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# The Fourier Transforms of a Coiled Coil and a Toroidal Helix

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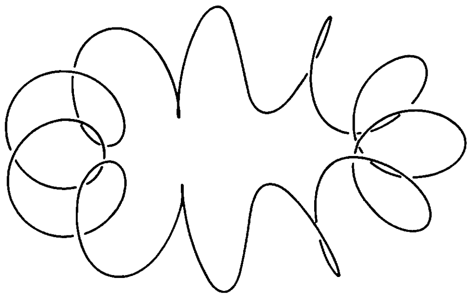
**Abstract**

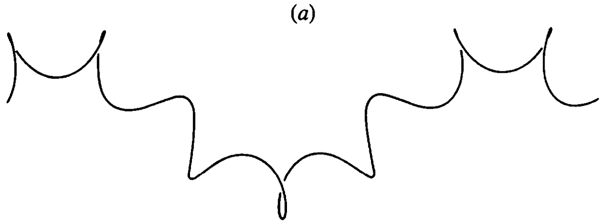
The Fourier transform of a finite coiled coil containing an integral number of repeat units is evaluated analytically. The special cases where the coiled coil reduces either to a pure helix or to a toroidal helix are specifically included.

A coiled coil is a linear, biperiodic structure consisting of a first-order helix whose central axis is deformed into a second-order helix. Two qualitatively distinct coiled-coil geometries are possible depending on the pitch angle $\alpha$ of the second order. If $\alpha = \pi/2$, the central axis of the first-order helix becomes a circle so that the coiled coil reduces to a toroidal helix, as shown in Fig. 1(*a*). Whenever $\alpha \neq \pi/2$, a shape of the type depicted in Fig. 1(*b*) arises.

The first calculation of the Fourier transform of a coiled coil was performed by Crick (1953*a*). That treatment applies to long coiled coils in which one of the orders imposes a small perturbation on the other, so that the overall structure is a slightly sinusoidally deformed helix. Crick's analysis applies quite well to many of the coiled coils found in nature, such as long multi-stranded 'ropes' of $\alpha$-helices (Crick, 1953*b*). However, other methods are required to handle cases where the pitch angle $\alpha$ is large or the two orders are comparable in size. Several useful approximate techniques have been developed to treat these situations. Lang (1956) treats an infinite coiled coil as a grating composed of repetitions of the first-order helix whose Fourier transform has a periodic modulation in amplitude and phase imposed by the second order. This approximate theory is used to explain the near-meridional diffraction from multistranded cables of $\alpha$-helices. More recently, Pardon (1967) has applied a correction factor to the results of Crick (1953*a*). His method computes to good accuracy the Fourier transforms of long coiled coils with intermediate second-order pitch angle $\alpha$. In this paper the exact Fourier transform is calculated for a continuous, infinitely thin wire of uniform electron density shaped as a coiled coil containing an integral number of repeat units, subject to a certain technical restriction. The present analysis specifically applies to coiled coils of large pitch angle $\alpha$, where the earlier approximate calculations can be inaccurate.



(*a*)



(*b*)

Fig. 1. A coiled coil consisting of a (first-order) helix whose central axis is itself deformed into a (second-order) helix. If the pitch angle of the second order is $\pi/2$, the coiled coil becomes a toroidal helix, as shown in (*a*). If the pitch angle of the second order is less than $\pi/2$, then the structure in (*b*) is representative of the coiled coil shape.

Structures involving multiple orders of coiling may arise in several biological systems. Current theories of chromatin structure posit the existence of higher orders of strand coiling with large pitch angles. Heirarchies of such structures are thought to occur in human mitotic chromosomes (Weintraub, Worcel & Alberts, 1976; Bak, Zeuthen & Crick, 1977). A solenoidal model of the chromatin fiber has been proposed in which the DNA traverses an approximately helical path around the nucleosomes, which in turn are stacked in a higher-order helix of pitch angle $\alpha = 75°$ (Finch & Klug, 1976). Closed circular SV40 viral DNA from infected cells also forms nucleosomal structures (Germond, Hirt, Oudet, Gross-Bellard & Chambon, 1975). These in turn can condense further to resemble toroidal helices (Müller, Zentgraf, Eicken & Keller, 1978). In fact, long strands of DNA spontaneously condense into compact toroids in the presence of polyamines (Laemmli, 1975; Gosule & Schellman, 1976; Chattoraj, Gosule & Schellman, 1978).

A coiled coil whose first order has radius $r_1$, whose second order has radius $r_0$ and pitch angle $\alpha$, and which has $\omega$ turns of the first order per turn of the second is

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depicted in Fig. 2. There the second order is the helical central axis about which the coiled coil is wound. The parameter $\omega$ is measured relative to the reference frame which travels along and rotates with the second-order helix. When $\omega > 0$ the first-order helix is right-handed in this reference frame, whereas when $\omega < 0$ it is left-handed. Expressed in coordinates, this coiled coil is

$$x(t) = (\cos t)(r_0 + r_1 \cos \omega t) - r_1 \cos \alpha \sin t \sin \omega t, \quad (1a)$$

$$y(t) = (\sin t)(r_0 + r_1 \cos \omega t) + r_1 \cos \alpha \cos t \sin \omega t, \quad (1b)$$

$$z(t) = at - r_1 \sin \alpha \sin \omega t, \quad (1c)$$

$$0 \le t \le 2\pi\lambda.$$

Here $t$ is the angular parameter which increases by $2\pi$ for each turn of the second-order helix, so the structure has $\lambda$ such turns in all. Also, the helical repeat distance of the second order is $2\pi a = 2\pi r_0 \cot \alpha$. This coiled coil is regarded as containing an integral number of structural repeats, which means that $\omega\lambda =$ integer. (An additional minor technical restriction on the choices of $\omega$, $\alpha$, $r_0$, $r_1$ is presented in the Appendix.) The present notation is used because it results in simpler expressions than that of previous treatments (Crick, 1953*a*; Pardon, 1967). To change variables from the notation of the previous authors involves specifying $\omega_0 = 1$, so that $\omega_1 = N_1/N_0 = \gamma$.

The Fourier transform of an infinitely thin 'wire' of uniform electron density (hereafter normalized to unity) is given by

$$F(X,Y,Z) = \int_0^L \exp[2\pi i(Xx + Yy + Zz)]\, dl, \quad (2)$$

where $(X,Y,Z)$ are the coordinates of reciprocal space, $l$ is the contour-length parameter and $L$ is the total contour length of the structure. The change of variables required to perform this integration is

$$dl = \frac{dl}{dt}\,dt = \left[\left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2 + \left(\frac{dz}{dt}\right)^2\right]^{1/2} dt$$
$$= [f(t)]^{1/2}\, dt. \quad (3)$$

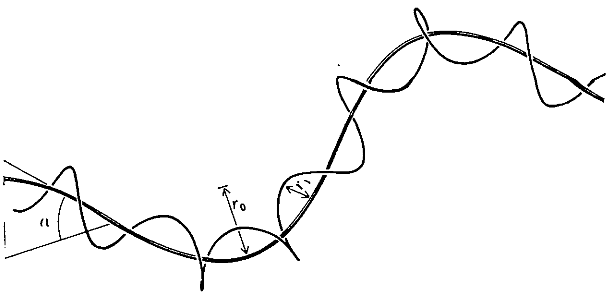

Fig. 2. A coiled coil consisting of a first-order helix winding about a central axis which is itself wound into a second-order helix. In this example the pitch angle of the second order is 45°, the radii are $r_0/r_1 = 2{\cdot}5$ and $\omega = 5$.

Direct computation shows $f$ to be quadratic in $T = \cos \omega t$:

$$f(t) = A + BT + CT^2, \quad (4a)$$

where

$$A = r_0^2 + a^2 + r_1^2(\omega + \cos\alpha)^2, \quad (4b)$$

$$B = 2r_0 r_1, \quad (4c)$$

$$C = r_1^2 \sin^2 \alpha. \quad (4d)$$

Therefore the Fourier transform of this coiled coil is

$$F(X,Y,Z) = \int_0^{2\pi\lambda} [f(t)]^{1/2} \exp\{2\pi i[Xx(t) + Yy(t) + Zz(t)]\}\, dt. \quad (5)$$

In the original treatment of Crick (1953*a*) the value of $f(t)$ was regarded as fixed. As $f(t)$ acts reasonably constant only when either $r_1$ or both $r_0$ and $\bar{a}$ are small, the applicability of his results is restricted accordingly. Pardon (1967) partially surmounted this problem by approximating $f(t)$ with an expression of the form

$$\bar{f}(t) = (A' + B'T)^2 \quad (6a)$$

where

$$2A' = (A + B + C)^{1/2} + (A - B + C)^{1/2}, \quad (6b)$$

$$2B' = (A + B + C)^{1/2} - (A - B + C)^{1/2}. \quad (6c)$$

The difference between the exact function $f(t)$ and Pardon's approximation is

$$f(t) - \bar{f}(t) = \frac{A - C - [(A + C)^2 - B^2]^{1/2}}{2} \times (1 + T)(1 - T). \quad (7)$$

The maximum value of this difference occurs when $T = \cos \omega t = 0$. Then the fractional error is

$$\frac{f(t) - \bar{f}(t)}{f(t)} = \frac{A - C - [(A + C)^2 - B^2]^{1/2}}{2A}. \quad (8)$$

Calculations in an extreme case ($r_0 \simeq r_1$, $\alpha = \pi/2$, $\omega = 1$) show that Pardon's approximation can lead to fractional errors in excess of 30%. This causes significant inaccuracies in the computed Fourier transforms.

In the present paper we develop the analytic solution of (5) subject to the restrictions that $\omega\lambda =$ integer and the satisfaction of the condition expressed in equation ($A$1) of the Appendix. Changing to cylindrical coordinates in reciprocal space by the transformation $X = R\cos\psi$, $Y = R\sin\psi$ yields

$$x(t)X + y(t)Y + z(t)Z = \frac{Rr_1}{2}(1+\cos\alpha) \times \cos[(\omega+1)t-\psi] + \frac{Rr_1}{2}(1-\cos\alpha) \times \cos[(\omega-1)t+\psi] + Rr_0\cos(t-\psi) + Zat - Zr_1\sin\alpha\sin\omega t.$$

The further substitution $\tau = t/\lambda$, $dt = \lambda d\tau$ transforms the integral of (5) to

$$F(R,\psi,Z) = \lambda\int_0^{2\pi}\prod_{j=1}^{6} g_j(\tau)\,d\tau, \tag{9}$$

where

$$g_1(\tau) = \exp\{\pi iRr_1(1+\cos\alpha)\cos[(\omega+1)\lambda\tau-\psi]\},$$

$$g_2(\tau) = \exp\{\pi iRr_1(1-\cos\alpha)\cos[(\omega-1)\lambda\tau+\psi]\},$$

$$g_3(\tau) = \exp\{2\pi iRr_0\cos(\lambda\tau-\psi)\},$$

$$g_4(\tau) = \exp\{-2\pi iZr_1\sin\alpha\sin\omega\lambda\tau\},$$

$$g_5(\tau) = \exp\{2\pi iZa\lambda\tau\},$$

$$g_6(\tau) = \{r_0^2 + a^2 + r_1^2(\omega+\cos\alpha)^2 + r_1^2\sin^2\alpha\cos^2\omega\lambda\tau + 2r_0r_1\cos\omega\lambda\tau\}^{1/2}.$$

Following the method of Crick (1953*a*), we evaluate this integral with a Parseval formula. A sufficient condition for the use of this technique is that all the functions $g_j(\tau)$ be $L^2(T)$ in the region of integration $0 \le \tau < 2\pi$ (Rudin, 1966). That is,

$$\int_0^{2\pi} g_j(\tau)\overline{g_j(\tau)}d\tau < \infty,$$

which is satisfied by all $g_j(\tau), j = 1, \ldots, 6$. The Parseval formula used is

$$\int_0^{2\pi}\prod_{j=1}^{6} g_j(\tau)\,d\tau = 2\pi\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\sum_{n_3=-\infty}^{\infty}\sum_{n_4=-\infty}^{\infty}\sum_{n_5=-\infty}^{\infty}\sum_{n_6=-\infty}^{\infty}\hat{g}_1(n_1) \times \hat{g}_2(n_2)\hat{g}_3(n_3)\hat{g}_4(n_4)\hat{g}_5(n_5)\hat{g}_6(n_6), \tag{10a}$$

subject to the restriction

$$n_1 + n_2 + n_3 + n_4 + n_5 + n_6 = 0. \tag{10b}$$

Here $\hat{g}_j(n_j)$ is the $n_j$th Fourier coefficient of $g_j$,

$$\hat{g}_j(n_j) = \frac{1}{2\pi}\int_0^{2\pi} g_j(\tau)\exp(-in_j\tau)\,d\tau.$$

To solve this problem we must compute the Fourier coefficients of the $g_j$'s above. With variables changed when necessary, the first four coefficients $\hat{g}_j(n)$ are all of the form

$$\hat{g}_j(n) = \frac{e^{i\varrho n}}{2\pi}\int_{-\varrho}^{2\pi-\varrho}\exp(iK\cos qT - inT)\,dT. \tag{11a}$$

This integral may be evaluated in a direct but tedious manner to be

$$\int_{-\varrho}^{2\pi-\varrho}\exp[iK\cos qT - inT]\,dT = \sum_{j=0}^{\infty} A_jJ_j(K), \tag{11b}$$

where $J_j$ is the $j$th Bessel function,

$$A_j = \begin{cases} 2\pi i^j, & jq = \pm n, j \ne 0 \\ ie^{i\varrho n}\left(\dfrac{e^{i\varrho jq}}{jq+n}(e^{-2\pi ijq}-1) - \dfrac{e^{-i\varrho jq}}{jq-n}(e^{2\pi ijq}-1)\right), & jq \ne \pm n, j \ne 0 \end{cases} \tag{11c}$$

$$A_0 = \begin{cases} 2\pi, & n = 0 \\ 0, & \text{otherwise.} \end{cases} \tag{11d}$$

If $q$ = integer, then $A_j = 2\pi i^j$ for $jq = \pm n$, $A_j = 0$ otherwise. This permits the evaluation of the Fourier coefficients $\hat{g}_i(n)$, $i = 1, \ldots, 4$ by appropriate designation of $K$, $q$ and $\rho$. These are given in Table 1.

The Fourier coefficient $\hat{g}_5(n)$ may be evaluated directly to be

$$\hat{g}_5(n) = \begin{cases} \dfrac{1}{2\pi(2\pi a\lambda Z - n)}\{\sin[2\pi(2\pi aZ\lambda - n)] - i\{\cos[2\pi(2\pi aZ\lambda - n)] - 1\}\}, & n \ne 2\pi a\lambda Z \\ 1, \quad n = 2\pi a\lambda Z. \end{cases}$$

Crick (1953*a*) originally let $\hat{g}_5(n)$ vanish except when $n = 2\pi a\lambda Z$, so that scattering was regarded as being confined to layer lines. This is rigorously correct for an infinite coiled coil. In the finite case $\hat{g}_4(n)$ is as above. For relatively short coiled coils the difference can be significant.

Table 1. *The first four Fourier coefficients $\hat{g}_i(n)$, $i$ = 1,...,4, which are all found by evaluation of the integral in equation* (11*a*) *with the variables K, q and ρ identified as shown*

| $i$ | $K$ | $q$ | $\rho$ |
|---|---|---|---|
| 1 | $\pi Rr_1(1+\cos\alpha)$ | $(\omega+1)\lambda$ | $-\psi/[(\omega+1)\lambda]$ |
| 2 | $\pi Rr_1(1-\cos\alpha)$ | $(\omega-1)\lambda$ | $\psi/[(\omega-1)\lambda]$ |
| 3 | $2\pi Rr_0$ | $\lambda$ | $-\psi/\lambda$ |
| 4 | $2\pi Zr_1\sin\alpha$ | $\omega\lambda$ | $\pi/2\omega\lambda$ |

To calculate $\hat{g}_6(n)$ we express $g_6(\tau) = [f(\tau)]^{1/2}$ as a Fourier series. By symmetry this will be a cosine series:

$$g_6(\tau) = F_0 + \sum_{m=1}^{\infty} F_m \cos m\tau.$$

Then the Fourier coefficients of $[f(\tau)]^{1/2} = g_6(\tau)$ are $\hat{g}_6(n) = \hat{g}_6(-n) = F_n/2$, $n \neq 0$ and $\hat{g}_6(0) = F_0$. The calculation of this Fourier series is intricate, and hence is relegated to the Appendix. To perform this computation, it is necessary to assume that $\omega\lambda$ = integer. With the substitutions $\beta = [r_0^2 + a^2 + r_1^2(\omega + \cos\alpha)^2]^{1/2}$ and $\delta = r_1 \sin^2\alpha$, the Fourier coefficients are

$$F_0 = \beta\left[1 + \sum_{n=1}^{\infty} \frac{(-1)^n\left(\prod_{j=0}^{n-1}(2j-1)\right)r_1^n}{2^n n!\beta^{2n}} \times \left\{\sum_{b=0}^{[n/2]} \frac{\binom{n}{2b}(2r_0)^{2b}(\delta)^{n-2b}\binom{2(n-b)}{n-b}}{2^{2(n-b)}}\right\}\right];$$

for $m$ an even multiple of $\omega\lambda$, $m = 2\eta\omega\lambda$,

$$F_m = \sum_{n=\eta}^{\infty} \frac{(-1)^m\left(\prod_{j=0}^{n-1}(2j-1)\right)r_1^n}{2^n n!\beta^{2n-1}} \times \left\{\sum_{b=0}^{\min([n/2],n-\eta)} \frac{\binom{n}{2b}(2r_0)^{2b}(\delta)^{n-2b}\binom{2n-2b}{n-b-\eta}}{2^{2n-2b-1}}\right\};$$

for $m$ an odd multiple of $\lambda\omega$, $m = (2\gamma - 1)\omega\lambda$,

$$F_m = \sum_{n=\gamma}^{\infty} \frac{(-1)^n\left(\prod_{j=0}^{n-1}(2j-1)\right)r_1^n}{2^n n!\beta^{2n-1}} \times \left\{\sum_{c=1}^{\min([(n+1)/2]\, n-\gamma+1)} \frac{\binom{n}{2c-1}(2r_0)^{2c-1}(\delta)^{n-2c+1}}{2^{2(n-c)}} \times \binom{2n-2c+1}{n-c-\gamma+1}\right\}.$$

For all other $m$, $F_m = 0$. (The square brackets in the limits of summation denote the greatest integer function.) Note that $F_{2\eta} = F_{2\gamma-1} = 0$ for all $\eta$, $\gamma > 0$ exactly when $r_1 \sin^2\alpha = 0$. That is, the terms $\hat{g}_6(n)$, $n \neq 0$, vanish from the Fourier transform exactly when the coiled coil reduces to a helix. More precisely, the first order may be regarded as vanishing ($r_1 = 0$), or the second order may be regarded as being straight ($\sin\alpha = 0$).

This calculation contains as special cases both the Fourier transforms of a pure helix and of a toroidal helix. More specifically, a toroidal helix is a coiled coil with pitch $\alpha = \pi/2$, second-order repeat distance zero (*i.e.* $a = 0$), $\omega$ an integer, and $\lambda = 1$. Therefore, $g_5(\tau) \equiv 1$ so the $\hat{g}_5(n_5)$ term does not appear in the Parseval formula for the Fourier transform, equation (10*a*). As $q_i$ is an integer for $i = 1, 2, 3, 4$, the terms $g_i(n_i)$, are easily computed from Table 1 and equations 11(*a* – *d*).

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## APPENDIX

We derive the Fourier series of

$$g_6(\tau) = [r_0^2 + a^2 + r_1^2(\omega + \cos\alpha)^2 + r_1^2\sin^2\alpha\cos^2\omega\lambda\tau + 2r_o r_1 \cos\omega\lambda\tau]^{1/2}.$$

To simplify notation we substitute $\beta = [r_0^2 + a^2 + r_1^2(\omega + \cos\alpha)^2]^{1/2}$, $\delta = r_1\sin^2\alpha$. Then

$$g_6(\tau) = \beta\left[1 + \frac{r_1\delta\cos^2\omega\lambda\tau + 2r_0 r_1\cos\omega\lambda\tau}{\beta^2}\right]^{1/2}.$$

One can show that (Gradshteyn & Ryzhik, 1965)

$$(1 + x)^{1/2} = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n\left(\prod_{j=0}^{n-1}(2j-1)\right)}{2^n n!} x^n,$$

which is uniformly convergent provided $|x|$ is bounded below 1. This implies the restriction that

$$r_1^2 + 2r_0 r_1 < r_0^2 + a^2 + r_1^2(\omega + \cos\alpha)^2. \qquad (A1)$$

This condition is satisfied, for example, when $(\omega + \cos\alpha)^2 > 2$ for any $r_1$ and $r_0$, or when $r_0 > r_1(\sqrt{2} - 1)$ for any $\omega$, $\alpha$. It is a very minor restriction which is likely to be satisfied in all situations of practical importance. Then

$$g_6(\tau) = \beta\left[1 + \sum_{n=1}^{\infty} \frac{(-1)^n\left(\prod_{j=0}^{n-1}(2j-1)\right)}{2^n n!} x^n\right],$$

where

$$x^n = \frac{r_1^n}{2n}\sum_{a=0}^{n}\binom{n}{a}\delta^{n-a}\cos^{2n-a}(\omega\lambda\tau)(2r)^a.$$

We separate the even and odd degree terms in the series for $x^n$:

$$x^n = \frac{r_1^n}{\beta^{2n}}\left(\sum_{b=0}^{[n/2]}\binom{n}{2b}\,\delta^{n-2b}\cos^{2(n-b)}(\omega\lambda\tau)(2r_0)^{2b} + \sum_{c=1}^{[(n+1)/2]}\binom{n}{2c-1}\delta^{n-2c+1} \times \cos^{(2n-c+1)-1}(\omega\lambda\tau)(2r_0)^{2c-1}\right).$$

But

$$\cos^{2p}(\omega\lambda\tau) = \frac{1}{2^{2p}}\left[\sum_{k=0}^{p-1} 2\binom{2p}{k} \times \cos[2(p-k)\,\omega\lambda\tau] + \binom{2p}{p}\right],$$

$$\cos^{2p-1}(\omega\lambda\tau) = \frac{1}{2^{2p-2}}\sum_{k=0}^{p-1}\binom{2p-1}{k} \times \cos[(2p-2k-1)\omega\lambda\tau].$$

Then

$$[f(\tau)]^{1/2} = \beta\left[1 + \sum_{n=1}^{\infty}\left(\frac{(-1)^n\left(\prod_{j=0}^{n-1}(2j-1)\right)r_1^n}{2^n\, n!\,\beta^{2n}} \times \left\{\sum_{b=0}^{[n/2]}\binom{n}{2b}(2r_0)^{2b}\,\delta^{n-2b} + \left\langle\frac{1}{2^{2(n-b)}}\left[\sum_{k=0}^{n-b-1} 2\binom{2(n-b)}{k} \times \cos[2(n-b-k)\omega\lambda\tau] + \binom{2(n-b)}{n-b}\right]\right\rangle + \sum_{c=1}^{[(n+1)/2]}\binom{n}{2c-1}\delta^{n-2c+1}(2r_0)^{2c-1} \times \left\langle\frac{1}{2^{2(n-c)}}\sum_{k=0}^{n-c}\binom{2(n-c)+1}{k} \times \cos[(2n-2c-2k+1)\omega\lambda\tau]\right\rangle\right\}\right)\right].$$

Finally, the coefficients $F_m$ of the $\cos m\tau$ terms give the Fourier coefficients which have been sought. For $m$ not a multiple of $\omega\lambda$, $F_m = 0$. Otherwise, they are

$$F_0 = \beta\left[1 + \sum_{n=1}^{\infty}\left(\frac{(-1)^n\left(\prod_{j=0}^{n-1}(2j-1)\right)r_1^n}{2^n\, n!\,\beta^{2n}} \times \left\{\sum_{b=0}^{[n/2]}\frac{\binom{n}{2b}(2r_0)^{2b}\,\delta^{n-2b}\binom{2(n-b)}{n-b}}{2^{2(n-b)}}\right\}\right)\right].$$

For $m$ an even multiple of $\omega\lambda$, $m = 2\eta\omega\lambda$, then

$$F_m = \sum_{n=\eta}^{\infty}\frac{(-1)^n\left(\prod_{j=0}^{n-1}(2j-1)\right)r_1^n}{2^n\, n!\,\beta^{2n-1}} \times \left\{\sum_{b=0}^{w}\frac{\binom{n}{2b}(2r_0)^{2b}\,\delta^{n-2b}}{2^{2(n-b)-1}}\binom{2(n-b)}{n-b-\eta}\right\},$$

where $w = \min([n/2], n-\eta)$.

Finally, for $m$ an odd multiple of $\omega\lambda$, $m = (2\gamma-1)\,\omega\lambda$, then

$$F_m = \sum_{n=\gamma}^{\infty}\frac{(-1)^n\left(\prod_{j=0}^{n-1}(2j-1)\right)r_1^n}{2^n\, n!\,\beta^{2n-1}} \times \left(\sum_{c=1}^{v}\frac{\binom{n}{2c-1}(2r_0)^{2c-1}\,\delta^{n-2c+1}}{2^{2(n-c)}} \times \binom{2(n-c)+1}{n-c-\gamma+1}\right),$$

where $v = \min([(n+1)/2], n-\gamma+1)$.

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# Diffraction of X-rays by Magnetic Materials. I. General Formulae and Measurements on Ferro- and Ferrimagnetic Compounds

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## Abstract

The calculation of the amplitude of X-rays scattered by a magnetically ordered substance, carried out in the relativistic quantum theory (*i.e.* taking the spin into account), is detailed. The effect of the orbital momentum is described in an appendix. The practical formulae dealing with the polarization of the beams are given both in a simple form for the usual experiments and in a complete form, using the Stokes vectors, for the most general case. The experiments show a change in the intensity of the X-rays diffracted by a ferromagnetic (pure iron) or a ferrimagnetic (zinc-substituted magnetite) powder when the magnetization, perpendicular to the diffraction plane, is reversed. The relative values of these intensity changes range from $10^{-4}$ to $5 \times 10^{-3}$ and agree in sign and magnitude with the predictions. They are proportional to the spin-density structure factor multiplied by the imaginary part of the charge-density structure factor; the large anomalous scattering of the Cu $K\alpha$ radiation in the iron-containing samples is used in the present experiments.

## Introduction

X-ray diffraction is usually interpreted through the Thomson scattering mechanism, *i.e.* the interaction between the electromagnetic radiation and the charge of the electrons. X-rays therefore seem to give information about the charge density only and not about the spin density. If one examines the phenomenon more thoroughly, it appears that the electronic spin also plays some role; the magnetic moment associated with the spin does interact with the magnetic field of the radiation (Fig. 1). This effect can

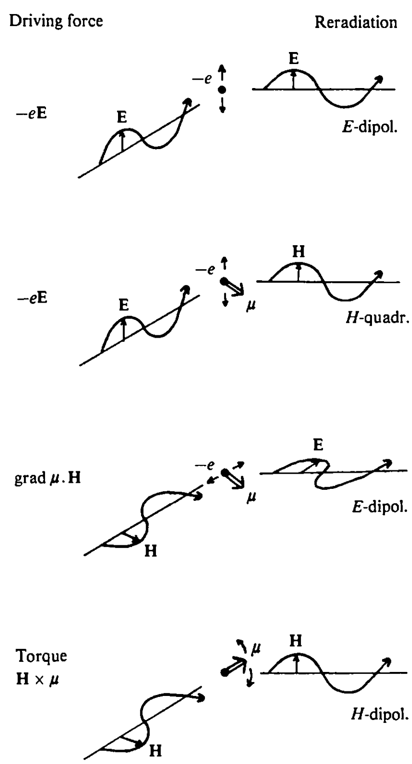


Fig. 1. The four mechanisms of scattering, in the classical description. The first one is the well known Thomson scattering. In each case, the electron (charge $-e$) or its magnetic moment $\mu$ is moved by the incident electromagnetic field. The force or torque is indicated in the left column. The type of reradiation (electric or magnetic, dipolar or quadrupolar) is given at the right.

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