattering by quasi-crystalline phases. Perhaps higher-dimensional X-ray crystallography will extend to the description of non-crystalline phases, too.

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TABLE 1. The Debye scattering formula for the dimensions n=2,...,8

	Dimension n	**Debye scattering formula** $F(k,n)$
(5)	$n=2$	$J(0,k\,r_{ij})$
(6)	$n=3$	$\frac{\sin(k\,r_{ij})}{k\,r_{ij}}$
(7)	$n=4$	$\frac{2J(1,k\,r_{ij})}{k\,r_{ij}}$
(8)	$n=5$	$\frac{3(\sin(k\,r_{ij})-k\,r_{ij}\cos(k\,r_{ij}))}{k^3r_{ij}^3}$
(9)	$n=6$	$\frac{8(2J(1,k\,r_{ij})-k\,r_{ij}J(0,k\,r_{ij}))}{k^3r_{ij}^3}$
(10)	$n=7$	$\frac{15(3\sin(k\,r_{ij})-3k\,r_{ij}\cos(k\,r_{ij})-k^2r_{ij}^2\sin(k\,r_{ij}))}{k^5r_{ij}^5}$
(11)	$n=8$	$\frac{48(8J(1,k\,r_{ij})-4k\,r_{ij}J(0,k\,r_{ij})-k^2r_{ij}^2J(1,k\,r_{ij}))}{k^5r_{ij}^5}$