Crystallographic Fourier Analysis

Crystallographic Diffraction

Laue diffraction by a three-dimensional *abc* lattice grating

$$\boxed{\begin{aligned} a\left(\cos\nu_1-\cos\mu_1\right)&=\mathbf{a}\bullet\left(\hat{\mathbf{s}}-\hat{\mathbf{s}}_0\right)=h\lambda\\ b\left(\cos\nu_2-\cos\mu_2\right)&=\mathbf{b}\bullet\left(\hat{\mathbf{s}}-\hat{\mathbf{s}}_0\right)=k\lambda\\ c\left(\cos\nu_3-\cos\mu_3\right)&=\mathbf{c}\bullet\left(\hat{\mathbf{s}}-\hat{\mathbf{s}}_0\right)=l\,\lambda \end{aligned}}$$

Walther Friedrich, Paul Knipping, and Max Laue (1912).

Bragg reflection from families of parallel *hkl* lattice planes

$$\boxed{2d_{hkl}\sin\theta=n\lambda\,,\qquad 2\left(\frac{d_{hkl}}{n}\right)\sin\theta=\lambda\,,\qquad 2d_{nh\,nk\,nl}\sin\theta=\lambda}$$

William Henry and William Lawrence Bragg (1913). (Father and son)

Integrated Bragg reflections

$$\boxed{\frac{E_{hkl}\omega}{I_0}=kALp\left|F_{hkl}\right|^2=\left(\frac{e^2}{mc^2}\right)^2\lambda^3\left(\frac{v_{\text{xtal}}}{V_{\text{cell}}}\right)^2\left[\int_{v_{\text{xtal}}}\mathrm{e}^{-\mu\left(t_0+t_1\right)}\mathrm{d}v\right]\frac{1}{\sin 2\theta}\left(\frac{1}{2}+\frac{1}{2}\cos^2 2\theta\right)\left|F_{hkl}\right|^2}$$

Charles G. Darwin (1914). (Grandson of the author of the theory of evolution)

Fourier analysis of crystal structure

"[Another fundamental early] contribution appeared in my father's Bakerian Lecture[1] in 1915; a quotation from it will show its significance:

> 'Let us imagine then that the periodic variation of density [in the crystal] has been analyzed into a series of periodic terms. The coefficient of any term will be proportional to the intensity[2] of the reflexion to which it corresponds.'

[This] was the start of [crystallographic] Fourier analysis…"[3]

[1] Wm. Henry Bragg. The Bakerian Lecture, 1915. X-Rays and Crystals. *Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character*, Vol. **215**, pp. 253-274 (13 July 1915).

[2] In fact, not the intensity but rather the amplitude, $\left|F_{hkl}\right| \propto \sqrt{I_{hkl}}$.

[3] Wm. Lawrence Bragg. The Rutherford Memorial Lecture, 1960. The Development of X-Ray Analysis. *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, Vol. **262**, No. 1309, pp. 145-158 (4 July 1961).

The "fundamental theorem" of structural crystallography

The fundamental theorem of arithmetic

Every integer greater that 1 has a unique expression as a product of primes.

The fundamental theorem of algebra

Every univariate polynomial of degree n with complex coefficients has exactly n complex roots.

The fundamental theorem of the calculus

If the derivative of $f(x)$ is $g(x)$, then the integral of $g(x)$ is $f(x)$.

$$\frac{\mathrm{d}}{\mathrm{d}x} f(x) = g(x) \quad \Rightarrow \quad \int_a^b g(x)\,\mathrm{d}x = f(x)\Big|_a^b = f(b) - f(a) \quad \Rightarrow \quad \int g(x)\,\mathrm{d}x = f(x) + C$$

The "fundamental theorem" of structural crystallography

The crystal structure factors F_{hkl} in diffraction or reciprocal hkl space and the unit-cell scattering density distribution $\rho(x,y,z)$ in crystal or direct xyz space are related by Fourier transformation,

$$F_{hkl} = |F_{hkl}| \mathrm{e}^{i\varphi_{hkl}} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x,y,z) \qquad \begin{cases} \mathcal{F}[F_{hkl}] = \rho(x,y,z) & \text{Fourier synthesis} \\ \mathcal{F}^{-1}[\rho(x,y,z)] = F_{hkl} & \text{Fourier analysis} \end{cases}$$

where the $|F_{hkl}|$ and φ_{hkl} are, respectively, the amplitudes and phases of the beams of Laue-Bragg scattered radiation diffracted by a crystal.

Fourier had shown in 1807 that a periodic function can be represented by a harmonic sum of sines and cosines.

If $\quad f(x) = f(x \pm 2n\pi)$,

then $\quad f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos(nx) + b_n \sin(nx)$

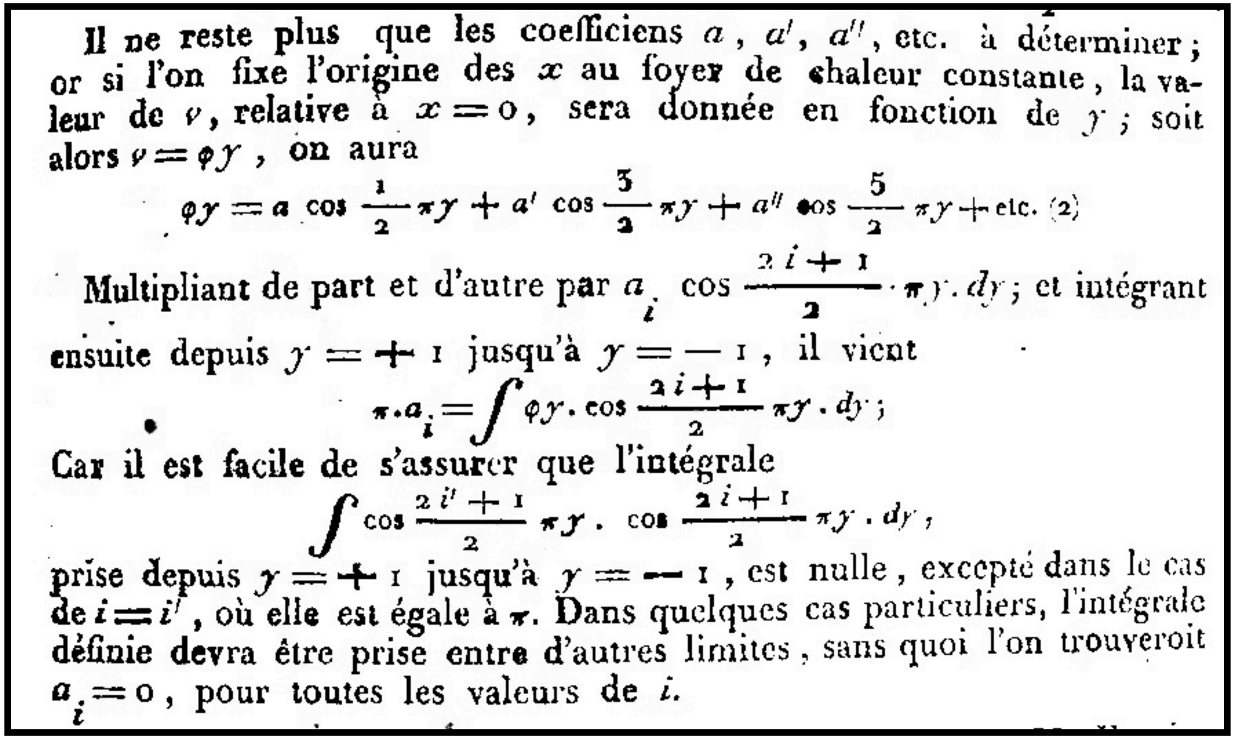
$$a_0 = \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\,\mathrm{d}x$$

$$a_n = \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\cos(nx)\,\mathrm{d}x$$

$$b_n = \frac{1}{\pi}\int_{-\pi}^{+\pi} f(x)\sin(nx)\,\mathrm{d}x$$

Lagrange, Laplace, Legendre, Malus *et al*. thought Fourier’s formulation of his theory lacked rigor.
Later, Dirichlet and Riemann expressed Fourier's results with greater precision and formality.

(Jean-Baptiste-) Joseph FOURIER, 1768-1830.



Il ne reste plus que les coefficiens a, a', a'', etc. à déterminer; or si l'on fixe l'origine des x au foyer de chaleur constante, la valeur de v, relative à $x = 0$, sera donnée en fonction de y; soit alors $v = \varphi y$, on aura

$$\varphi y = a \cos \frac{1}{2} \pi y + a' \cos \frac{3}{2} \pi y + a'' \cos \frac{5}{2} \pi y + \text{etc.} \quad (2)$$

Multipliant de part et d'autre par $a_i \cos \frac{2i+1}{2} \cdot \pi y . dy$; et intégrant ensuite depuis $y = +1$ jusqu'à $y = -1$, il vient

$$\pi . a_i = \int \varphi y . \cos \frac{2i+1}{2} \pi y . dy;$$

Car il est facile de s'assurer que l'intégrale

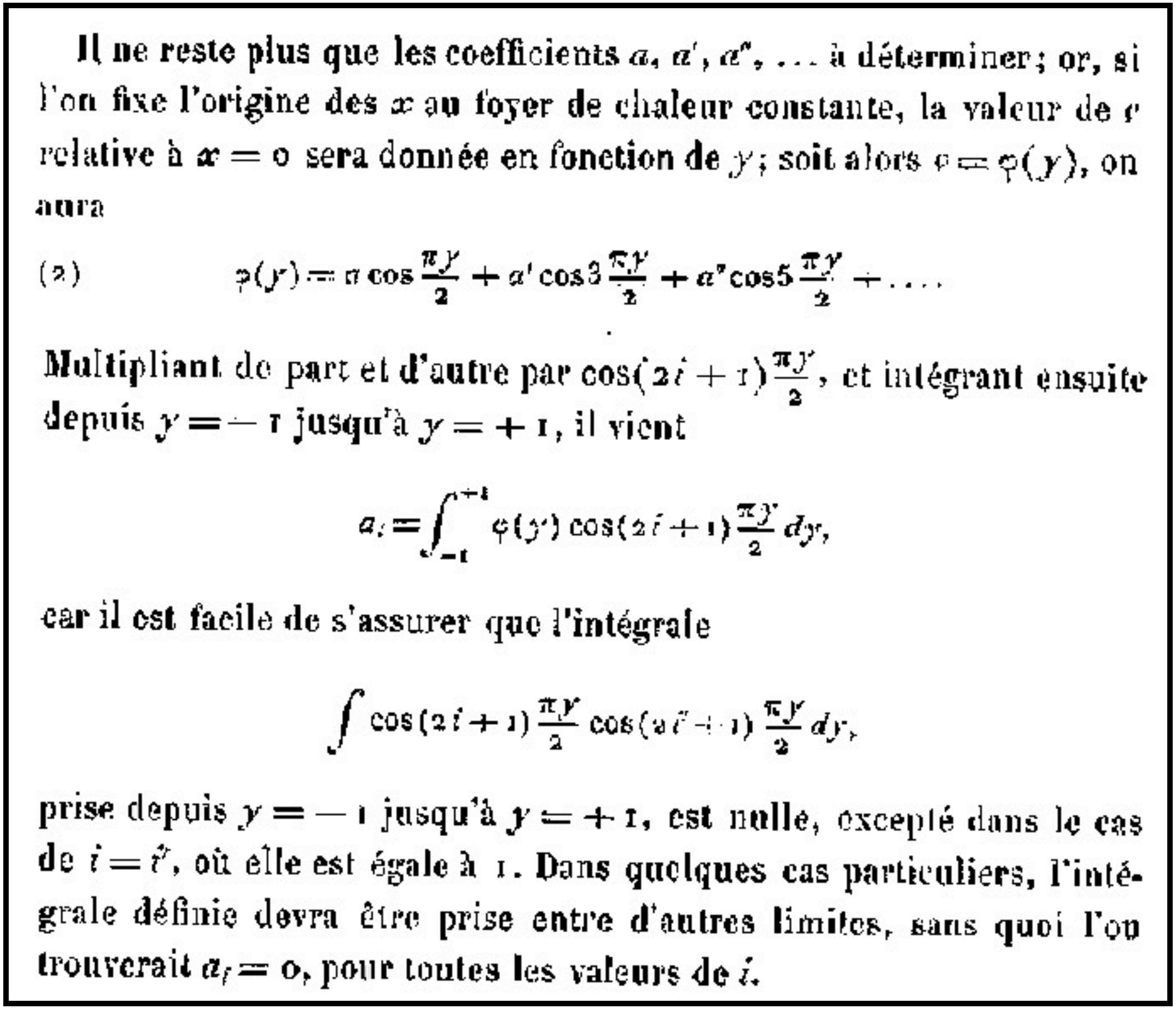
$$\int \cos \frac{2i'+1}{2} \pi y . \cos \frac{2i+1}{2} \pi y . dy,$$

prise depuis $y = +1$ jusqu'à $y = -1$, est nulle, excepté dans le cas de $i = i'$, où elle est égale à π. Dans quelques cas particuliers, l'intégrale définie devra être prise entre d'autres limites, sans quoi l'on trouveroit $a_i = 0$, pour toutes les valeurs de i.

"Mémoire sur la propagation de la Chaleur dans les corps solides, présenté le 21 décembre 1807 à l'institute national." Nouveau Bulletin des sciences par la Société philomathique de Paris, N^o. 6, Paris (Bernard), March 1808, pp. 112-116.

http://www.ujf-grenoble.fr/images/photos/0005/img_1118050034589.jpg
http://pagesperso-orange.fr/alta.mathematica/fourier1807.html

Fourier (1807). Memoir on the conduction of heat in solid bodies.



Il ne reste plus que les coefficients $a, a', a'', \ldots$ à déterminer; or, si l'on fixe l'origine des x au foyer de chaleur constante, la valeur de v relative à $x = 0$ sera donnée en fonction de y; soit alors $v = \varphi(y)$, on aura

$$(2) \qquad \varphi(y) = a \cos \frac{\pi y}{2} + a' \cos 3 \frac{\pi y}{2} + a'' \cos 5 \frac{\pi y}{2} + \ldots.$$

Multipliant de part et d'autre par $\cos(2i + 1)\frac{\pi y}{2}$, et intégrant ensuite depuis $y = -1$ jusqu'à $y = +1$, il vient

$$a_i = \int_{-1}^{+1} \varphi(y) \cos(2i + 1) \frac{\pi y}{2} \, dy,$$

car il est facile de s'assurer que l'intégrale

$$\int \cos(2i + 1) \frac{\pi y}{2} \cos(2i' + 1) \frac{\pi y}{2} \, dy,$$

prise depuis $y = -1$ jusqu'à $y = +1$, est nulle, excepté dans le cas de $i = i'$, où elle est égale à 1. Dans quelques cas particuliers, l'intégrale définie devra être prise entre d'autres limites, sans quoi l'on trouverait $a_i = 0$, pour toutes les valeurs de i.

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Fourier (1807) translated

For the variation of temperature $\varphi(y)$ along the length y of a heated metal bar…

"… one has

$$\varphi(y) = a_0 \cos\left(\frac{1}{2}\pi y\right) + a_1 \cos\left(\frac{3}{2}\pi y\right) + a_2 \cos\left(\frac{5}{2}\pi y\right) + \cdots .$$

Multiplying both sides by $\cos\left(\frac{2n+1}{2}\pi y\right)$, and integrating from $y = -1$ to $y = +1$ yields

$$a_n = \int_{-1}^{+1} \varphi(y) \cos\left(\frac{2n+1}{2}\pi y\right) \mathrm{d}y \,,$$

since it is easy to show that the integral

$$\int_{-1}^{+1} \cos\left(\frac{2n+1}{2}\pi y\right) \cos\left(\frac{2n'+1}{2}\pi y\right) \mathrm{d}y$$

is equal to zero, except in the case $n' = n$, where it equals unity."

Oeuvres de Fourier, publiées par les soins de M. Gaston Darboux (1842-1917), sous les auspices du ministère de l'Instruction publique au ministère de l' Éducation nationale de France…, Gauthier-Villars (Paris), 1888-1890. Bibliothèque nationale de France.

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>
> Multiplying both sides by $\cos\left(\frac{2n+1}{2}\pi y\right)$, and integrating from $y=-1$ to $y=+1$ yields
>
> $$a_n = \int_{-1}^{+1} \varphi(y)\cos\left(\frac{2n+1}{2}\pi y\right)\mathrm{d}y\,,$$
>
> since it is easy to show that the integral
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Fourier series expansion of a 2π periodic function $f(x)=f(x\pm 2n\pi)$, $\forall x\in\mathbb{R}$

Trigonometric series

$$f(x)=\frac{1}{2}a_0+\sum_{n=1}^{\infty}a_n\cos(nx)+b_n\sin(nx)$$

$$a_0=\frac{1}{\pi}\int_{-\pi}^{+\pi}f(x)\mathrm{d}x\,,\quad a_n=\frac{1}{\pi}\int_{-\pi}^{+\pi}f(x)\cos(nx)\mathrm{d}x\,,\quad b_n=\frac{1}{\pi}\int_{-\pi}^{+\pi}f(x)\sin(nx)\mathrm{d}x$$

$$\mathrm{e}^{i\varphi}=\cos\varphi+i\sin\varphi\,,\qquad \cos\varphi=\frac{1}{2}\left(\mathrm{e}^{i\varphi}+\mathrm{e}^{-i\varphi}\right),\qquad \sin\varphi=\frac{1}{2i}\left(\mathrm{e}^{i\varphi}-\mathrm{e}^{-i\varphi}\right)=-\frac{i}{2}\left(\mathrm{e}^{i\varphi}-\mathrm{e}^{-i\varphi}\right)$$

$$f(x)=\frac{1}{2}a_0+\frac{1}{2}\sum_{n=1}^{\infty}\left[a_n\left(\mathrm{e}^{inx}+\mathrm{e}^{-inx}\right)-ib_n\left(\mathrm{e}^{inx}-\mathrm{e}^{-inx}\right)\right]$$

$$f(x)=\frac{1}{2}a_0+\frac{1}{2}\sum_{n=1}^{\infty}\left[\left(a_n-ib_n\right)\mathrm{e}^{inx}+\left(a_n+ib_n\right)\mathrm{e}^{-inx}\right]$$

$$\frac{1}{2}\left(a_n+ib_n\right)=c_n\,,\qquad \frac{1}{2}\left(a_n-ib_n\right)=c_n^*\equiv c_{-n}$$

Complex exponential series

$$f(x)=c_0+\sum_{n=1}^{\infty}\left(c_{-n}\,\mathrm{e}^{inx}+c_n\,\mathrm{e}^{-inx}\right)=\sum_{n=-\infty}^{+\infty}c_n\,\mathrm{e}^{-inx}$$

$$c_n=\frac{1}{2\pi}\int_{-\pi}^{+\pi}f(x)\mathrm{e}^{+inx}\,\mathrm{d}x\,,\quad n=0,\pm1,\pm2,\ldots$$

Fourier series expansion of a periodic function with arbitrary period $f\left(x\right)=f\left(x\pm nL\right),\ \forall\ x\in\mathbb{R}$

Trigonometric series

$$f\left(x\right)=\frac{1}{2}a_0+\sum_{n=1}^{\infty}\left[a_n\cos\left(2\pi\frac{nx}{L}\right)+b_n\sin\left(2\pi\frac{nx}{L}\right)\right]$$

$$a_0=\frac{2}{L}\int_{-L/2}^{+L/2}f\left(x\right)\mathrm{d}x\ ,\quad a_n=\frac{2}{L}\int_{-L/2}^{+L/2}f\left(x\right)\cos\left(2\pi\frac{nx}{L}\right)\mathrm{d}x\ ,\quad b_n=\frac{2}{L}\int_{-L/2}^{+L/2}f\left(x\right)\sin\left(2\pi\frac{nx}{L}\right)\mathrm{d}x$$

$$\mathrm{e}^{i\varphi}=\cos\varphi+i\sin\varphi\ ,\qquad \cos\varphi=\frac{1}{2}\left(\mathrm{e}^{i\varphi}+\mathrm{e}^{-i\varphi}\right),\qquad \sin\varphi=\frac{1}{2i}\left(\mathrm{e}^{i\varphi}-\mathrm{e}^{-i\varphi}\right)=-\frac{i}{2}\left(\mathrm{e}^{i\varphi}-\mathrm{e}^{-i\varphi}\right)$$

$$f\left(x\right)=\frac{1}{2}a_0+\sum_{n=1}^{\infty}\left\{\frac{1}{2}a_n\left[\exp\left(2\pi i\frac{nx}{L}\right)+\exp\left(-2\pi i\frac{nx}{L}\right)\right]-\frac{i}{2}b_n\left[\exp\left(2\pi i\frac{nx}{L}\right)-\exp\left(-2\pi i\frac{nx}{L}\right)\right]\right\}$$

$$f\left(x\right)=\frac{1}{2}a_0+\sum_{n=1}^{\infty}\left[\frac{1}{2}\left(a_n-ib_n\right)\exp\left(2\pi i\frac{nx}{L}\right)+\frac{1}{2}\left(a_n+ib_n\right)\exp\left(-2\pi i\frac{nx}{L}\right)\right]$$

$$\frac{1}{2}\left(a_n+ib_n\right)=c_n\ ,\qquad \frac{1}{2}\left(a_n-ib_n\right)=c_n^*\equiv c_{-n}$$

Complex exponential series

$$f\left(x\right)=c_0+\sum_{n=1}^{\infty}\left[c_{-n}\exp\left(2\pi i\frac{nx}{L}\right)+c_n\exp\left(-2\pi i\frac{nx}{L}\right)\right]=\sum_{n=-\infty}^{+\infty}c_n\exp\left(-2\pi i\frac{nx}{L}\right)$$

$$c_n=\frac{1}{L}\int_{-L/2}^{+L/2}f\left(x\right)\exp\left(+2\pi i\frac{nx}{L}\right)\mathrm{d}x\ ,\quad n=0,\pm1,\pm2,...$$

Orthogonality of the sine and cosine functions

$$\forall\, m,n: \quad m,n \in \mathbb{Z} \neq 0\,,$$

$$\int_{-\pi}^{+\pi} \cos(mx)\cos(nx)\,\mathrm{d}x = \int_{-\pi}^{+\pi} \sin(mx)\sin(nx)\,\mathrm{d}x = \pi\,\delta_{mn} = \begin{cases} 0 & \text{if} \quad m \neq n \\ \pi & \text{iff} \quad m = n \end{cases}$$

$$\int_{-\pi}^{+\pi} \cos(mx)\sin(nx)\,\mathrm{d}x = 0$$

Orthonormality
of
$f(x)$ and $g(x)$
in $[a \leq x \leq b]$

$$\int_a^b f(x)g(x)\mathrm{d}x = \delta_{fg} = \begin{cases} 0 & \text{if} \quad f(x) \neq g(x) \\ 1 & \text{iff} \quad f(x) = g(x) \end{cases}$$

Kronecker delta $\delta_{ij} = \begin{cases} 0\,, & i \neq j \\ 1\,, & i = j \end{cases}$

Sine and cosine orthogonality integrals

$$\cos(x+y)=\cos x\cos y-\sin x\sin y$$

$$\cos(x-y)=\cos x\cos y+\sin x\sin y$$

$$\cos(x+y)+\cos(x-y)=2\cos x\cos y$$

$$\cos(x-y)-\cos(x+y)=2\ \sin x\ \sin y$$

$$\begin{aligned}\int_{-\pi}^{+\pi}\cos(mx)\cos(nx)\,\mathrm{d}x&=\frac{1}{2}\int_{-\pi}^{+\pi}\left[\cos(m+n)x\right]+\cos\left[(m-n)x\right]\mathrm{d}x\\&=\begin{cases}0+0 & \text{if}\quad m\neq n\\ 0+\frac{1}{2}\int_{-\pi}^{+\pi}\mathrm{d}x=\frac{1}{2}x\Big|_{-\pi}^{+\pi}=\pi & \text{iff}\quad m=n\end{cases}\\&=\pi\delta_{mn}\end{aligned}$$

$$\begin{aligned}\int_{-\pi}^{+\pi}\sin(mx)\sin(nx)\,\mathrm{d}x&=\frac{1}{2}\int_{-\pi}^{+\pi}\left[\cos(m-n)x\right]-\cos\left[(m+n)x\right]\mathrm{d}x\\&=\begin{cases}0+0 & \text{if}\quad m\neq n\\ \frac{1}{2}\int_{-\pi}^{+\pi}\mathrm{d}x+0=\frac{1}{2}x\Big|_{-\pi}^{+\pi}=\pi & \text{iff}\quad m=n\end{cases}\\&=\pi\delta_{mn}\end{aligned}$$

$$\sin(x+y)=\sin x\cos y+\cos x\sin y$$

$$\sin(x-y)=\sin x\cos y-\cos x\sin y$$

$$\sin(x+y)+\sin(x-y)=2\sin x\cos y$$

$$\sin(x+y)-\sin(x-y)=2\cos x\sin y$$

$$\int_{-\pi}^{+\pi}\sin(mx)\cos(nx)\,\mathrm{d}x=\frac{1}{2}\int_{-\pi}^{+\pi}\left[\sin(m+n)x\right]+\sin\left[(m-n)x\right]\mathrm{d}x=0$$

Sine and cosine orthogonality integrals

$$\cos(x+y) = \cos x \cos y - \sin x \sin y$$

$$\cos(x-y) = \cos x \cos y + \sin x \sin y$$

$$\cos(x+y) + \cos(x-y) = 2\cos x \cos y$$

$$\cos(x-y) - \cos(x+y) = 2\,\sin x\;\sin y$$

$$\int_{-\pi}^{+\pi} \cos(mx)\cos(nx)\,\mathrm{d}x = \frac{1}{2}\int_{-\pi}^{+\pi} \left[\cos(m+n)x\right] + \cos\left[(m-n)x\right]\mathrm{d}x$$

$$= \begin{cases} 0+0\,, & m \neq n \\ 0 + \frac{1}{2}\int_{-\pi}^{+\pi}\mathrm{d}x = \frac{1}{2}x\Big|_{-\pi}^{+\pi} = \pi\,, & m = n \end{cases}$$

$$= \pi\,\delta_{mn}$$

$$\int_{-\pi}^{+\pi} \sin(mx)\sin(nx)\,\mathrm{d}x = \frac{1}{2}\int_{-\pi}^{+\pi} \left[\cos(m-n)x\right] - \cos\left[(m+n)x\right]\mathrm{d}x$$

$$= \begin{cases} 0+0\,, & m \neq n \\ \frac{1}{2}\int_{-\pi}^{+\pi}\mathrm{d}x + 0 = \frac{1}{2}x\Big|_{-\pi}^{+\pi} = \pi\,, & m = n \end{cases}$$

$$= \pi\,\delta_{mn}$$

(cont’ d)

Sine and cosine orthogonality integrals (cont' d)

$$\sin(x+y)=\sin x\cos y+\cos x\sin y$$

$$\sin(x-y)=\sin x\cos y-\cos x\sin y$$

$$\sin(x+y)+\sin(x-y)=2\sin x\cos y$$

$$\sin(x+y)-\sin(x-y)=2\cos x\sin y$$

$$\int_{-\pi}^{+\pi}\sin(mx)\cos(nx)\,\mathrm{d}x=\frac{1}{2}\int_{-\pi}^{+\pi}\left[\sin(m+n)x\right]+\sin\left[(m-n)x\right]\mathrm{d}x=0$$

The Euler formula

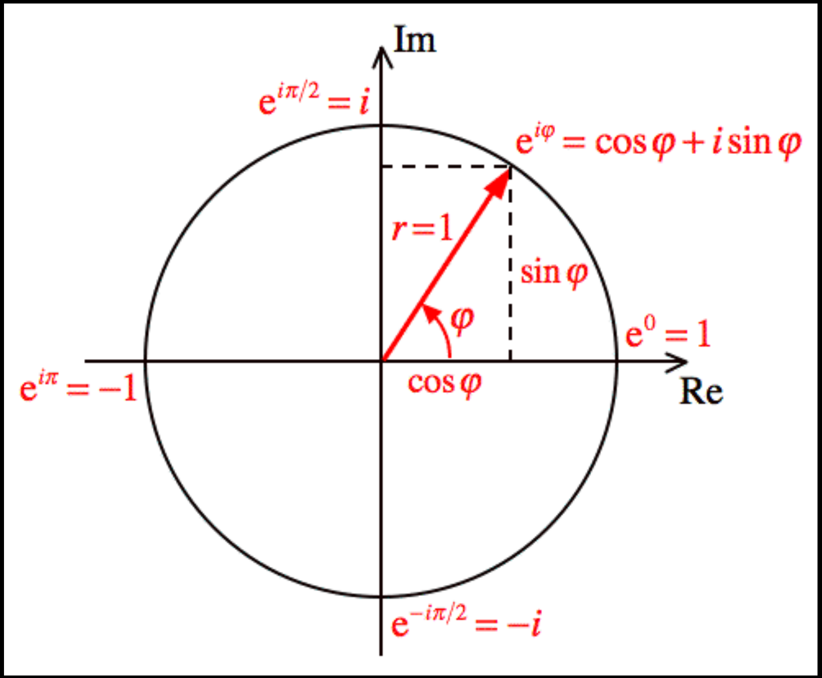
$$\boxed{e^{i\varphi} = \cos\varphi + i\sin\varphi}$$

Feynman called this "… the most remarkable formula in mathematics…, our jewel".

The Euler identity

$$\boxed{e^{i\pi} + 1 \equiv 0}$$

Gauss reportedly said that anyone to whom this formula is not immediately obvious could never be a first-class mathematician.



The Euler formula is a thing of *deep mathematical meaning*. It unites algebra and geometry by linking complex exponential functions and the trigonometric functions.

$$e^{i\varphi} = \cos\varphi + i\sin\varphi \qquad \cos\varphi = \frac{1}{2}\left(e^{i\varphi} + e^{-i\varphi}\right)$$

$$e^{-i\varphi} = \cos\varphi - i\sin\varphi \qquad \sin\varphi = \frac{1}{2i}\left(e^{i\varphi} - e^{-i\varphi}\right)$$

The Euler identity is a thing of *great mathematical beauty*. It links the real numbers 0 and –1 , the transcendental numbers *π* and e , and the imaginary unit *i* .

The Euler Formula and the Euler Identity

$$e^{i\varphi} = \cos\varphi + i\,\sin\varphi$$

$$e^{i\pi} = 0 - 1$$

$$e^{i\pi} + 1 \equiv 0$$

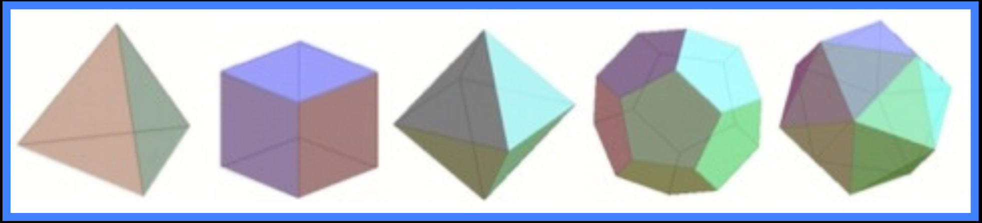
$$\cos\varphi = \frac{1}{2}\left(e^{i\varphi} + e^{-i\varphi}\right)$$

$$\sin\varphi = \frac{1}{2i}\left(e^{i\varphi} - e^{-i\varphi}\right)$$

$$e^{i\varphi} = \cos\varphi + i\sin\varphi$$

$$e^{i\pi} = 0 - 1$$

$$e^{i\pi} + 1 \equiv 0$$

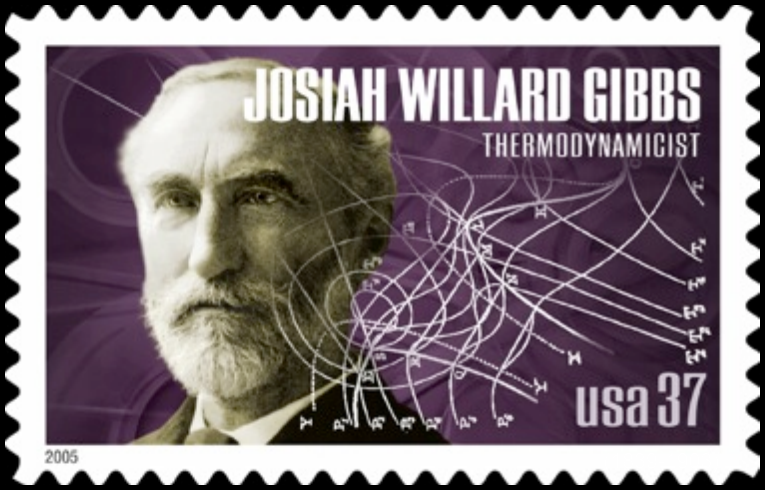


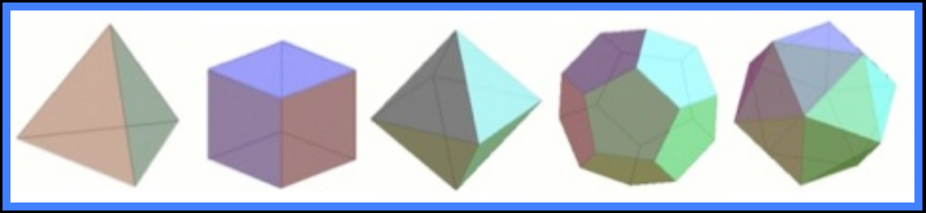
$e - k + f = 2$
die Ecken – die Kanten + die Flächen = 2

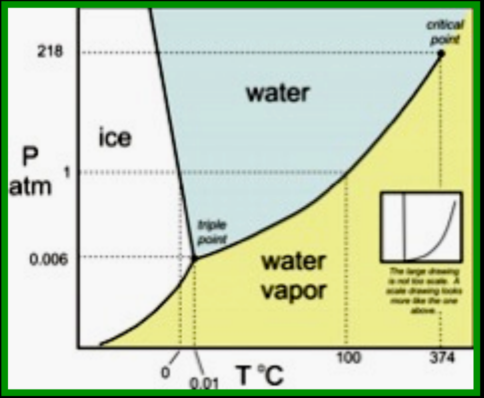
$v - e + f = 2$
vertices – edges + faces = 2

Gibbs phase rule
$F - C + P = 2$
degrees of freedom – components + phases = 2

Platonic solids, Euler's formula, and Gibbs' phase rule





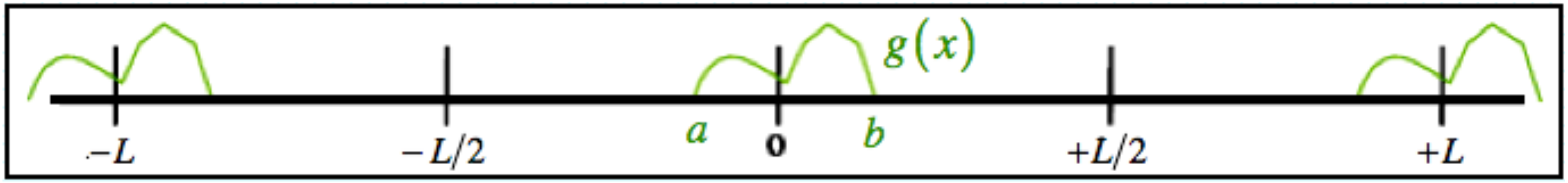


e – k + f = 2
die Ecken – die Kanten + die Flächen = 2

v – e + f = 2
vertices – edges + faces = 2

Gibbs phase rule
F – C + P = 2
degrees of – components + phases = 2
freedom

An aperiodic signal can be viewed as a periodic signal with an infinite period.



$$f_L(x)=\left\{\begin{array}{ll}0 & -L/2<x<a\\ g(x) & a\le x\le b\\ 0 & b<x<+L/2\end{array}\right.$$

$$f_L(x\pm nL)=f_L(x)\,,\qquad L\gg b-a$$

$$\left\{\begin{array}{l} f_L(x)=\displaystyle\sum_{n=-\infty}^{+\infty} c_n \exp\left(-2\pi i\frac{nx}{L}\right)\\ c_n=\displaystyle\frac{1}{L}\int_{-L/2}^{+L/2} f_L(x)\exp\left(+2\pi i\frac{nx}{L}\right)\mathrm{d}x\end{array}\right.$$

$$\left\{\begin{array}{l}x\in\mathbb{R}\\ n\in\mathbb{Z}\qquad n=0,\pm1,\pm2,\dots\end{array}\right.$$

$$g(x)=\lim_{L\to\infty} f_L(x)$$

$$f_L(x)=\sum_{n=-\infty}^{+\infty}\left[\frac{1}{L}\int_{-L/2}^{+L/2} f_L(u)\exp\left(+2\pi i\frac{nu}{L}\right)\mathrm{d}u\right]\exp\left(-2\pi i\frac{nx}{L}\right)$$

$$f_L(x)=\sum_{n=-\infty}^{+\infty}\left[\frac{1}{L}\int_{-L/2}^{+L/2} f_L(u)\exp\left(+2\pi i\frac{nu}{L}\right)\mathrm{d}u\right]\exp\left(-2\pi i\frac{nx}{L}\right)$$

$$\frac{n}{L}=h_n\qquad\Rightarrow\qquad \Delta h=(h_{n+1}-h_n)=\frac{1}{L}$$

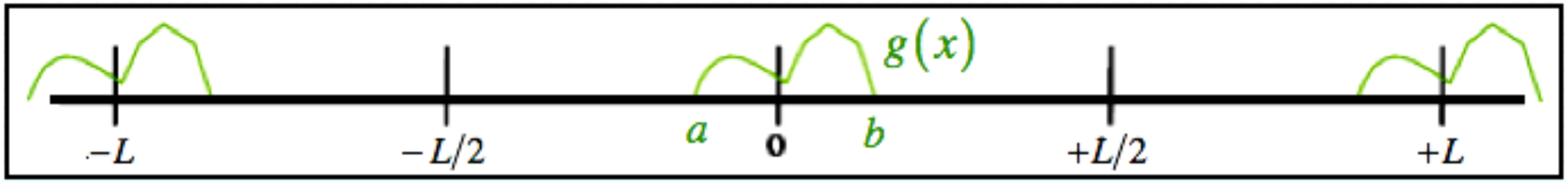
$$f_L(x)=\sum_{n=-\infty}^{+\infty}\Delta h\,\underbrace{\left[\int_{-L/2}^{+L/2} f_L(u)\exp(+2\pi i h_n u)\mathrm{d}u\right]}_{F(h_n)}\exp(-2\pi i h_n x)$$

$$f_L(x)=\sum_{n=-\infty}^{+\infty}\Delta h\,F(h_n)\exp(-2\pi i h_n x)$$

$$\lim_{L\to\infty} f_L(x)=\lim_{\Delta h\to 0}\sum_{n=-\infty}^{+\infty}F(h_n)\exp(-2\pi i h_n x)\Delta h=\int_{-\infty}^{+\infty}F(h)\exp(-2\pi i h x)\mathrm{d}h$$

$$\left\{\begin{array}{l} f(x)=\displaystyle\int_{-\infty}^{+\infty}F(h)\exp(-2\pi i h x)\mathrm{d}h=\mathcal{F}\left[F(h)\right]\\ F(h)=\displaystyle\int_{-\infty}^{+\infty}f(x)\exp(+2\pi i h x)\mathrm{d}x=\mathcal{F}^{-1}\left[f(x)\right]\end{array}\right.$$

An aperiodic signal can be viewed as a periodic signal with an infinite period.



$$\begin{cases} f_L(x) = \begin{cases} 0 & -L/2 < x < a \\ g(x) & a \le x \le b \\ 0 & b < x < +L/2 \end{cases} \\ f_L(x \pm nL) = f_L(x) \qquad L \gg b - a \end{cases}$$

$$g(x) = \lim_{L \to \infty} f_L(x)$$

$$\begin{cases} f_L(x) = \sum_{n=-\infty}^{+\infty} c_n \exp\left(-2\pi i \frac{nx}{L}\right) \qquad \begin{cases} x \in \mathbb{R} \\ n \in \mathbb{Z}, \quad n = 0, \pm 1, \pm 2, \ldots \end{cases} \\ c_n = \frac{1}{L} \int_{-L/2}^{+L/2} f_L(x) \exp\left(+2\pi i \frac{nx}{L}\right) \mathrm{d}x \end{cases}$$

$$g(x) = \lim_{L \to \infty} f_L(x) = \lim_{L \to \infty} \sum_{n=-\infty}^{+\infty} \left[\frac{1}{L} \int_{-L/2}^{+L/2} f_L(u) \exp\left(+2\pi i \frac{nu}{L}\right) \mathrm{d}u \right] \exp\left(-2\pi i \frac{nx}{L}\right)$$

(cont’d)

Aperiodic signal (cont'd)

$$g(x)=\lim_{L\to\infty} f_L(x)=\lim_{L\to\infty}\sum_{n=-\infty}^{+\infty}\left[\frac{1}{L}\int_{-L/2}^{+L/2} f_L(u)\exp\left(+2\pi i\frac{nu}{L}\right)\mathrm{d}u\right]\exp\left(-2\pi i\frac{nx}{L}\right)$$

$$f_L(x)=\sum_{n=-\infty}^{+\infty}\left[\frac{1}{L}\int_{-L/2}^{+L/2} f_L(u)\exp\left(+2\pi i\frac{nu}{L}\right)\mathrm{d}u\right]\exp\left(-2\pi i\frac{nx}{L}\right)$$

$$f_L(x)=\sum_{n=-\infty}^{+\infty}\left[\frac{1}{L}\int_{-L/2}^{+L/2} f_L(u)\exp\left(+2\pi i\frac{nu}{L}\right)\mathrm{d}u\right]\exp\left(-2\pi i\frac{nx}{L}\right)$$

$$\frac{n}{L}=h_n \qquad \Rightarrow \qquad \Delta h=\left(h_{n+1}-h_n\right)=\frac{1}{L}$$

$$f_L(x)=\sum_{n=-\infty}^{+\infty}\Delta h\underbrace{\left[\int_{-L/2}^{+L/2} f_L(u)\exp\left(+2\pi i h_n u\right)\mathrm{d}u\right]}_{F\left(h_n\right)}\exp\left(-2\pi i h_n x\right)$$

$$f_L(x)=\sum_{n=-\infty}^{+\infty}F\left(h_n\right)\exp\left(-2\pi i h_n x\right)\Delta h$$

$$\lim_{L\to\infty} f_L(x)=\lim_{\Delta h\to 0}\sum_{n=-\infty}^{+\infty}F\left(h_n\right)\exp\left(-2\pi i h_n x\right)\Delta h=\int_{-\infty}^{+\infty}F(h)\exp\left(-2\pi i h x\right)\mathrm{d}h$$

$$\begin{cases} f(x)=\int_{-\infty}^{+\infty}F(h)\exp\left(-2\pi i h x\right)\mathrm{d}h=\mathcal{F}\left[F(h)\right] \\ F(h)=\int_{-\infty}^{+\infty}f(x)\exp\left(+2\pi i h x\right)\mathrm{d}x=\mathcal{F}^{-1}\left[f(x)\right] \end{cases}$$

From Fourier series (sums) to Fourier transforms (integrals)

$$\left.\begin{array}{l} f_L(x) = \begin{cases} 0\,, & -L/2 < x < a \\ g(x)\,, & a \le x \le b \\ 0\,, & b < x < +L/2 \end{cases} \\ f_L(x \pm nL) = f_L(x)\,, \qquad L \gg b - a \end{array}\right\} \qquad \begin{cases} f_L(x) = \displaystyle\sum_{n=-\infty}^{+\infty} c_n \exp\left(-2\pi i \frac{nx}{L}\right), & \begin{cases} x \in \mathbb{R} \\ n \in \mathbb{Z}\,, \quad n = 0, \pm 1, \pm 2, \ldots \end{cases} \\ c_n = \displaystyle\frac{1}{L}\int_{-L/2}^{+L/2} f_L(x) \exp\left(+2\pi i \frac{nx}{L}\right) \mathrm{d}x \end{cases}$$

$$g(x) = \lim_{L\to\infty} f_L(x)$$

$$f_L(x) = \sum_{n=-\infty}^{+\infty} \left[\frac{1}{L}\int_{-L/2}^{+L/2} f_L(u) \exp\left(+2\pi i \frac{nu}{L}\right) \mathrm{d}u\right] \exp\left(-2\pi i \frac{nx}{L}\right)$$

$$f_L(x) = \sum_{n=-\infty}^{+\infty} \left[\frac{1}{L}\int_{-L/2}^{+L/2} f_L(u) \exp\left(+2\pi i \frac{nu}{L}\right) \mathrm{d}u\right] \exp\left(-2\pi i \frac{nx}{L}\right)$$

$$\frac{n}{L} = h_n \qquad \Rightarrow \qquad \Delta h = \left(h_{n+1} - h_n\right) = \frac{1}{L}$$

$$f_L(x) = \sum_{n=-\infty}^{+\infty} \Delta h \underbrace{\left[\int_{-L/2}^{+L/2} f_L(u) \exp\left(+2\pi i h_n u\right) \mathrm{d}u\right]}_{F(h_n)} \exp\left(-2\pi i h_n x\right)$$

$$f_L(x) = \sum_{n=-\infty}^{+\infty} \Delta h\, F(h_n) \exp\left(-2\pi i h_n x\right)$$

$$\lim_{L\to\infty} f_L(x) = \lim_{\Delta h\to 0} \sum_{n=-\infty}^{+\infty} F(h_n) \exp\left(-2\pi i h_n x\right) \Delta h = \int_{-\infty}^{+\infty} F(h) \exp\left(-2\pi i h x\right) \mathrm{d}h$$

$$\begin{cases} f(x) = \displaystyle\int_{-\infty}^{+\infty} F(h) \exp\left(-2\pi i h x\right) \mathrm{d}h = \mathcal{F}\left[F(h)\right] \\ F(h) = \displaystyle\int_{-\infty}^{+\infty} f(x) \exp\left(+2\pi i h x\right) \mathrm{d}x = \mathcal{F}^{-1}\left[f(x)\right] \end{cases}$$

In the Fourier series representation of a periodic function, the Fourier coefficients are Fourier transforms of the function.

$$\begin{cases} f(x) = \sum_{n=-\infty}^{+\infty} c_n \exp\left(-2\pi i \frac{nx}{T}\right), & \begin{cases} x \in \mathbb{R} \\ n \in \mathbb{Z}, \quad n = 0, \pm 1, \pm 2, \ldots \end{cases} \\ c_n = \frac{1}{T}\int_{-T/2}^{+T/2} f(x) \exp\left(+2\pi i \frac{nx}{T}\right) \mathrm{d}x = \mathcal{F}^{-1}\left[f(x)\right] \end{cases}$$

$$\begin{cases} \rho(x) = \frac{1}{a}\sum_{h=-\infty}^{+\infty} F_{h00} \exp(-2\pi i h x), & \begin{cases} x \in \mathbb{R}, \quad 0 \le x < 1 \\ h \in \mathbb{Z}, \quad h = 0, \pm 1, \pm 2, \ldots \end{cases} \\ F_{h00} = a\int_0^1 \rho(x) \exp(+2\pi i h x) \mathrm{d}x = \mathcal{F}^{-1}\left[\rho(x)\right] \end{cases}$$

$$\begin{cases} \rho(x,y,z) = \frac{1}{V_{\text{cell}}} \sum_{\substack{-\infty \\ h}}^{+\infty} \sum_{\substack{-\infty \\ k}}^{+\infty} \sum_{\substack{-\infty \\ l}}^{+\infty} F_{hkl} \exp\left[-2\pi i (hx + ky + lz)\right], & \begin{cases} x,y,z \in \mathbb{R}^3 \\ hkl \in \mathbb{Z}^3 \end{cases} \\ F_{hkl} = V_{\text{cell}} \int_0^1 \int_0^1 \int_0^1 \rho(x,y,z) \exp\left[+2\pi i (hx + ky + lz)\right] \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \mathcal{F}^{-1}\left[\rho(x,y,z)\right] \end{cases}$$

- Each and every value of the function depends on the whole (in principle, infinite) set of Fourier coefficients, and
- Each and every Fourier coefficient depends on all of the points (in principle, an infinite number of points) in one period of the function.

Vocabulary and syntax of Fourier transformation terminology

$$F(h) \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x) \quad \begin{cases} \rho(x) = \mathcal{F}\left[F(h)\right] = \int_{-\infty}^{+\infty} F(h)\exp(-2\pi i h x)\,\mathrm{d}h \approx \sum\limits_{j=-\infty}^{+\infty} F\left(h_j\right)\exp\left(-2\pi i h_j x\right)\Delta h_j \\ F(h) = \mathcal{F}^{-1}\left[\rho(x)\right] = \int_{-\infty}^{+\infty} \rho(x)\exp(+2\pi i h x)\,\mathrm{d}x \approx \sum\limits_{k=-\infty}^{+\infty} \rho\left(x_k\right)\exp\left(+2\pi i h x_k\right)\Delta x_k \end{cases}$$

$$\begin{cases} \mathcal{F} \\ \mathcal{F}^{-1} \end{cases} \text{is the} \begin{cases} \text{forward } (-i) \\ \text{reverse } (+i) \end{cases} \text{Fourier transform } \textit{operator}$$

$$\begin{cases} \rho(x) \\ F(h) \end{cases} \text{is given by Fourier} \begin{cases} \text{transformation} \\ \text{inversion} \end{cases} \text{or Fourier} \begin{cases} \text{synthesis} \\ \text{analysis} \end{cases} \text{of} \begin{cases} F(h) \\ \rho(x) \end{cases}$$

$$\begin{cases} \rho(x) \\ F(h) \end{cases} \text{is the Fourier} \begin{cases} \text{transform} \\ \text{inverse} \end{cases} \text{of} \begin{cases} F(h) \\ \rho(x) \end{cases}$$

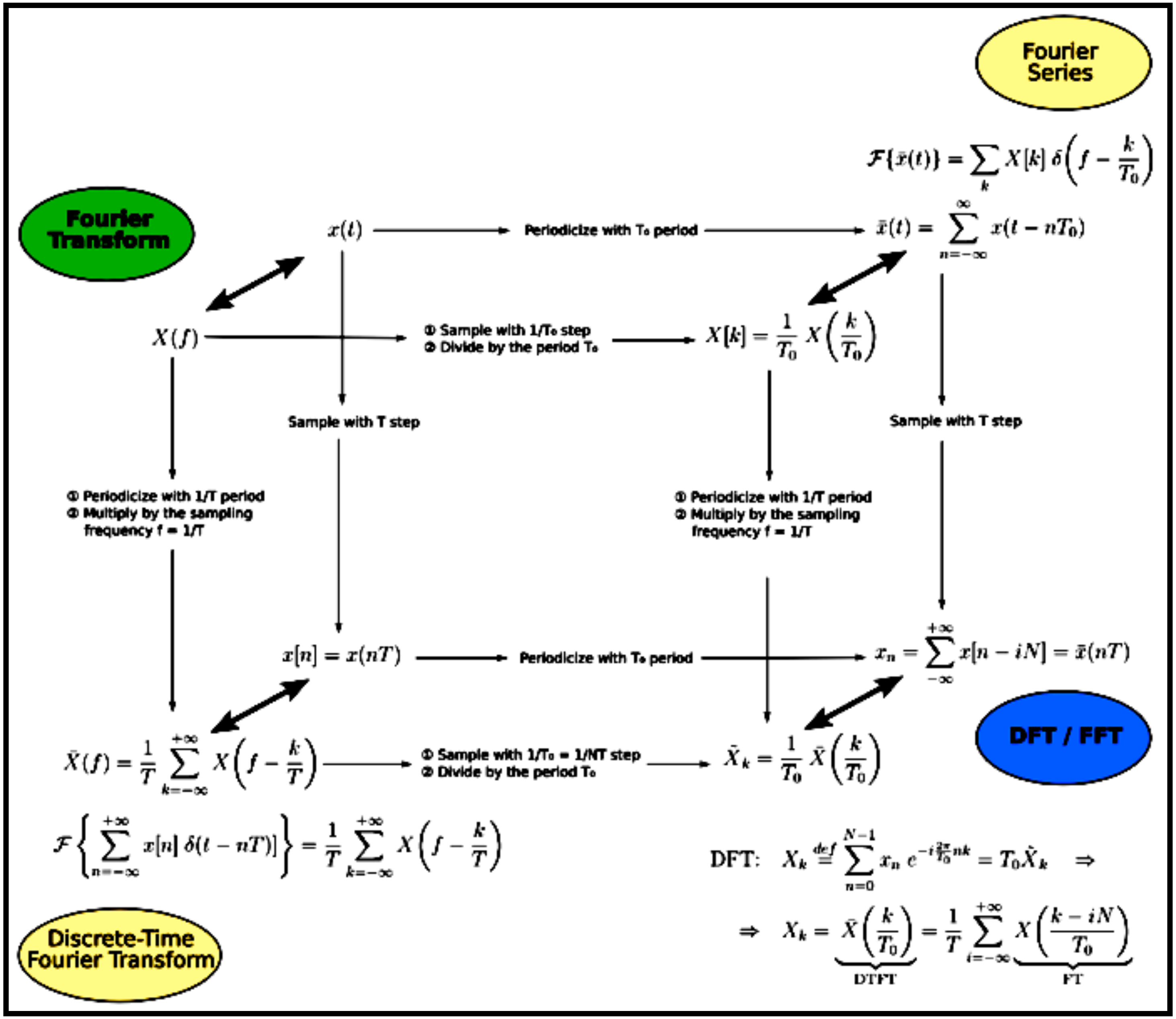
The complex exponential quantity $\begin{cases} \exp(-2\pi i h x) \\ \exp(+2\pi i h x) \end{cases}$

is the Fourier transformation *kernel* for the $\begin{cases} \text{forward } (-i) \\ \text{reverse } (+i) \end{cases}$

transform operator for Fourier $\begin{cases} \text{synthesis} \\ \text{analysis} \end{cases}$

The *conjugate, dual* variables *x* and *h* have dimensions that are reciprocally related, since the products *hx* must be *dimensionless* arguments of the exponential function

$$\exp(\pm 2\pi i h x) = \cos(2\pi h x) \pm i \sin(2\pi h x) \; .$$



Fourier Series

$$\mathcal{F}\{\tilde{x}(t)\} = \sum_k X[k]\,\delta\left(f - \frac{k}{T_0}\right)$$

Fourier Transform

$x(t)$ → Periodicize with T₀ period → $\tilde{x}(t) = \sum_{n=-\infty}^{\infty} x(t - nT_0)$

$X(f)$ → ① Sample with 1/T₀ step ② Divide by the period T₀ → $X[k] = \frac{1}{T_0} X\left(\frac{k}{T_0}\right)$

Sample with T step

Sample with T step

① Periodicize with 1/T period
② Multiply by the sampling frequency f = 1/T

① Periodicize with 1/T period
② Multiply by the sampling frequency f = 1/T

$x[n] = x(nT)$ → Periodicize with T₀ period → $\tilde{x}_n = \sum_{-\infty}^{+\infty} x[n - iN] = \tilde{x}(nT)$

DFT / FFT

$\tilde{X}(f) = \frac{1}{T} \sum_{k=-\infty}^{+\infty} X\left(f - \frac{k}{T}\right)$ → ① Sample with 1/T₀ = 1/NT step ② Divide by the period T₀ → $\tilde{X}_k = \frac{1}{T_0} \tilde{X}\left(\frac{k}{T_0}\right)$

$$\mathcal{F}\left\{\sum_{n=-\infty}^{+\infty} x[n]\,\delta(t - nT)\right\} = \frac{1}{T} \sum_{k=-\infty}^{+\infty} X\left(f - \frac{k}{T}\right)$$

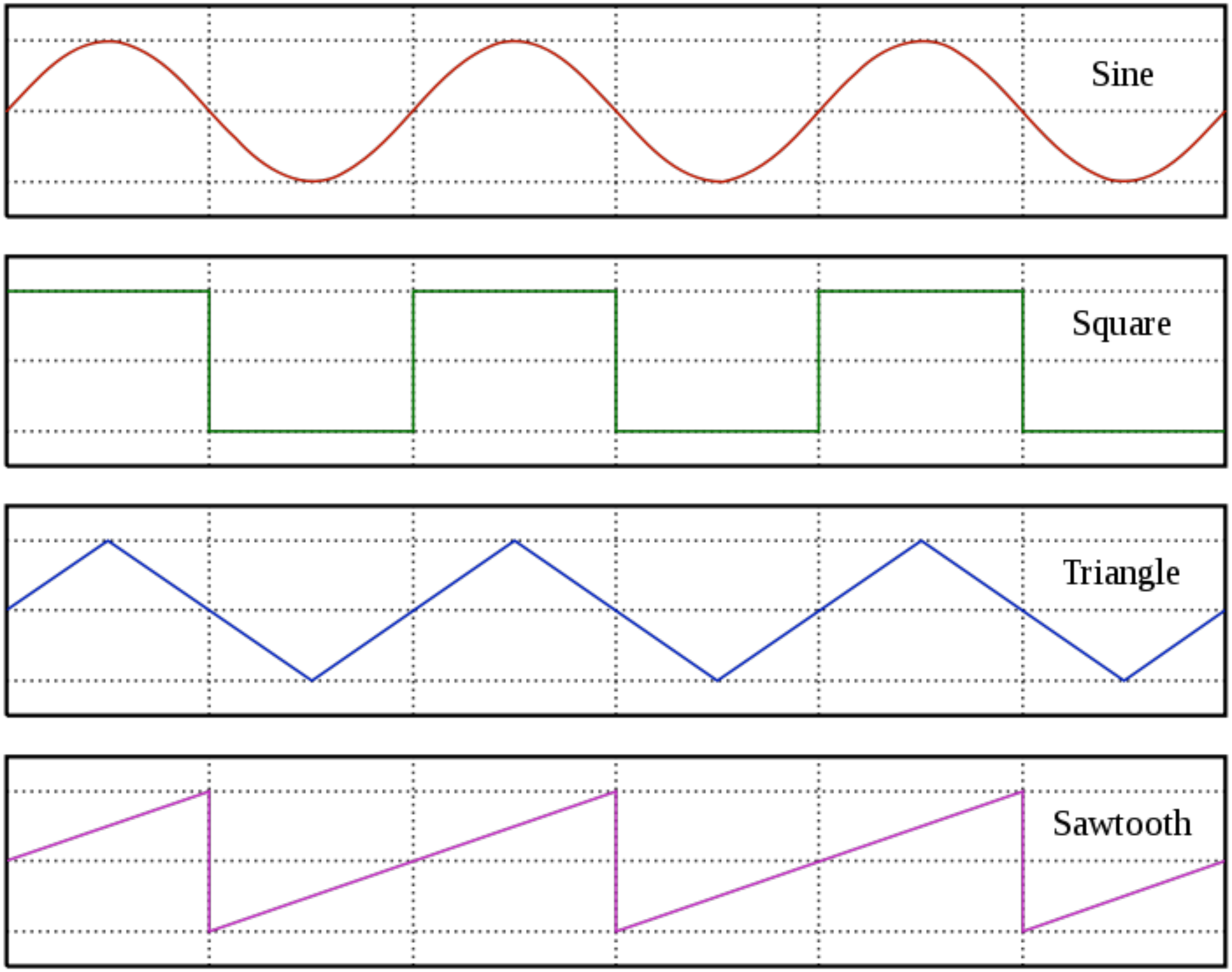
$$\text{DFT:}\quad X_k \overset{def}{=} \sum_{n=0}^{N-1} x_n\, e^{-i\frac{2\pi}{T_0}nk} = T_0 \tilde{X}_k \quad \Rightarrow$$

$$\Rightarrow\quad X_k = \underbrace{\tilde{X}\left(\frac{k}{T_0}\right)}_{\text{DTFT}} = \frac{1}{T} \sum_{i=-\infty}^{+\infty} \underbrace{X\left(\frac{k - iN}{T_0}\right)}_{\text{FT}}$$

Discrete-Time Fourier Transform

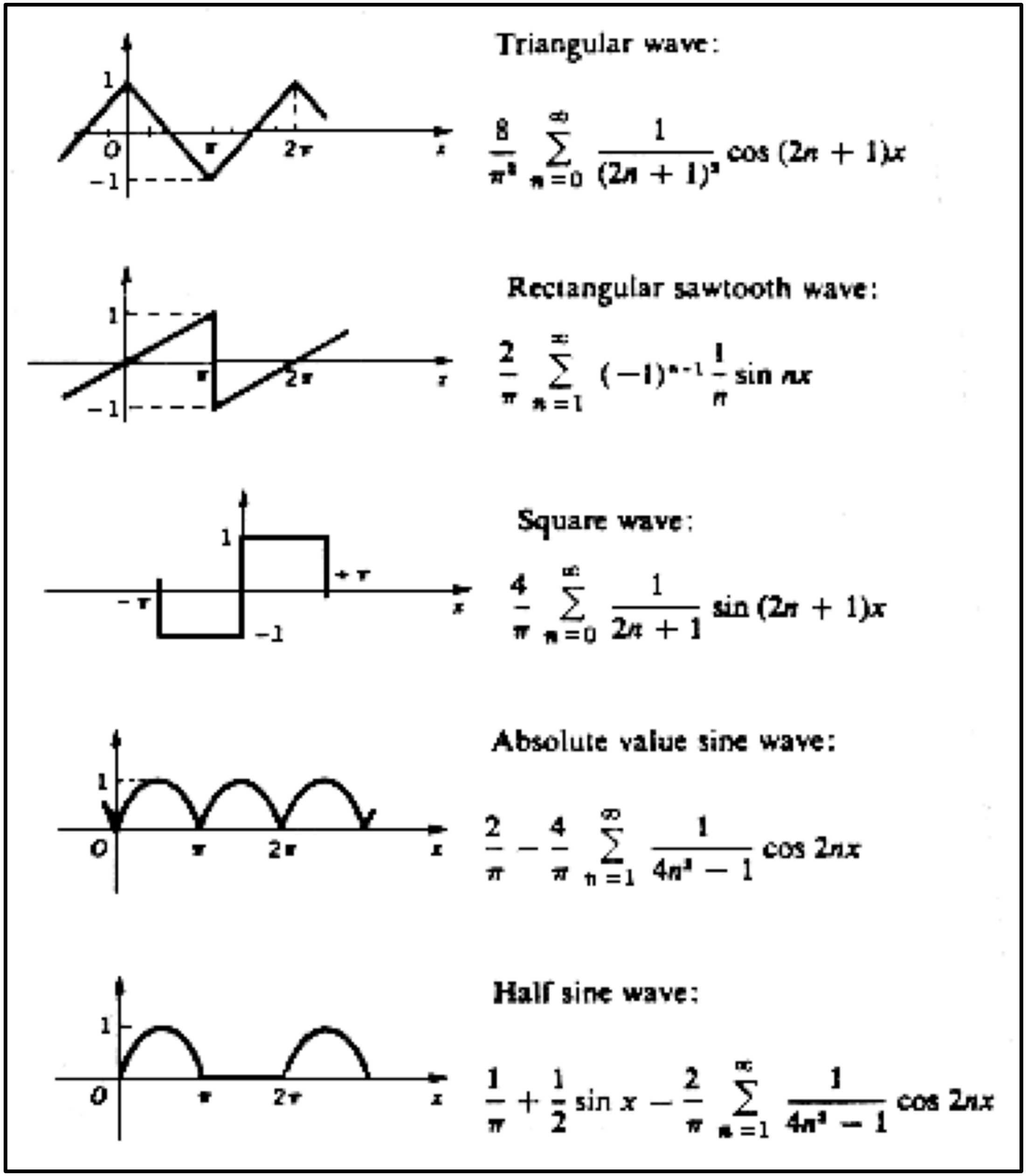
http://en.wikipedia.org/wiki/Relations_between_Fourier_transforms_and_Fourier_series

Simple Waveforms



http://upload.wikimedia.org/wikipedia/commons/thumb/7/77/Waveforms.svg/760px-Waveforms.svg.png
http://en.wikipedia.org/wiki/Waveform

Some simple waveforms and their Fourier series



Triangular wave:

$$\frac{8}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\cos(2n+1)x$$

Rectangular sawtooth wave:

$$\frac{2}{\pi}\sum_{n=1}^{\infty}(-1)^{n-1}\frac{1}{n}\sin nx$$

Square wave:

$$\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\sin(2n+1)x$$

Absolute value sine wave:

$$\frac{2}{\pi}-\frac{4}{\pi}\sum_{n=1}^{\infty}\frac{1}{4n^2-1}\cos 2nx$$

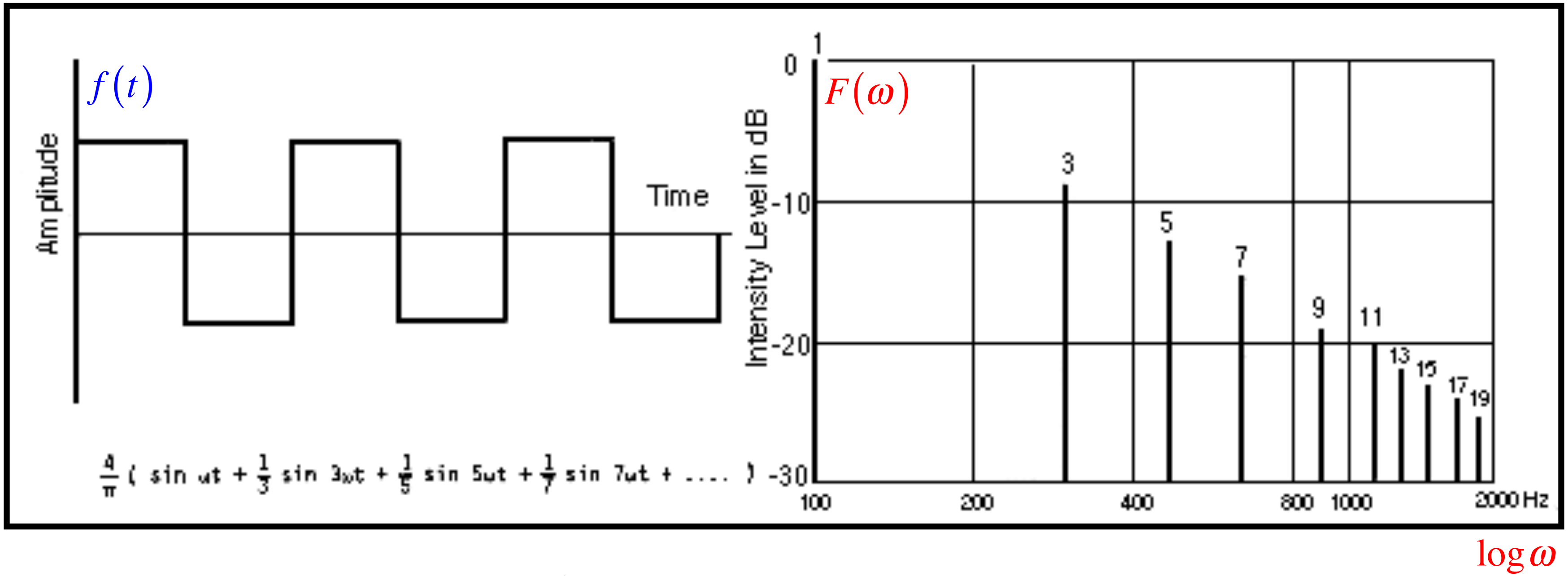
Half sine wave:

$$\frac{1}{\pi}+\frac{1}{2}\sin x-\frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{4n^2-1}\cos 2nx$$

http://www.sfu.ca/sonic-studio/handbook/Fourier_Theorem.html

Time and frequency domains

$$\begin{cases} \text{signal} & f(t)=\mathcal{F}\left[F(\omega)\right] \\ \text{spectrum} & F(\omega)=\mathcal{F}^{-1}\left[f(t)\right] \end{cases}$$



$$f(t)=\begin{cases} \pi\,, & 0<t<\pi \\ -\pi\,, & \pi<t<2\pi \end{cases}$$

$$f(t \pm 2n\pi)=f(t)$$

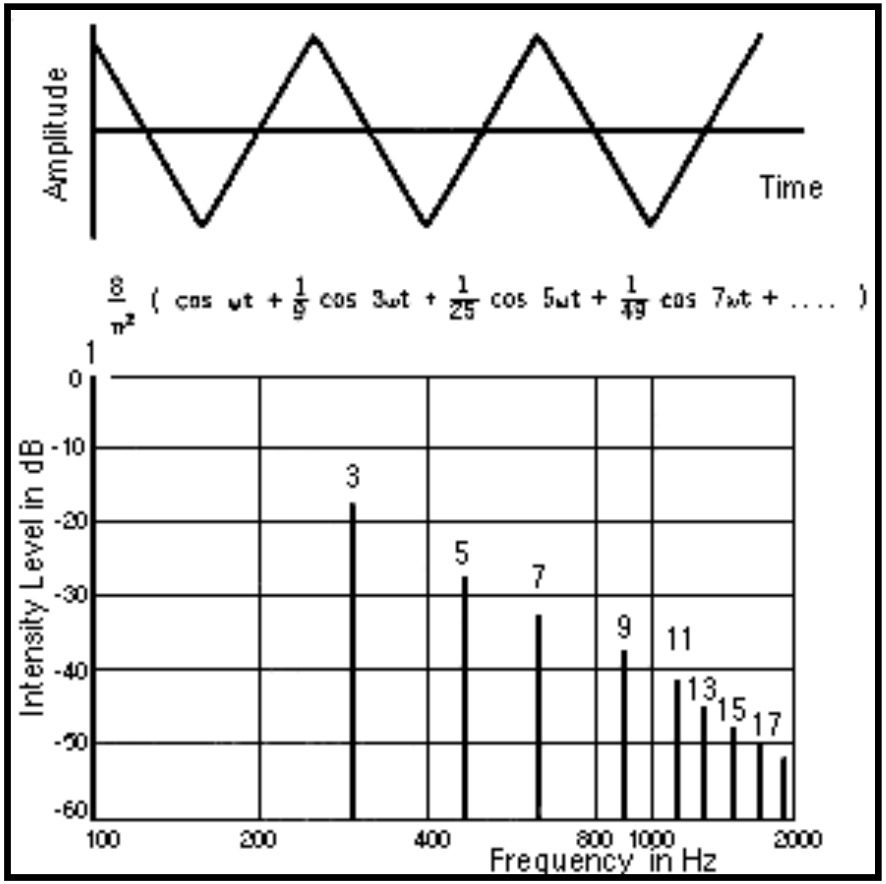
$$f(t)=\frac{4}{\pi}\left[\sin(\omega t)+\frac{1}{3}\sin(3\omega t)+\frac{1}{5}\sin(5\omega t)+\cdots\right]$$

http://www.sfu.ca/sonic-studio/handbook/Fourier_Theorem.html

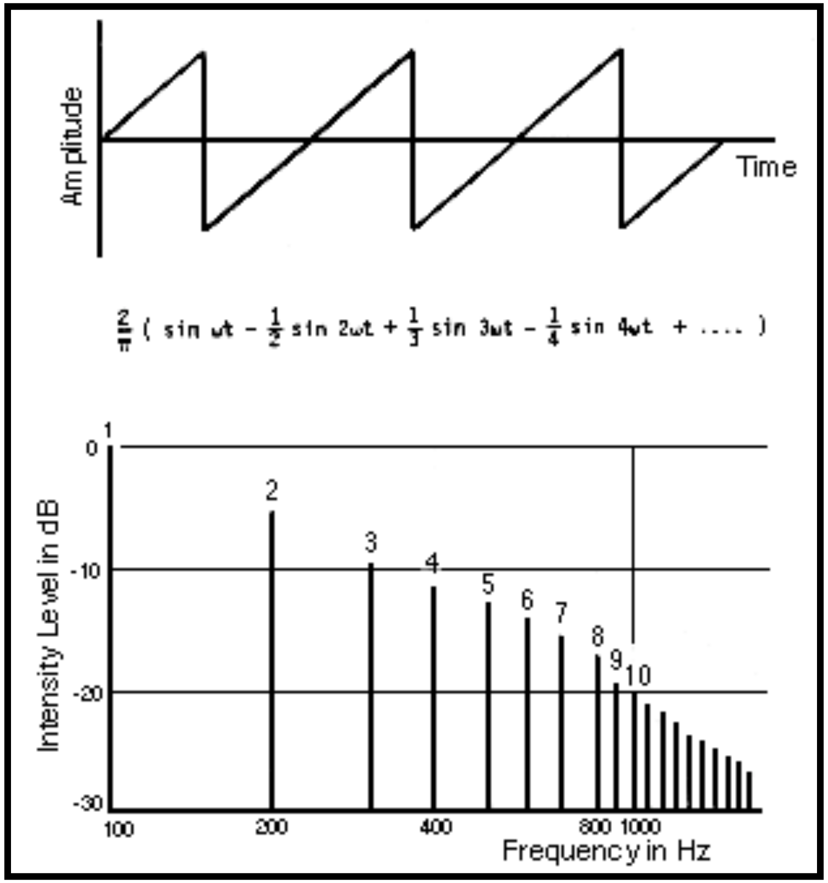
Time and frequency domains

signal $f(t) = \mathcal{F}\left[F(\omega)\right]$

spectrum $F(\omega) = \mathcal{F}^{-1}\left[f(t)\right]$



$\log \omega$



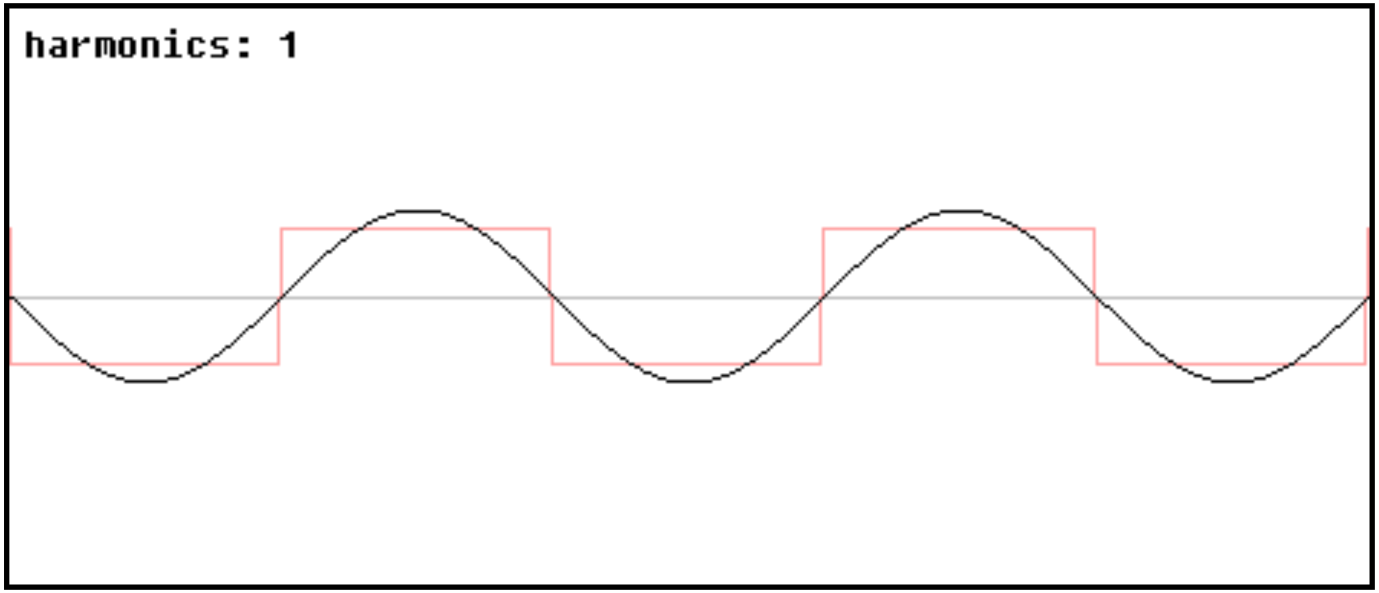
$\log \omega$

$$f(t) = \frac{8}{\pi^2}\left(\cos\omega t + \frac{1}{9}\cos 3\omega t + \frac{1}{25}\cos 5\omega t + \cdots\right)$$

$$f(t) = \frac{2}{\pi}\left(\sin\omega t - \frac{1}{2}\sin 2\omega t + \frac{1}{3}\cos 3\omega t - \frac{1}{4}\cos 4\omega t + \cdots\right)$$

http://www.sfu.ca/sonic-studio/handbook/Triangle_Wave.html http://www.sfu.ca/sonic-studio/handbook/Sawtooth_Wave.html

Square-wave function
$$\begin{cases} f(t) = \operatorname{sgn}(\sin t) = \begin{cases} -1, & -\pi < t < 0 \\ 0, & t = 0 \\ +1, & 0 < t < \pi \end{cases} \\ f(t \pm 2n\pi) = f(t) \end{cases}$$



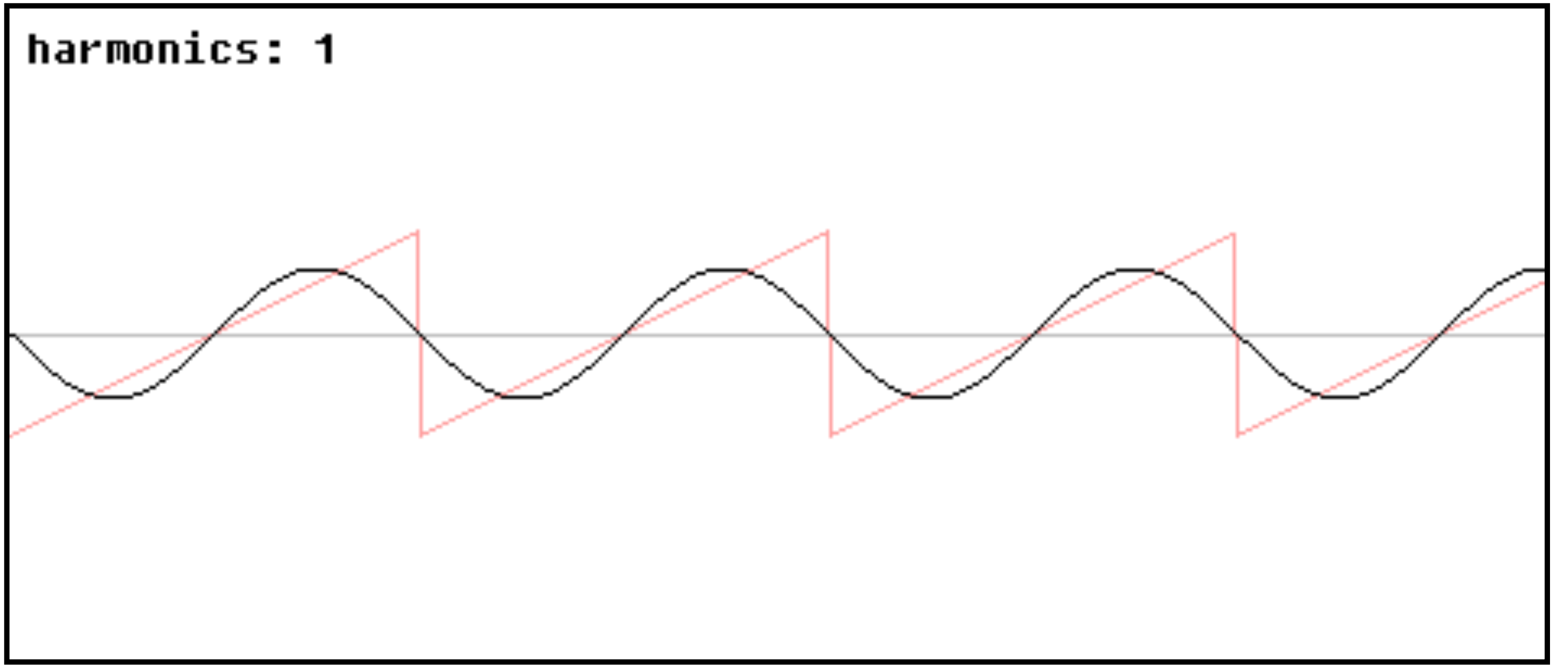
Fourier series representation $f(t) = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\sin\left[2\pi(2n-1)\omega t\right]}{2n-1}$

$$f(t) = \frac{4}{\pi}\left[\sin(2\pi\omega t) + \frac{1}{3}\sin(6\pi\omega t) + \frac{1}{5}\sin(10\pi\omega t) + \cdots\right]$$

http://commons.wikimedia.org/wiki/Image:Synthesis_square.gif

Sawtooth-wave function

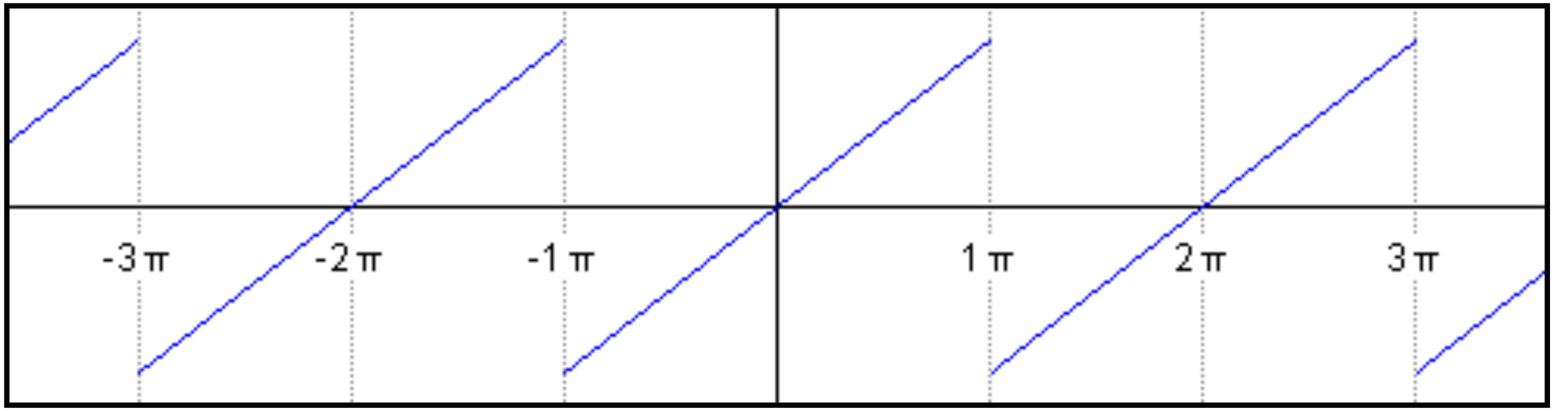
$$\begin{cases} f(t) = t/2\,, & -\pi < t < +\pi \\ f(t \pm 2n\pi) = f(t) \end{cases}$$

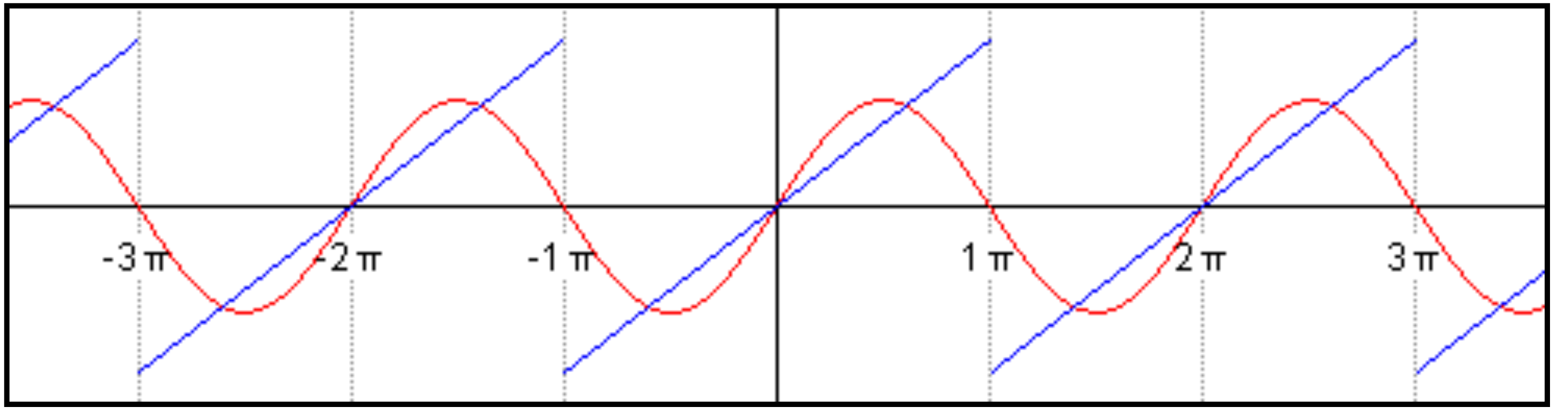


Fourier series representation $$f(t) = \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{\sin(nt)}{n}$$

http://commons.wikimedia.org/wiki/Image:Synthesis_sawtooth.gif

Periodic identity function $$\begin{cases} f(x) = x\,, & -\pi \le x \le \pi \\ f(x \pm 2n\pi) = f(x) \end{cases}$$

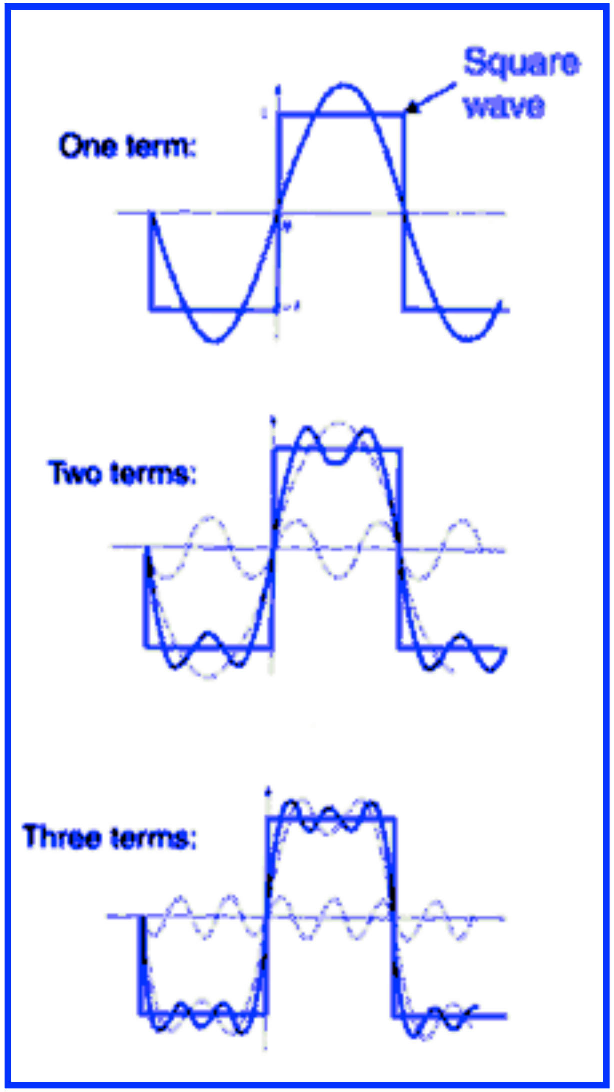




Fourier series representation $$f(x) = 2\sum_{n=1}^{\infty}(-1)^{n+1}\frac{\sin(nx)}{n}$$

http://en.wikipedia.org/wiki/Image:Periodic_identity_function.gif

Approximation of a square-wave function by a Fourier sum of three sinusoidal harmonic components

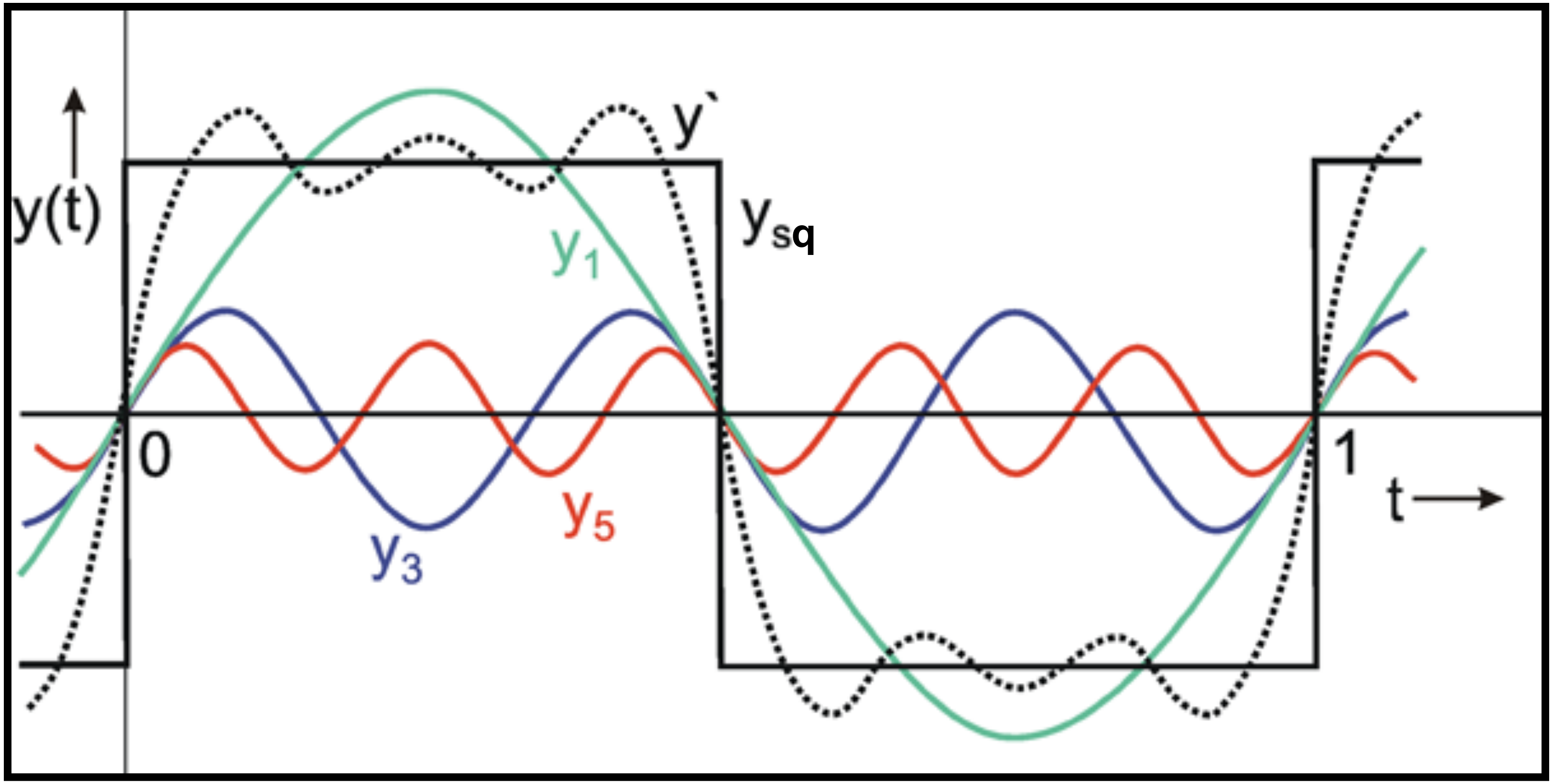


$$y_1 = \sin x$$

$$y_2 = \sin x + \frac{1}{3}\sin 3x$$

$$y_3 = \sin x + \frac{1}{3}\sin 3x + \frac{1}{5}\sin 5x$$

Approximation of a square-wave function by a Fourier sum of three sinusoidal harmonic components



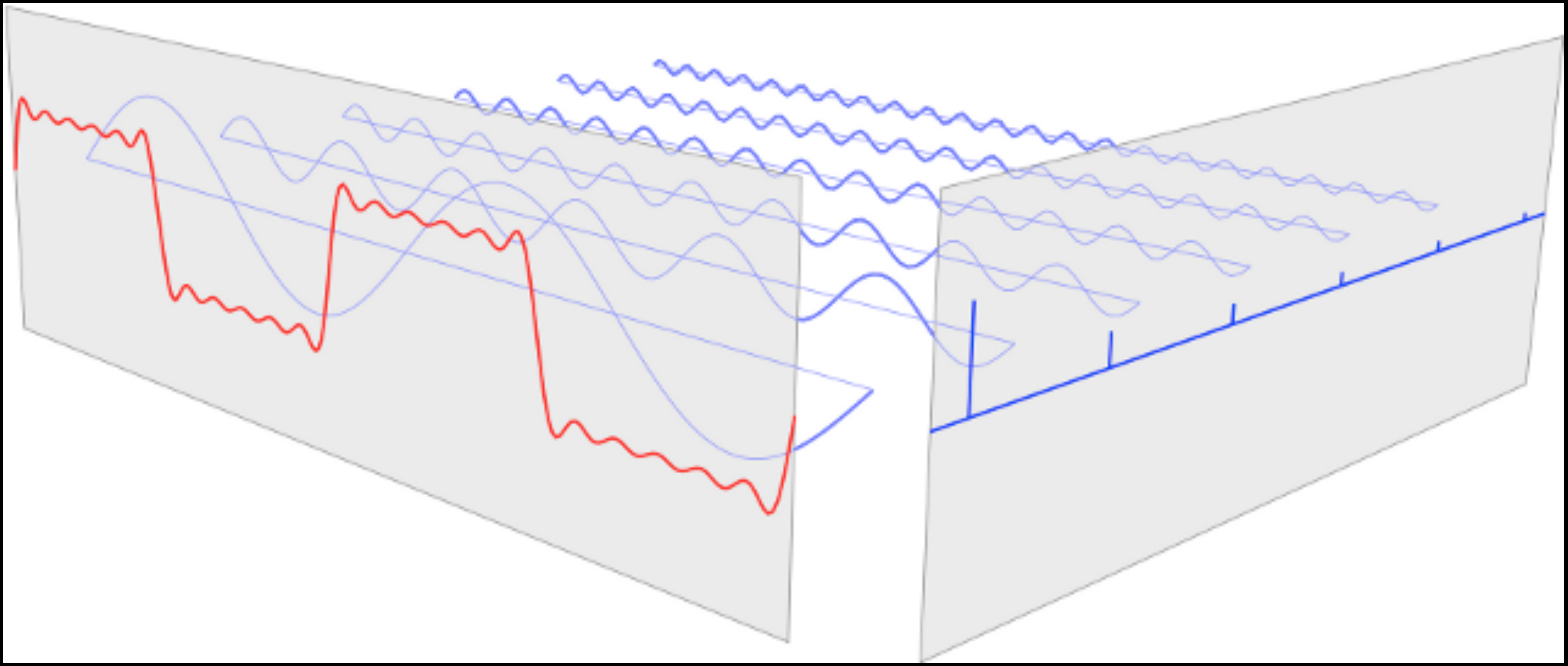
$$y_{\text{sq}} \approx y' = y_1 + y_3 + y_5 = \sin(2\pi t) + \frac{1}{3}\sin[3(2\pi t)] + \frac{1}{5}\sin[5(2\pi t)]$$

http://www.brains-minds-media.org/archive/1988/

$$\mathrm{FT}\left[f(t)\right]=\hat{f}(\omega)$$

http://tex.stackexchange.com/questions/127375/replicate-the-fourier-transform-time-frequency-domains-correspondence-illustrati

http://i.stack.imgur.com/27HVo.gif



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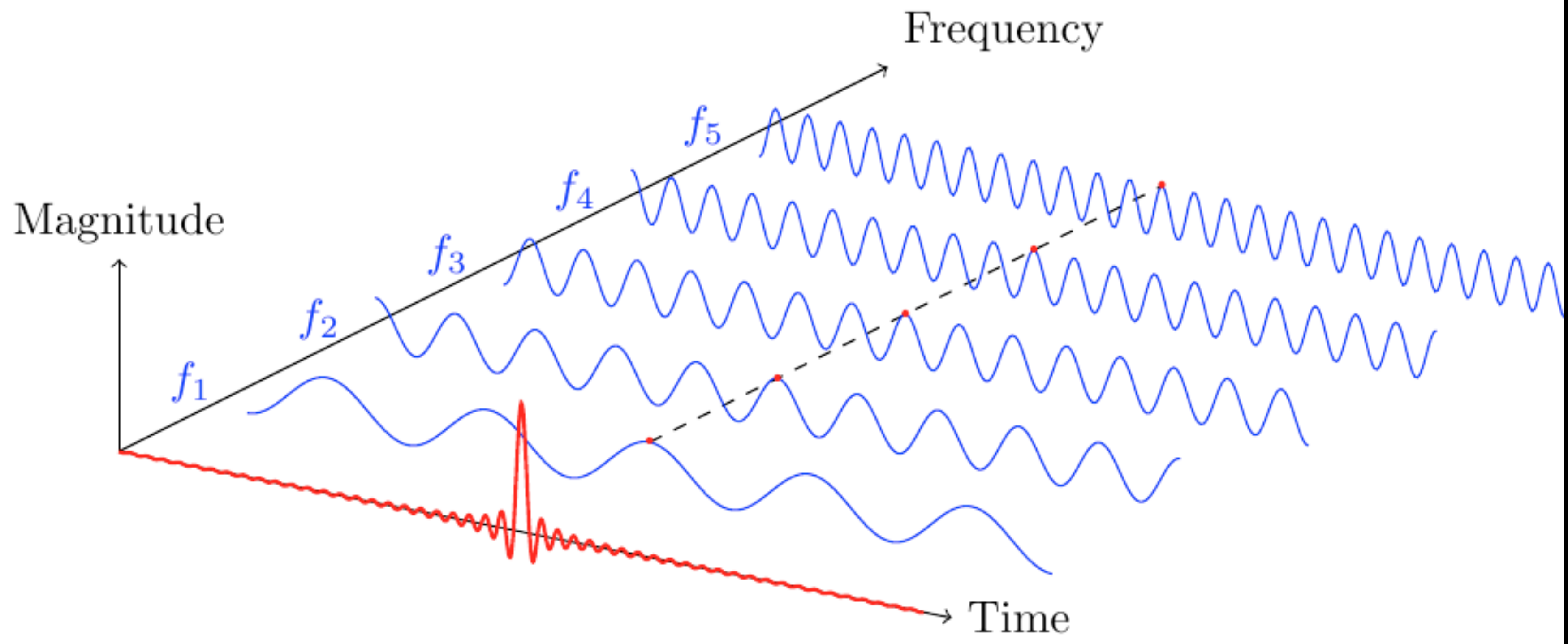
http://tex.stackexchange.com/questions/127375/replicate-the-fourier-transform-time-frequency-domains-correspondence-illustrati



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http://tex.stackexchange.com/questions/127375/replicate-the-fourier-transform-time-frequency-domains-correspondence-illustrati

The "fundamental theorem" of structural crystallography

The fundamental theorem of arithmetic

Every integer greater that 1 has a unique expression as a product of primes.

The fundamental theorem of algebra

Every univariate polynomial of degree n with complex coefficients has exactly n complex roots.

The fundamental theorem of the calculus

If the derivative of $f(x)$ is $g(x)$, then the integral of $g(x)$ is $f(x)$.

$$\frac{\mathrm{d}}{\mathrm{d}x} f(x) = g(x) \quad \Rightarrow \quad \int_a^b g(x)\mathrm{d}x = f(x)\Big|_a^b = f(b) - f(a) \quad \Rightarrow \quad \int g(x)\mathrm{d}x = f(x) + C$$

The "fundamental theorem" of structural crystallography

The crystal structure factors F_{hkl} in diffraction or reciprocal *hkl* space and the unit-cell scattering density distribution $\rho(x,y,z)$ in crystal or direct xyz space are related by Fourier transformation,

$$F_{hkl} = |F_{hkl}|\mathrm{e}^{i\varphi_{hkl}} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x,y,z) \qquad \begin{cases} \mathcal{F}[F_{hkl}] = \rho(x,y,z) & \text{Fourier synthesis} \\ \mathcal{F}^{-1}[\rho(x,y,z)] = F_{hkl} & \text{Fourier analysis} \end{cases}$$

where the $|F_{hkl}|$ and φ_{hkl} are, respectively, the amplitudes and phases of the beams of Laue-Bragg scattered radiation diffracted by a crystal.

The “fundamental theorem” of structural crystallography

$$F_{hkl} = \left|F_{hkl}\right| \mathrm{e}^{i\varphi_{hkl}} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x,y,z) \qquad \begin{cases} \rho(x,y,z) = \mathcal{F}\left[F_{hkl}\right] & \text{Fourier synthesis} \\ F_{hkl} = \mathcal{F}^{-1}\left[\rho(x,y,z)\right] & \text{Fourier analysis} \end{cases}$$

$$\begin{cases} \rho(x,y,z) = \dfrac{1}{V_{\text{cell}}} \displaystyle\sum_{\substack{-\infty \\ h}}^{+\infty} \sum_{\substack{-\infty \\ k}}^{+\infty} \sum_{\substack{-\infty \\ l}}^{+\infty} F_{hkl} \exp\left[-2\pi i(hx+ky+lz)\right] \\ F_{hkl} = V_{\text{cell}} \displaystyle\int_0^1 \int_0^1 \int_0^1 \rho(x,y,z) \exp\left[+2\pi i(hx+ky+lz)\right] \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \end{cases}$$

$$\begin{cases} F_{hkl} = \displaystyle\sum_{a=1}^{N} f_a(S_{hkl}) \exp\left[2\pi i(hx_a+ky_a+lz_a)\right] = \left|F_{hkl}\right| \mathrm{e}^{i\varphi_{hkl}} \\ \rho(x,y,z) = \dfrac{1}{V_{\text{cell}}} \displaystyle\sum_{\substack{-\infty \\ h}}^{+\infty} \sum_{\substack{-\infty \\ k}}^{+\infty} \sum_{\substack{-\infty \\ l}}^{+\infty} \left|F_{hkl}\right| \cos\left[\varphi_{hkl} - 2\pi(hx+ky+lz)\right] \end{cases}$$

$$S_{hkl} = \frac{1}{d_{hkl}} = 2\left(\frac{\sin\theta_{hkl}}{\lambda}\right) \qquad \text{and} \qquad \begin{cases} \left|F_{\bar{h}\bar{k}\bar{l}}\right| = \left|F_{hkl}\right| \\ \varphi_{\bar{h}\bar{k}\bar{l}} = -\varphi_{hkl} \end{cases}$$

The “fundamental theorem” of structural crystallography

$$F_{hkl} = \left|F_{hkl}\right| \mathrm{e}^{i\varphi_{hkl}} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x,y,z) \qquad \begin{cases} \rho(x,y,z) = \mathcal{F}\left[F_{hkl}\right] & \text{Fourier synthesis} \\ F_{hkl} = \mathcal{F}^{-1}\left[\rho(x,y,z)\right] & \text{Fourier analysis} \end{cases}$$

$$\begin{cases} F_{\mathbf{h}} = \int_V \rho(\mathbf{r}) \exp(+2\pi i \mathbf{h} \bullet \mathbf{r}) \mathrm{d}^3\mathbf{r} = \sum_{a=1}^{N} f_a(\mathbf{h}) \exp(2\pi i \mathbf{h} \bullet \mathbf{r}_a) = \left|F_{\mathbf{h}}\right| \mathrm{e}^{i\varphi_{\mathbf{h}}} \\ \rho(\mathbf{r}) = \dfrac{1}{V} \sum_{\mathbf{h}} F_{\mathbf{h}} \exp(-2\pi i \mathbf{h} \bullet \mathbf{r}) = \dfrac{1}{V} \sum_{\mathbf{h}} \left|F_{\mathbf{h}}\right| \cos(\varphi_{\mathbf{h}} - 2\pi \mathbf{h} \bullet \mathbf{r}), \qquad \begin{cases} \left|F_{-\mathbf{h}}\right| = \left|F_{+\mathbf{h}}\right| \\ \varphi_{-\mathbf{h}} = -\varphi_{+\mathbf{h}} \end{cases} \end{cases}$$

$$\begin{cases} \mathbf{r} = \sum_{i=1}^{3} r^i \mathbf{a}_i = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}, \qquad r^i \in \mathbb{R}, \quad \mathbf{r} \in \mathbb{R}^3, \qquad V = \mathbf{a} \bullet (\mathbf{b} \times \mathbf{c}) \quad \circlearrowright \\ \begin{cases} \mathbf{h} = \sum_{i=1}^{3} h_i \mathbf{a}^{*i} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*, \qquad h_i \in \mathbb{Z}, \quad \mathbf{h} \in \mathbb{Z}^3, \qquad \mathbf{a}^* = \dfrac{\mathbf{b} \times \mathbf{c}}{V} \quad \circlearrowright \\ \left|\mathbf{h}\right| = d^*_{hkl} = \dfrac{1}{d_{hkl}} = 2\left(\dfrac{\sin\theta_{hkl}}{\lambda}\right) \end{cases} \\ \begin{cases} \mathbf{a}^{*i} \bullet \mathbf{a}_j = \delta^i_j = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases} \\ \mathbf{h} \bullet \mathbf{r} = hx + ky + lz \end{cases} \\ f_a(\mathbf{h}) = \mathcal{F}^{-1}\left[\rho_a(\mathbf{r})\right] = \int_{V_{\mathbf{r}}} \rho_a(\mathbf{r}) \exp(2\pi i \mathbf{h} \bullet \mathbf{r}) \mathrm{d}^3\mathbf{r} \end{cases}$$

The unit cell scattering density distribution $\rho(x,y,z) = \rho(\mathbf{r})$ and the crystal structure factors $F_{hkl} = F_{\mathbf{h}}$ as atomic summations

$$\rho(\mathbf{r}) = \sum_{a=1}^{N} \rho_a(\mathbf{r}-\mathbf{r}_a) = \sum_{a=1}^{N} \rho_a(\mathbf{r}) * \delta^3(\mathbf{r}-\mathbf{r}_a)$$

$$\begin{aligned}
F_{\mathbf{h}} &= \mathcal{F}^{-1}\left[\rho(\mathbf{r})\right] \\
&= \mathcal{F}^{-1}\left[\sum_{a=1}^{N} \rho_a(\mathbf{r}-\mathbf{r}_a)\right] \\
&= \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r}-\mathbf{r}_a)\right] \\
&= \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r}) * \delta^3(\mathbf{r}-\mathbf{r}_a)\right] \\
F_{\mathbf{h}} &= \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r})\right] \mathcal{F}^{-1}\left[\delta(\mathbf{r}-\mathbf{r}_a)\right]
\end{aligned}$$

$$\mathcal{F}^{-1}\left[\rho_a(\mathbf{r})\right] = f_a(\mathbf{h})$$

$$\mathcal{F}^{-1}\left[\delta^3(\mathbf{r}-\mathbf{r}_a)\right] = \exp(2\pi i\mathbf{h}\bullet\mathbf{r}_a)$$

$$F_{\mathbf{h}} = \sum_{a=1}^{N} f_a(\mathbf{h}) \exp(2\pi i\mathbf{h}\bullet\mathbf{r}_a)$$

The crystal structure factors $F_{hkl} = F_{\mathbf{h}}$ and the unit cell scattering density distribution $\rho(x,y,z) = \rho(\mathbf{r})$ as Fourier series cosine and sine summations

$$F_{\mathbf{h}} = \sum_{a=1}^{N} f_a(\mathbf{h}) \exp\left(2\pi i \mathbf{h} \bullet \mathbf{r}_a\right)$$

$$= \sum_{a=1}^{N} f_a(\mathbf{h}) \left[\cos\left(2\pi \mathbf{h} \bullet \mathbf{r}_a\right) + i \sin\left(2\pi \mathbf{h} \bullet \mathbf{r}_a\right)\right]$$

$$= A_{\mathbf{h}} + iB_{\mathbf{h}}$$

$$F_{\mathbf{h}} = \left|F_{\mathbf{h}}\right| \mathrm{e}^{i\varphi_{\mathbf{h}}}$$

$$\left|F_{\mathbf{h}}\right| = \sqrt{A_{\mathbf{h}}{}^2 + B_{\mathbf{h}}{}^2}, \qquad \varphi_{\mathbf{h}} = \arctan\left(B_{\mathbf{h}}/A_{\mathbf{h}}\right)$$

$$F_{\mathbf{h}}^* F_{\mathbf{h}} = \left(A_{\mathbf{h}} - iB_{\mathbf{h}}\right)\left(A_{\mathbf{h}} + iB_{\mathbf{h}}\right) = \left|F_{\mathbf{h}}\right| \mathrm{e}^{-i\varphi_{\mathbf{h}}} \left|F_{\mathbf{h}}\right| \mathrm{e}^{i\varphi_{\mathbf{h}}} = \left|F_{\mathbf{h}}\right|^2$$

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{h}} F_{\mathbf{h}} \exp\left(-2\pi i \mathbf{h} \bullet \mathbf{r}\right)$$

$$= \frac{1}{V} \sum_{\mathbf{h}} \left|F_{\mathbf{h}}\right| \exp\left[i\left(\varphi_{\mathbf{h}} - 2\pi \mathbf{h} \bullet \mathbf{r}\right)\right]$$

$$= \frac{1}{V} \sum_{\mathbf{h}} \left|F_{\mathbf{h}}\right| \left[\cos\left(\varphi_{\mathbf{h}} - 2\pi \mathbf{h} \bullet \mathbf{r}\right) + i \sin\left(\varphi_{\mathbf{h}} - 2\pi \mathbf{h} \bullet \mathbf{r}\right)\right]$$

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{h}} \left|F_{\mathbf{h}}\right| \cos\left(\varphi_{\mathbf{h}} - 2\pi \mathbf{h} \bullet \mathbf{r}\right), \quad \text{if} \quad \begin{cases} \left|F_{-\mathbf{h}}\right| = \left|F_{+\mathbf{h}}\right| \\ \varphi_{-\mathbf{h}} = -\varphi_{+\mathbf{h}} \end{cases}$$

Physical (*X*,*Y*,*Z*) Ångström and dimensionless (*x*,*y*,*z*) fractional coordinates

$$F_{hkl} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho\left(x,y,z\right) \qquad \left\{ \begin{array}{rl} \rho\left(x,y,z\right) = \mathcal{F}\left[F_{hkl}\right] & \text{Fourier synthesis} \\ F_{hkl} = \mathcal{F}^{-1}\left[\rho\left(x,y,z\right)\right] & \text{Fourier analysis} \end{array} \right.$$

$$\left\{ \begin{aligned} \rho\left(\mathbf{r}\right) &= \frac{1}{V_{\text{cell}}} \sum_{\substack{-\infty \\ \mathbf{h}}}^{+\infty} F_{\mathbf{h}} \exp\left(-2\pi i \mathbf{h} \bullet \mathbf{r}\right) \\ F_{\mathbf{h}} &= \int_{V_{\text{cell}}} \rho\left(\mathbf{r}\right) \exp\left(+2\pi i \mathbf{h} \bullet \mathbf{r}\right) \mathrm{d}^3\mathbf{r} \end{aligned} \right.$$

$$\left\{ \begin{aligned} \rho\left(X,Y,Z\right) &= \frac{1}{V_{\text{cell}}} \sum_{\substack{-\infty \\ h}}^{+\infty} \sum_{\substack{-\infty \\ k}}^{+\infty} \sum_{\substack{-\infty \\ l}}^{+\infty} F_{hkl} \exp\left[-2\pi i \left(h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*\right) \bullet \left(x\mathbf{a} + y\mathbf{b} + z\mathbf{c}\right)\right] \\ F_{hkl} &= \int_0^a \int_0^b \int_0^c \rho\left(X,Y,Z\right) \exp\left[+2\pi i \left(h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*\right) \bullet \left(x\mathbf{a} + y\mathbf{b} + z\mathbf{c}\right)\right] \mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}Z \\ & \left\{ \begin{array}{l} X = xa\,, \qquad Y = yb\,, \qquad Z = zc\,, \qquad 0 \le x,y,z < 1 \\ \mathrm{d}X = a\,\mathrm{d}x\,, \quad \mathrm{d}Y = b\,\mathrm{d}y\,, \quad \mathrm{d}Z = c\,\mathrm{d}z \\ \mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}Z = abc\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = V_{\text{cell}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \\ \mathbf{a}^{*j} \bullet \mathbf{a}_k = \delta_k^j = \left\{ \begin{array}{ll} 0\,, & j \neq k \\ 1\,, & j = k \end{array} \right. \end{array} \right. \\ F_{hkl} &= V_{\text{cell}} \int_0^1 \int_0^1 \int_0^1 \rho\left(x,y,z\right) \exp\left[+2\pi i \left(hx + ky + lz\right)\right] \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \end{aligned} \right.$$

Continuous and discrete Fourier synthesis

$$F_{hkl} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x,y,z)$$

$$\begin{cases} \rho(x,y,z) = \mathcal{F}\left[F_{hkl}\right] & \text{Fourier synthesis} \\ F_{hkl} = \mathcal{F}^{-1}\left[\rho(x,y,z)\right] & \text{Fourier analysis} \end{cases}$$

$$\rho(\mathbf{r}) = \int_{V_{\mathrm{cell}}} F_{\mathbf{h}} \exp(-2\pi i \mathbf{h}\bullet\mathbf{r})\,\mathrm{d}^3\mathbf{h}$$

$$\rho(x,y,z) = \int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty} F_{hkl} \exp\left[-2\pi i\left(h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*\right)\bullet\left(x\mathbf{a} + y\mathbf{b} + z\mathbf{c}\right)\right]\mathrm{d}(ha^*)\,\mathrm{d}(kb^*)\,\mathrm{d}(lc^*)$$

$$\begin{cases} \mathrm{d}(ha^*)\,\mathrm{d}(kb^*)\,\mathrm{d}(lc^*) = a^*\, b^*\, c^*\,\mathrm{d}h\,\mathrm{d}k\,\mathrm{d}l = V^*_{\mathrm{cell}}\,\mathrm{d}h\,\mathrm{d}k\,\mathrm{d}l = \dfrac{1}{V_{\mathrm{cell}}}\,\mathrm{d}h\,\mathrm{d}k\,\mathrm{d}l \\ h,k,l \in \mathbb{Z} \quad \Rightarrow \quad \mathrm{d}h = \mathrm{d}k = \mathrm{d}l = \Delta h = \Delta k = \Delta l = 1 \\ \mathbf{a}^{*j}\bullet\mathbf{a}_k = \delta_k^j = \begin{cases} 0\,, & j \neq k \\ 1\,, & j = k \end{cases} \\ F_{hkl} = \left|F_{hkl}\right| \mathrm{e}^{i\varphi_{hkl}} \end{cases}$$

$$\rho(x,y,z) = \frac{1}{V_{\mathrm{cell}}} \sum_{\substack{-\infty \\ h}}^{+\infty}\sum_{\substack{-\infty \\ k}}^{+\infty}\sum_{\substack{-\infty \\ l}}^{+\infty} \left|F_{hkl}\right| \mathrm{e}^{i\varphi_{hkl}} \exp\left[-2\pi i\left(hx + ky + lz\right)\right],$$

$$\begin{cases} \left|F_{\bar{h}\bar{k}\bar{l}}\right| = \left|F_{hkl}\right| \\ \varphi_{\bar{h}\bar{k}\bar{l}} = -\varphi_{hkl} \end{cases}$$

$$\rho(x,y,z) = \frac{1}{V_{\mathrm{cell}}} \sum_{\substack{-\infty \\ h}}^{+\infty}\sum_{\substack{-\infty \\ k}}^{+\infty}\sum_{\substack{-\infty \\ l}}^{+\infty} \left|F_{hkl}\right| \cos\left[\varphi_{hkl} - 2\pi\left(hx + ky + lz\right)\right]$$

Fourier transformations by numerical grid summations

$$F_{hkl} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x,y,z) \qquad \begin{cases} \rho(x,y,z) = \mathcal{F}\left[F_{hkl}\right] \\ F_{hkl} = \mathcal{F}^{-1}\left[\rho(x,y,z)\right] \end{cases}$$

Fourier synthesis

Fourier analysis

Fourier Synthesis

$$\rho\left(x_p, y_q, z_r\right) = \frac{1}{V_{\text{cell}}} \sum_{h_{\min}}^{h_{\max}} \sum_{k_{\min}}^{k_{\max}} \sum_{l_{\min}}^{l_{\max}} \left|F_{hkl}\right| \cos\left[\varphi_{hkl} - 2\pi\left(hx_p + ky_q + lz_r\right)\right]$$

$$0 \le x_p, y_q, z_r < 1 \quad \begin{cases} x_p = p/N_{\text{x}}\,, & y_q = q/N_{\text{y}}\,, & z_r = r/N_{\text{z}} \\ p = 0,1,2,...,N_{\text{x}} - 1, & q = 0,1,2,...,N_{\text{y}} - 1, & r = 0,1,2,...,N_{\text{z}} - 1 \\ \Delta x = a/N_{\text{x}}\,, & \Delta y = b/N_{\text{y}} & \Delta z = c/N_{\text{z}} \end{cases}$$

Shannon sampling: $d_{hkl} \ge d_{\min} = \dfrac{\lambda}{2\sin\theta_{\max}}$ and $\max\left(\Delta x, \Delta y, \Delta z\right) \lesssim \dfrac{1}{2} d_{\min}$

Fourier Analysis

$$F_{hkl} = \frac{V_{\text{cell}}}{N_{\text{x}} N_{\text{y}} N_{\text{z}}} \sum_{p=0}^{N_{\text{x}}-1} \sum_{q=0}^{N_{\text{y}}-1} \sum_{r=0}^{N_{\text{z}}-1} \rho\left(x_p, y_q, z_r\right) \exp\left[+2\pi i\left(hx_p + ky_q + lz_r\right)\right]$$

Shannon sampling: $d_{hkl} \ge d_{\min} \gtrsim 2\max\left(\Delta x, \Delta y, \Delta z\right) = 2\max\left(a/N_{\text{x}}\,, b/N_{\text{y}}\,, c/N_{\text{z}}\right)$

Structure factor amplitudes and phases by numerical Fourier inversion of a grid density

Fourier Analysis

$$F_{hkl}=\frac{V_{\mathrm{cell}}}{N_{\mathrm{x}}N_{\mathrm{y}}N_{\mathrm{z}}}\sum_{p=0}^{N_{\mathrm{x}}-1}\sum_{q=0}^{N_{\mathrm{y}}-1}\sum_{r=0}^{N_{\mathrm{z}}-1}\rho\left(x_p,y_q,z_r\right)\exp\left[+2\pi i\left(hx_p+ky_q+lz_r\right)\right]$$

$$F_{hkl}=\left|F_{hkl}\right|\mathrm{e}^{i\varphi_{hkl}}=\left|F_{hkl}\right|\left(\cos\varphi_{hkl}+i\sin\varphi_{hkl}\right)=A_{hkl}+iB_{hkl}$$

$$\begin{cases} A_{hkl}=\dfrac{V_{\mathrm{cell}}}{N_{\mathrm{x}}N_{\mathrm{y}}N_{\mathrm{z}}}\displaystyle\sum_{p=0}^{N_{\mathrm{x}}-1}\sum_{q=0}^{N_{\mathrm{y}}-1}\sum_{r=0}^{N_{\mathrm{z}}-1}\rho\left(x_p,y_q,z_r\right)\cos\left[+2\pi\left(hx_p+ky_q+lz_r\right)\right] \\ B_{hkl}=\dfrac{V_{\mathrm{cell}}}{N_{\mathrm{x}}N_{\mathrm{y}}N_{\mathrm{z}}}\displaystyle\sum_{p=0}^{N_{\mathrm{x}}-1}\sum_{q=0}^{N_{\mathrm{y}}-1}\sum_{r=0}^{N_{\mathrm{z}}-1}\rho\left(x_p,y_q,z_r\right)\sin\left[+2\pi\left(hx_p+ky_q+lz_r\right)\right] \end{cases}$$

$$\begin{cases} \left|F_{hkl}\right|=\sqrt{A_{hkl}^2+B_{hkl}^2} \\ \varphi_{hkl}=\tan^{-1}\left(\dfrac{B_{hkl}}{A_{hkl}}\right) \end{cases}$$

Shannon sampling : $d_{hkl}\geq d_{\min}\gtrsim 2\max\left(\Delta x,\Delta y,\Delta z\right)=2\max\left(a/N_{\mathrm{x}},b/N_{\mathrm{y}},c/N_{\mathrm{z}}\right)$

Shannon sampling

$$\begin{cases} \textbf{Reciprocal lattice}: & \max\left|\mathbf{h}_j\right| = \dfrac{1}{d_{\min}} = 2\left(\dfrac{\sin\theta_{\max}}{\lambda}\right), & j = 1,2,\ldots,n \\ \textbf{Density grid}: & \min\left|\mathbf{r}_{j+1} - \mathbf{r}_j\right| = \dfrac{d_{\min}}{2} = \dfrac{\lambda}{4\sin\theta_{\max}}, & j = 0,1,\ldots,2n-1 \end{cases}$$

n points in **h**-space ⇔ $2n$ points in **r**-space

Claude E. Shannon, "Communication in the presence of noise", *Proc. Institute of Radio Engineers*, vol. **37**, no. 1, pp. 10–21, (Jan. 1949). Reprint as classic paper in: *Proc. IEEE*, vol. **86**, no. 2, (Feb. 1998)

http://en.wikipedia.org/wiki/Nyquist–Shannon_sampling_theorem

$$F_{hkl} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x,y,z)$$

Basic principle of the FFT

A sum of N terms can be decomposed into two sums of $N/2$ terms.

$$F_{hkl} \underset{\mathrm{FFT}^{-1}}{\overset{\mathrm{FFT}}{\rightleftarrows}} \rho(x,y,z)$$

The projection of a unit-cell scattering density distribution onto the *a* axis is given by Fourier transformation of the axial structure factors,

$$\begin{aligned}
\rho(x) &= \mathcal{F}\left[F_{h\,0\,0}\right] \\
&= \frac{1}{a}\sum_{h=0}^{N_h-1} F_{h\,0\,0}\exp(-2\pi i h x) \\
&= \frac{1}{a}\sum_{h=0}^{(N_h/2)-1} F_{2h\;0\;0}\exp\left[-2\pi i(2h)x\right] + \frac{1}{a}\sum_{h=0}^{(N_h/2)-1} F_{(2h+1)\;0\;0}\exp\left[-2\pi i(2h+1)x\right] \\
&= \frac{1}{a}\sum_{h=0}^{(N_h/2)-1} F_{2h\;0\;0}\exp\left[-2\pi i(2h)x\right] + \frac{1}{a}\exp(-2\pi i x)\sum_{h=0}^{(N_h/2)-1} F_{(2h+1)\;0\;0}\exp\left[-2\pi i(2h)x\right].
\end{aligned}$$

Thus $\exp\left[-2\pi i(2h)x\right]$ needs be evaluated only $N_h/2$ times but can be used N_h times.

Similarly, the axial structure factors are given by Fourier inversion of the one-dimensional projected density,

$$\begin{aligned}
F_{h00} &= \mathcal{F}^{-1}\left[\rho(x)\right] \\
&= a\sum_{n=0}^{N_x-1}\rho(x_n)\exp(+2\pi i h x_n) \\
&= a\sum_{n=0}^{N_x-1}\rho(n/N_x)\exp(2\pi i h\, n/N_x) \\
&= a\sum_{n=0}^{(N_x/2)-1}\rho\left(\frac{2n}{N_x}\right)\exp\left[2\pi i h(2n)/N_x\right] + a\sum_{n=0}^{(N_x/2)-1}\rho\left(\frac{2n+1}{N_x}\right)\exp\left[2\pi i h(2n+1)/N_x\right] \\
&= a\sum_{n=0}^{(N_x/2)-1}\rho\left(\frac{2n}{N_x}\right)\exp\left[2\pi i h(2n)/N_x\right] + a\exp(+2\pi i h)\sum_{n=0}^{(N_x/2)-1}\rho\left(\frac{2n+1}{N_x}\right)\exp\left[2\pi i h(2n)/N_x\right],
\end{aligned}$$

and $\exp\left[2\pi i h(2n)/N_x\right]$ needs be evaluated only $N_x/2$ times but can be used N_x times.

Basic principle of the FFT (cont'd)

- Subdivision of a sum of N terms into separate even-index and odd-index sums of $N/2$ terms can be repeated recursively.

- Each of the sums of $N/2$ terms can be subdivided into sums of $N/4$ terms over even-index and odd-index terms, and the process of subdivision can be continued until finally only two-term sums remain to be summed.

- The net effect of economies in evaluations of $\mathrm{e}^{i\theta}$ by subdivision in FFT algorithms is a reduction of the size of a calculation for N data points from order N^2 to order $N \log_2 N$. As shown in the table below, this represents for large N an enormous reduction.

- Depending on the factorability of N, subdivisions into other than two sums of $N/2$ terms indexed by $2n$ and $2n+1$, such as three sums of $N/3$ terms indexed by $3n$, $3n+1$, and $3n+2$, are also possible.

- After the advent of high-speed digital electronic computing, the invention of the Cooley-Tukey FFT algorithm (Cooley and Tukey, 1965) made large-scale Fourier transform calculations important and commonplace in many, many areas of science and engineering.

- The *N*-factorization/divide-and-conquer principle for series evaluation had in fact been discovered by Gauss (1777-1855), but its practical exploitation had to await the appearance of fast computers.

Basic principle of the FFT (cont'd)

The net effect of the computational economies in FFT algorithms is a reduction of the size of the calculation from order N^2 to order $N \log_2 N$.

N	N	N^2	$N \log_2 N$
1	2^0	1	1
2	2^1	4	2
4	2^2	16	8
8	2^3	64	24
$\vdots$			
1,024	2^{10}	$104{,}856 \approx 10^5$	$10{,}240 \approx 10^4$
2,048	2^{11}		
4,096	2^{12}		
8,192	2^{13}		
16,383	2^{14}		
32,768	2^{15}	$1{,}073{,}741{,}824 \approx 10^9$	$491{,}520 \approx 0.5\times10^6$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

The unit cell scattering density distribution $\rho(\mathbf{r}) = \rho(x,y,z)$ and the crystal structure factors $F_{\mathbf{h}} = F_{hkl}$ as atomic summations

$$\rho(\mathbf{r}) = \sum_{a=1}^{N} \rho_a(\mathbf{r} - \mathbf{r}_a) = \sum_{a=1}^{N} \rho_a(\mathbf{r}) * \delta(\mathbf{r} - \mathbf{r}_a)$$

$$\begin{aligned} F_{\mathbf{h}} &= \mathcal{F}^{-1}\left[\rho(\mathbf{r})\right] \\ &= \mathcal{F}^{-1}\left[\sum_{a=1}^{N} \rho_a(\mathbf{r} - \mathbf{r}_a)\right] \\ &= \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r} - \mathbf{r}_a)\right] \\ &= \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r}) * \delta(\mathbf{r} - \mathbf{r}_a)\right] \end{aligned}$$

$$F_{\mathbf{h}} = \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r})\right] \mathcal{F}^{-1}\left[\delta(\mathbf{r} - \mathbf{r}_a)\right]$$

$$\mathcal{F}^{-1}\left[\rho_a(\mathbf{r})\right] = f_a(\mathbf{h})$$

$$\mathcal{F}^{-1}\left[\delta(\mathbf{r} - \mathbf{r}_a)\right] = \exp\left(2\pi i \mathbf{h} \bullet \mathbf{r}_a\right)$$

$$F_{\mathbf{h}} = \sum_{a=1}^{N} f_a(\mathbf{h}) \exp\left(2\pi i \mathbf{h} \bullet \mathbf{r}_a\right)$$

The Kronecker Delta

$$\delta_{ij} = \begin{cases} 0\,, & i \neq j \\ 1\,, & i = j \end{cases}$$

The Dirac Delta Function

$$\delta(x - x_0) = 0\,, \quad \forall x \neq x_0$$

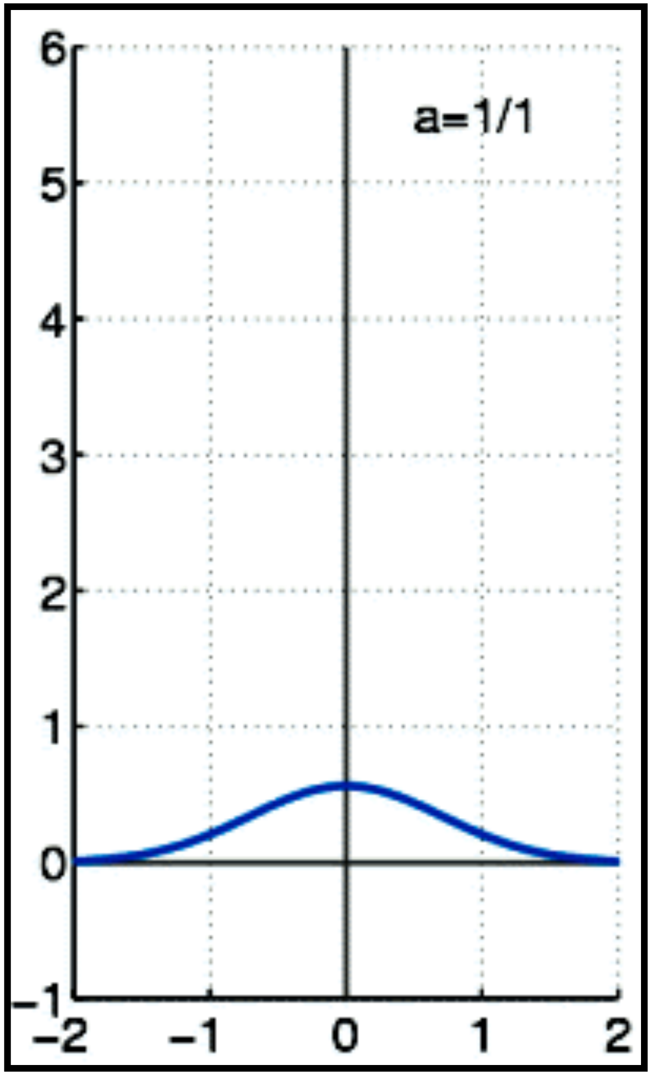
$$\int_{-\infty}^{+\infty} \delta(x - x_0)\,\mathrm{d}x = 1$$

$$\int_{-\infty}^{+\infty} f(x)\,\delta(x - x_0)\,\mathrm{d}x = f(x_0)$$

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} \delta(x - x_0)\,\mathrm{d}x = 1\,, \qquad \varepsilon > 0$$

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} f(x)\,\delta(x - x_0)\,\mathrm{d}x = f(x_0)\,, \quad \varepsilon > 0$$

a = σ



$$\delta(x) = \lim_{\sigma\to 0}\left\{\frac{1}{\sigma\sqrt{2\pi}}\exp\left[-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2\right]\right\}$$

The Dirac Delta Function and its Fourier Transform

$$\delta\left(x-x_0\right)=0\,,\qquad \forall\ x\neq x_0$$

$$\int_{-\infty}^{+\infty}\delta\left(x-x_0\right)\mathrm{d}x=\int_{x_0-\varepsilon}^{x_0+\varepsilon}\delta\left(x-x_0\right)\mathrm{d}x=1\,,\qquad \varepsilon>0$$

$$\int_{-\infty}^{+\infty}f\left(x\right)\delta\left(x-x_0\right)\mathrm{d}x=\int_{x_0-\varepsilon}^{x_0+\varepsilon}f\left(x\right)\delta\left(x-x_0\right)\mathrm{d}x=f\left(x_0\right),\qquad \varepsilon>0$$

$$\mathcal{F}\left[f\left(x\right)\right]=\int_{-\infty}^{+\infty}f\left(x\right)\exp\left(-2\pi ihx\right)\mathrm{d}x=F\left(h\right)$$

$$\begin{aligned}\mathcal{F}\left[\delta\left(x-x_0\right)\right]&=\int_{-\infty}^{+\infty}\delta\left(x-x_0\right)\exp\left(-2\pi ihx\right)\mathrm{d}x\\&=\exp\left(-2\pi ihx_0\right)\\&=\cos\left(2\pi hx_0\right)-i\sin\left(2\pi hx_0\right)\end{aligned}$$

The Fourier transform of an array of delta functions in direct space is an array of delta functions in reciprocal space.

$$F(h) \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x) \qquad \begin{cases} \rho(x) = \ \mathcal{F}\left[F(h)\right] = \int_{-\infty}^{+\infty} F(h)\exp(-2\pi i h x)\,\mathrm{d}h \\ F(h) = \mathcal{F}^{-1}\left[\rho(x)\right] = \int_{-\infty}^{+\infty} \rho(x)\exp(+2\pi i h x)\,\mathrm{d}x \end{cases}$$

Origin shift ⇒ Phase shift

$$\begin{aligned} \mathcal{F}^{-1}\left[\rho(x-x_0)\right] &= \mathcal{F}^{-1}\left[\rho(x) * \delta(x-x_0)\right] \\ &= \mathcal{F}^{-1}\left[\rho(x)\right]\mathcal{F}^{-1}\left[\delta(x-x_0)\right] = F(h)\exp(2\pi i h x_0) \end{aligned}$$

“Dirac comb”
a linear array of
delta functions

$$\rho(x) = \sum_{\substack{-\infty \\ n}}^{+\infty} \delta(x-na) \quad \Rightarrow \quad \mathcal{F}^{-1}\left[\rho(x)\right] = \mathcal{F}^{-1}\left[\sum_{\substack{-\infty \\ n}}^{+\infty} \delta(x-na)\right] = \sum_{\substack{-\infty \\ n}}^{+\infty} \delta\left(h - \frac{n}{a}\right) = F(h)$$

$$\begin{cases} \mathbf{R} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c} & \text{Bravais crystal lattice vector,} \quad n_1, n_2, n_3 \in \mathbb{Z} \\ \mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* & \text{Reciprocal lattice vector,} \quad h, k, l \in \mathbb{Z} \end{cases}$$

$$\begin{aligned} \mathbf{H}\bullet\mathbf{R} = {} & hn_1\,\mathbf{a}^*\bullet\mathbf{a} + hn_2\,\mathbf{a}^*\bullet\mathbf{b} + hn_3\,\mathbf{a}^*\bullet\mathbf{c} \\ & + kn_1\,\mathbf{b}^*\bullet\mathbf{a} + kn_2\,\mathbf{b}^*\bullet\mathbf{b} + kn_3\,\mathbf{b}^*\bullet\mathbf{c} \\ & + ln_1\,\mathbf{c}^*\bullet\mathbf{a} + ln_2\,\mathbf{c}^*\bullet\mathbf{b} + ln_3\,\mathbf{c}^*\bullet\mathbf{c} \end{aligned}$$

Choose $\mathbf{a}^* \perp \mathbf{b},\mathbf{c} \quad \wedge \quad \mathbf{b}^* \perp \mathbf{c},\mathbf{a} \quad \wedge \quad \mathbf{c}^* \perp \mathbf{a},\mathbf{b}$

$$\mathbf{a}^* = \frac{\mathbf{b}\times\mathbf{c}}{V}, \quad \mathbf{b}^* = \frac{\mathbf{c}\times\mathbf{a}}{V}, \quad \mathbf{c}^* = \frac{\mathbf{a}\times\mathbf{b}}{V}, \qquad V = \mathbf{a}\bullet(\mathbf{b}\times\mathbf{c}) \quad \circlearrowright$$

Then $\mathbf{H}\bullet\mathbf{R} = hn_1 + kn_2 + ln_3 \quad \Rightarrow \quad (\mathbf{H}\bullet\mathbf{R}) \in \mathbb{Z} \quad \Rightarrow \quad \exp(2\pi i\,\mathbf{H}\bullet\mathbf{R}) = 1$

Direct space

Position Vector $\mathbf{r} = x\,\mathbf{a} + y\,\mathbf{b} + z\,\mathbf{c}$

Space Lattice $\mathcal{L}_{\mathbf{r}} = \sum_{n1}^{-\infty}{}^{+\infty} \sum_{n2}^{-\infty}{}^{+\infty} \sum_{n3}^{-\infty}{}^{+\infty} \delta^3\left(\mathbf{r} - n_1\mathbf{a} - n_2\mathbf{b} - n_3\mathbf{c}\right)$

$$= \sum_{\substack{-\infty \\ n1}}^{+\infty} \delta\left(x - n_1 a\right) \sum_{\substack{-\infty \\ n2}}^{+\infty} \delta\left(y - n_2 b\right) \sum_{\substack{-\infty \\ n3}}^{+\infty} \delta\left(z - n_3 c\right)$$

Reciprocal space

Position Vector $\mathbf{h} = h\,\mathbf{a}^* + k\,\mathbf{b}^* + l\,\mathbf{c}^*$

Space Lattice $\mathcal{L}_{\mathbf{h}} = \mathcal{F}\left[\mathcal{L}_{\mathbf{r}}\right]$

$$= \sum_{\substack{-\infty \\ m1}}^{+\infty} \sum_{\substack{-\infty \\ m2}}^{+\infty} \sum_{\substack{-\infty \\ m3}}^{+\infty} \delta^3\left(\mathbf{h} - m_1\mathbf{a}^* - m_2\mathbf{b}^* - m_3\mathbf{c}^*\right)$$

$$= \sum_{\substack{-\infty \\ m1}}^{+\infty} \delta\left(h - \frac{m_1}{a}\right) \sum_{\substack{-\infty \\ m2}}^{+\infty} \delta\left(k - \frac{m_2}{b}\right) \sum_{\substack{-\infty \\ m3}}^{+\infty} \delta\left(l - \frac{m_3}{c}\right)$$

D. Thompson (1996). The reciprocal lattice as the Fourier transform of the direct lattice. *Am. J. Phys.* **64**(3), 333-334.

Friedel's Law

Le loi de Friedel

Three-dimensional crystallographic diffraction patterns are centrosymmetric.

$$\boxed{\left(I_{\bar{h}\bar{k}\bar{l}} = I_{hkl}\right) \Rightarrow \left(\left|F_{\bar{h}\bar{k}\bar{l}}\right|^2 = \left|F_{hkl}\right|^2\right) \Rightarrow \left(\left|F_{\bar{h}\bar{k}\bar{l}}\right| = \left|F_{hkl}\right| \wedge \varphi_{\bar{h}\bar{k}\bar{l}} = -\varphi_{hkl}\right)}$$

Given that

$$\begin{cases} F_{+\mathbf{h}} = \int_V \rho(\mathbf{r})\exp(+2\pi i\mathbf{h}\bullet\mathbf{r})\mathrm{d}^3\mathbf{r} = \sum_{a=1}^{N} f_a(+\mathbf{h})\exp(+2\pi i\mathbf{h}\bullet\mathbf{r}_a) \\ F_{-\mathbf{h}} = \int_V \rho(\mathbf{r})\exp(-2\pi i\mathbf{h}\bullet\mathbf{r})\mathrm{d}^3\mathbf{r} = \sum_{a=1}^{N} f_a(-\mathbf{h})\exp(-2\pi i\mathbf{h}\bullet\mathbf{r}_a) = F_{+\mathbf{h}}^* \end{cases},$$

and that spherical atoms are centrosymmetric so that,

$$\rho_a\left[-(\mathbf{r}-\mathbf{r}_a)\right] = \rho_a\left[+(\mathbf{r}-\mathbf{r}_a)\right] \Rightarrow f_a(-\mathbf{h}) = f_a(+\mathbf{h}) = f_a(|\mathbf{h}|) = f_a(h),$$

it follows that

$$F_{-\mathbf{h}} = F_{+\mathbf{h}}^*$$

$$|F_{-\mathbf{h}}|\mathrm{e}^{i\varphi_{-\mathbf{h}}} = |F_{+\mathbf{h}}|\mathrm{e}^{-i\varphi_{+\mathbf{h}}}$$

and

$$\boxed{\begin{cases} |F_{-\mathbf{h}}| = |F_{+\mathbf{h}}| \\ \varphi_{-\mathbf{h}} = -\varphi_{+\mathbf{h}} \end{cases}}$$

Georges Friedel (1913). Sur les symmétries cristallines que peut révéler la diffraction des rayons X. *C.R. Acad. Sci. Paris*, **157**, 1533-1536.

Friedel's Law

Le loi de Friedel

$$\left(I_{\bar{h}\bar{k}\bar{l}} = I_{hkl} \right) \Rightarrow \left(\left|F_{\bar{h}\bar{k}\bar{l}}\right|^2 = \left|F_{hkl}\right|^2 \right) \Rightarrow \begin{cases} \left|F_{\bar{h}\bar{k}\bar{l}}\right| = \left|F_{hkl}\right| \\ \varphi_{\bar{h}\bar{k}\bar{l}} = -\varphi_{hkl} \end{cases}$$

Friedel's law holds if the atomic scattering factors are real-valued, even functions, which is the case if:

- The radiation frequency radiation greatly exceeds the natural resonant atomic absorption frequencies of the crystal, so that resonant or "anomalous" scattering is negligible;
- The atomic electron density distributions are spherical, or at least centrosymmetric about the atom-centers; and
- The atomic Debye-Waller factors are real-valued, as is the case for atomic displacement distributions that are centrosymmetric about the mean atomic positions, in particular, for atomic displacement distributions that are Gaussian, as they are for harmonic thermal vibrations.

Georges Friedel (1913). Sur les symétries cristallines que peut reveler la diffraction des rayons X. *C.R. Acad. Sci. Paris*, **157**, 1533-1536.

Phase restrictions for centrosymmetric structures or structure projections

- If the unit-cell scattering density distribution is centrosymmetric about the unit-cell origin, then

$$\rho(-\mathbf{r}) = \rho(+\mathbf{r}) \;,$$

and

$$F_{\mathbf{h}} = \int_V \rho(\mathbf{r}) \exp(2\pi i \mathbf{h}\bullet\mathbf{r}) \,\mathrm{d}^3\mathbf{r}$$

$$= \int_V \rho(-\mathbf{r}) \exp\left[2\pi i \mathbf{h}\bullet(-\mathbf{r})\right] \mathrm{d}^3\mathbf{r} = \int_V \rho(\mathbf{r}) \exp\left[2\pi i (-\mathbf{h})\bullet\mathbf{r}\right] \mathrm{d}^3\mathbf{r} = F_{-\mathbf{h}} \;.$$

- Equivalently, if the atomic electron density distributions are centrosymmetric about the atomic nuclei so that

$$\rho_a(-\mathbf{r}) = \rho_a(+\mathbf{r}) \quad \text{and} \quad f_a(-\mathbf{h}) = f_a(+\mathbf{h}) \;,$$

then, since centrosymmetrically related pairs of atoms have positions $+\mathbf{r}_a$ and $-\mathbf{r}_a$,

$$F_{\mathbf{h}} = \sum_{a=1}^{N} f_a(\mathbf{h}) \exp(2\pi i \mathbf{h}\bullet\mathbf{r}_a) = \sum_{a=1}^{N} f_a(\mathbf{h}) \exp(-2\pi i \mathbf{h}\bullet\mathbf{r}_a) = F_{-\mathbf{h}} \;.$$

- It therefore follows that

$$\left(F_{-\mathbf{h}} = F_{\mathbf{h}}\right) \;\Rightarrow\; \left(\mathrm{e}^{i\varphi_{-\mathbf{h}}} = \mathrm{e}^{i\varphi_{\mathbf{h}}}\right) \;\Rightarrow\; \left(\varphi_{-\mathbf{h}} = \varphi_{\mathbf{h}}\right) \;,$$

while by Friedel’s law,

$$\varphi_{-\mathbf{h}} = -\varphi_{\mathbf{h}} \;.$$

Thus,

$$\left[\left(\varphi_{-\mathbf{h}} = \varphi_{\mathbf{h}}\right) \wedge \left(\varphi_{-\mathbf{h}} = -\varphi_{\mathbf{h}}\right)\right] \;\Rightarrow\; \left(\varphi_{\mathbf{h}} = -\varphi_{\mathbf{h}}\right) \;\Rightarrow\; \varphi_{\mathbf{h}} = 0 \;\text{ or }\; \pi \;,$$

and

$$\mathrm{e}^{i\varphi_{\mathbf{h}}} = \pm 1 \;, \qquad F_{\mathbf{h}} = \left|F_{\mathbf{h}}\right| \mathrm{e}^{i\varphi_{\mathbf{h}}} = s_{\mathbf{h}} \left|F_{\mathbf{h}}\right| \;, \qquad s_{\mathbf{h}} = \pm 1 \,.$$

Real-valued electron density from complex-valued structure factors

$$\rho(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{h}} F_{\mathbf{h}} \exp(-2\pi i\mathbf{h}\bullet\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{h}} |F_{\mathbf{h}}| \mathrm{e}^{i\varphi_{\mathbf{h}}} \exp(-2\pi i\mathbf{h}\bullet\mathbf{r})$$

$$= \frac{1}{V}\sum_{\mathbf{h}} |F_{\mathbf{h}}| \exp\left[i\left(\varphi_{\mathbf{h}} - 2\pi\mathbf{h}\bullet\mathbf{r}\right)\right]$$

$$= \frac{1}{V}\sum_{\mathbf{h}} |F_{\mathbf{h}}| \cos\left(\varphi_{\mathbf{h}} - 2\pi\mathbf{h}\bullet\mathbf{r}\right) + i\,|F_{\mathbf{h}}| \sin\left(\varphi_{\mathbf{h}} - 2\pi\mathbf{h}\bullet\mathbf{r}\right).$$

If Friedel’s law holds,

$$|F_{-\mathbf{h}}| = |F_{+\mathbf{h}}| \qquad \text{and} \qquad \varphi_{-\mathbf{h}} = -\varphi_{+\mathbf{h}} \; .$$

Therefore, the imaginary, sine terms in +**h** and **–h** sum pairwise to zero, and

$$\rho(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{h}} |F_{\mathbf{h}}| \cos\left(\varphi_{\mathbf{h}} - 2\pi\mathbf{h}\bullet\mathbf{r}\right) ,$$

which is real-valued.