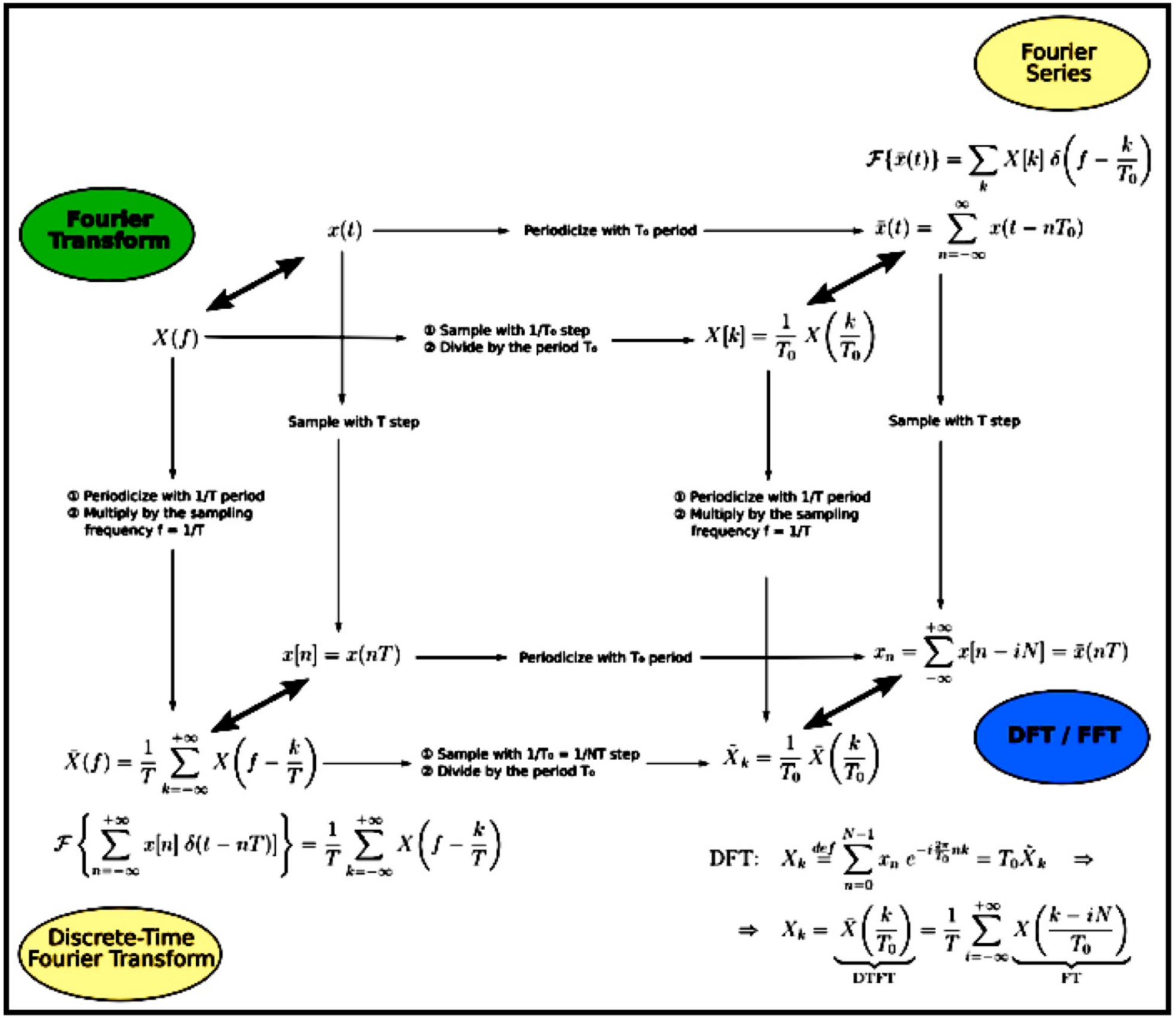
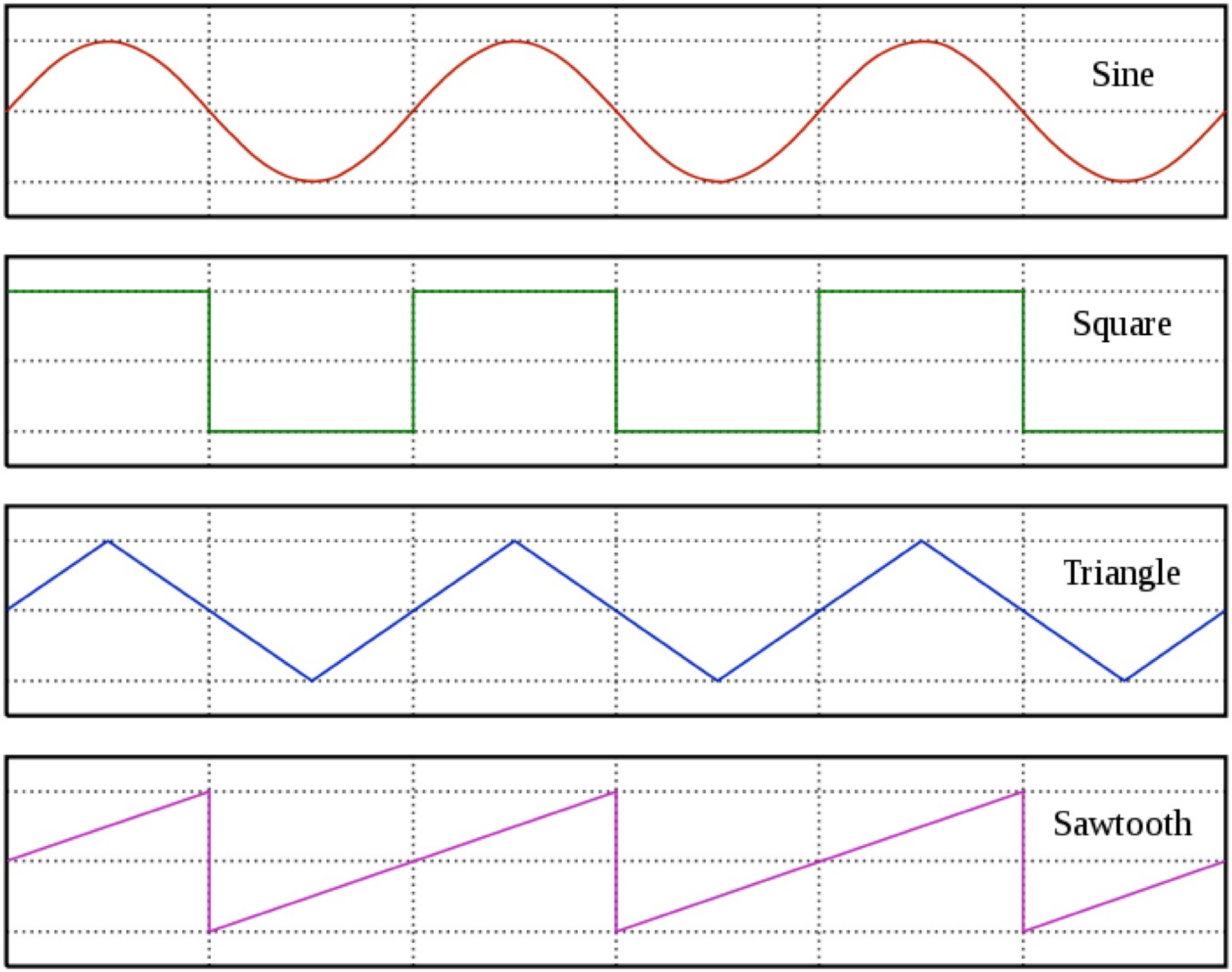


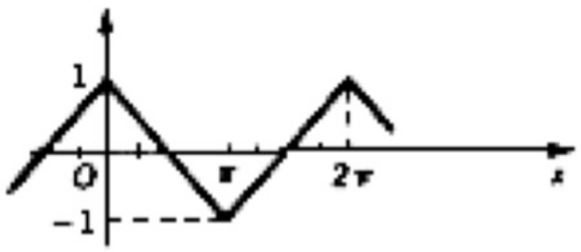
http://en.wikipedia.org/wiki/Relations_between_Fourier_transforms_and_Fourier_series

Simple Waveforms



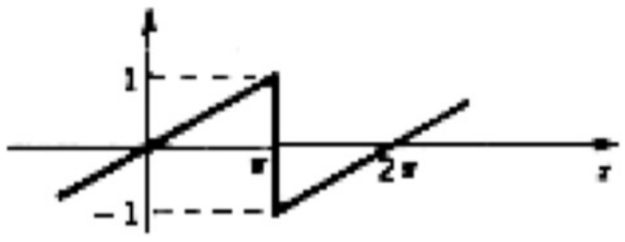
http://upload.wikimedia.org/wikipedia/commons/thumb/7/77/Waveforms.svg/760px-Waveforms.svg.png
http://en.wikipedia.org/wiki/Waveform

Some simple waveforms and their Fourier series



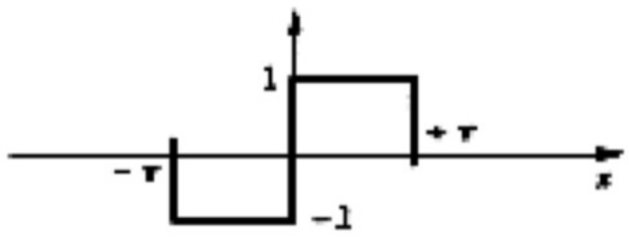
Triangular wave:

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



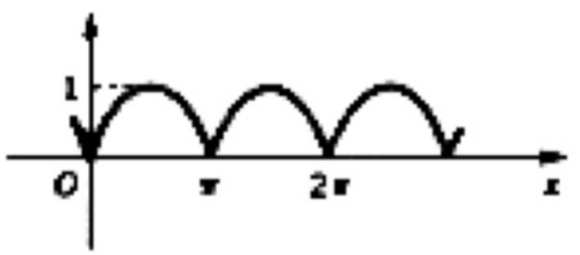
Rectangular sawtooth wave:

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



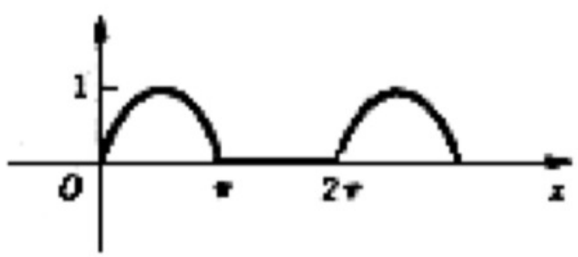
Square wave:

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



Absolute value sine wave:

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

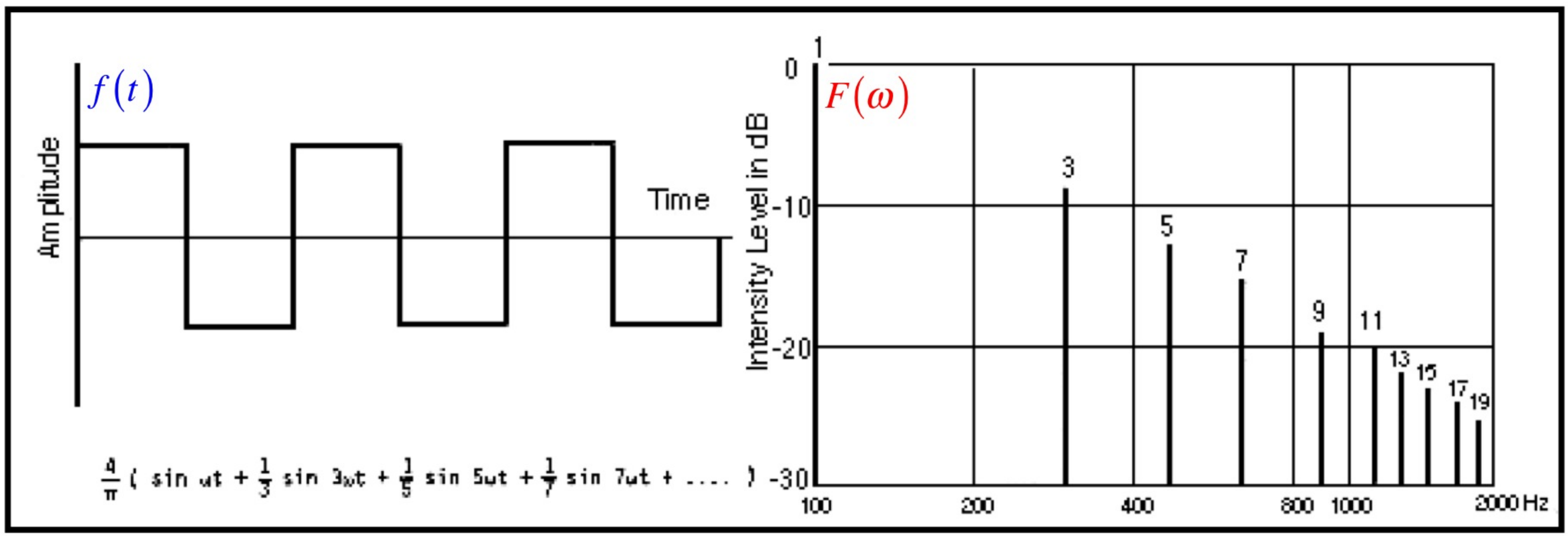


Half sine wave:

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

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

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



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

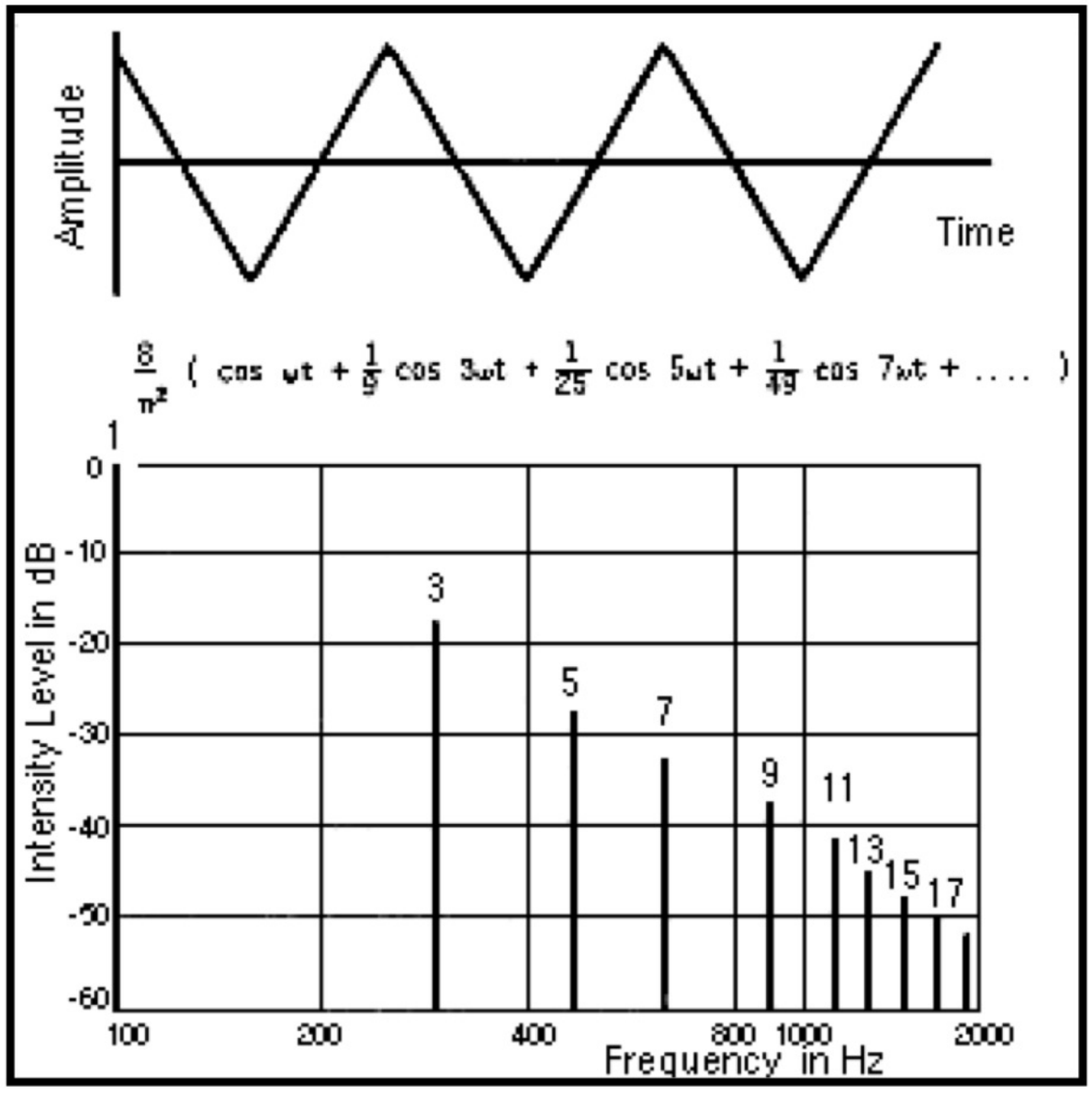
$$f(t \pm 2n\pi) = f(t)$$

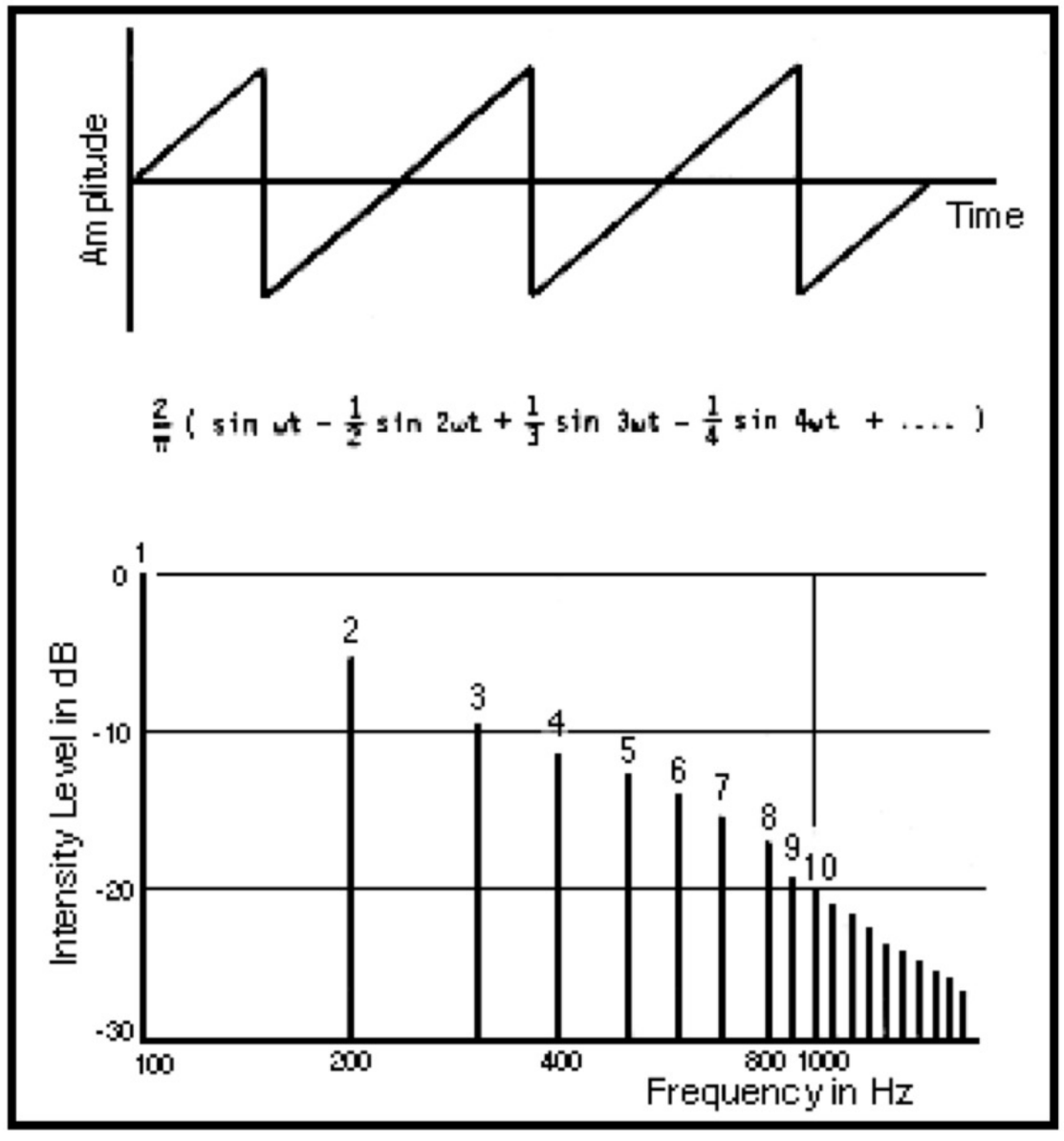
$$f(t) = \frac{4}{\pi}\left[\sin(\omega t) + \frac{1}{3}\sin(3\omega t) + \frac{1}{5}\sin(5\omega t) + \cdots\right]$$

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

Time and frequency domains

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





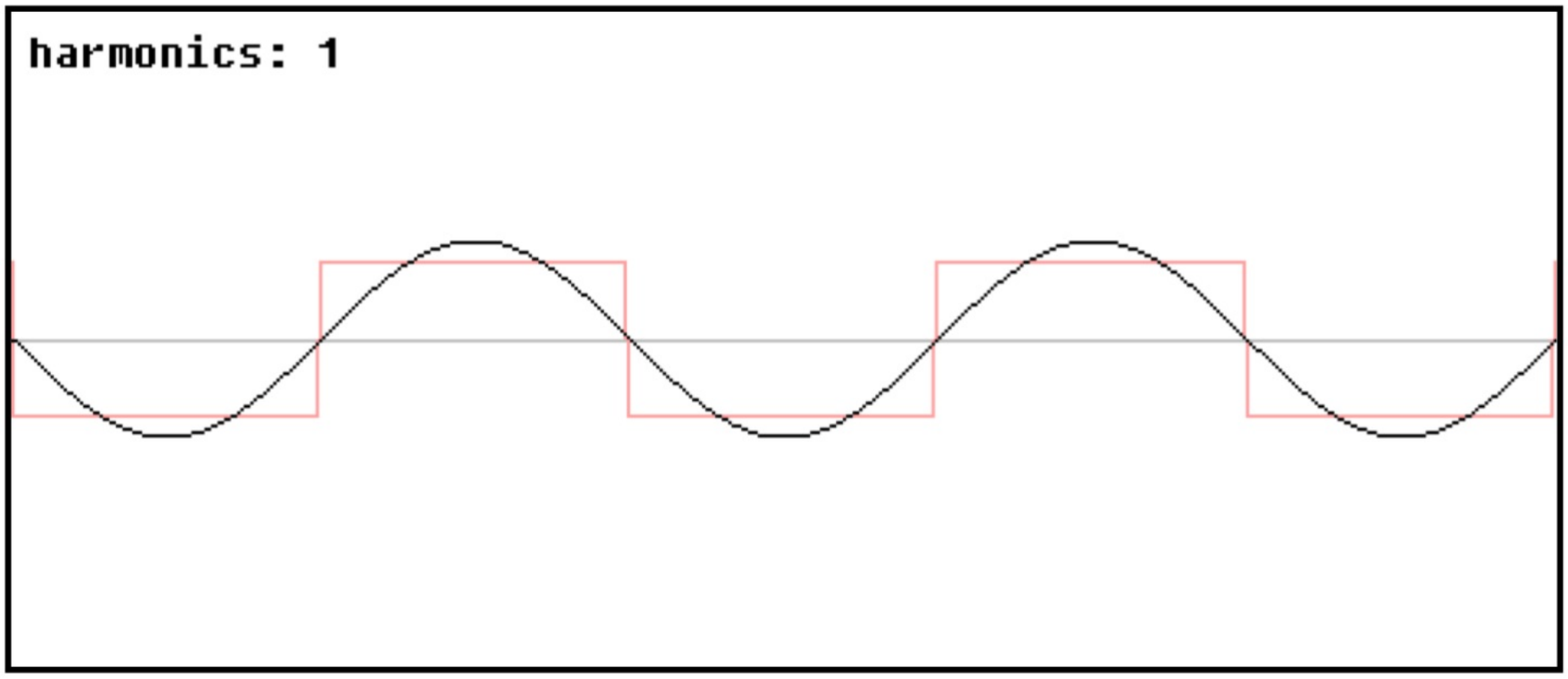
$$f(t) = \frac{8}{\pi^2}\left(\cos\omega t + \frac{1}{9}\cos 3\omega t + \frac{1}{25}\cos 5\omega t + \cdots\right)$$

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

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

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

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

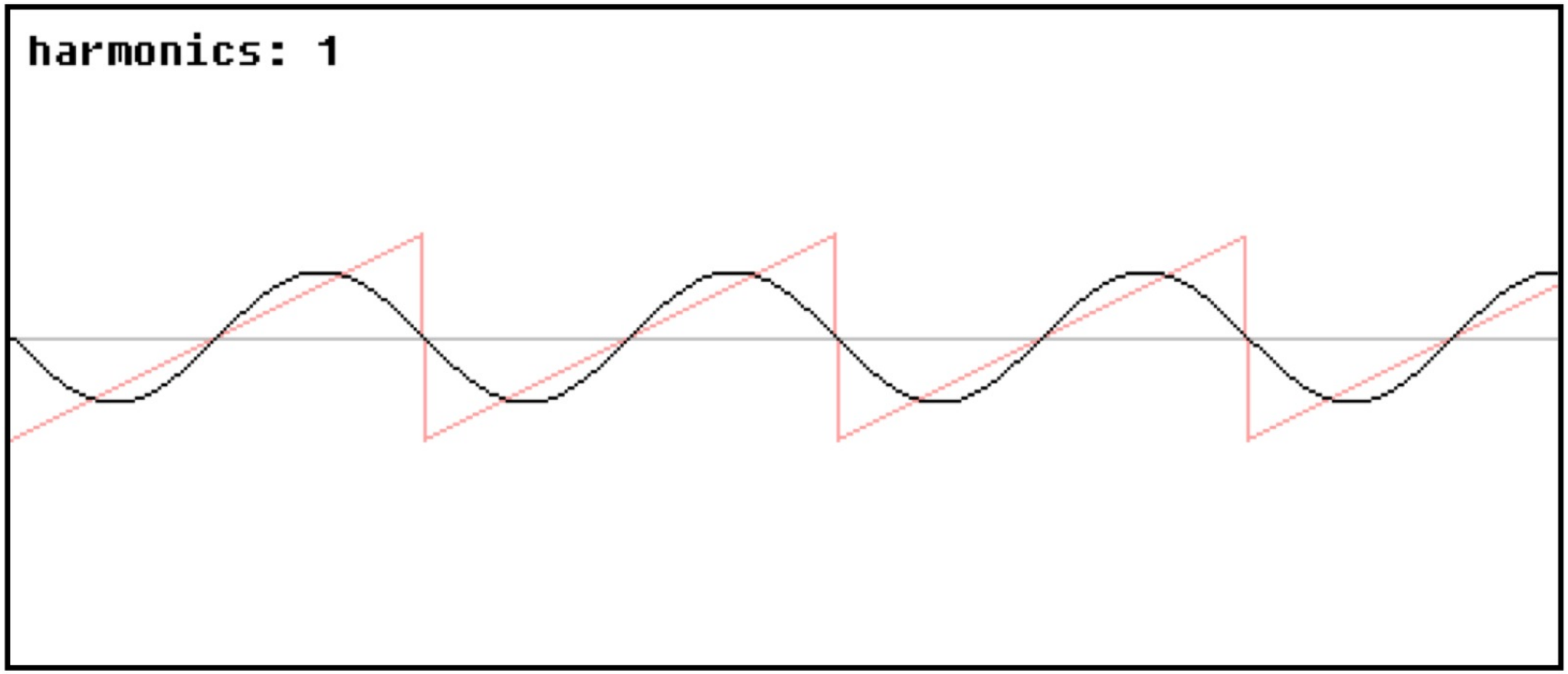


Fourier series representation $f(t) = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\sin[2\pi(2n-1)\omega t]}{2n-1}$

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

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

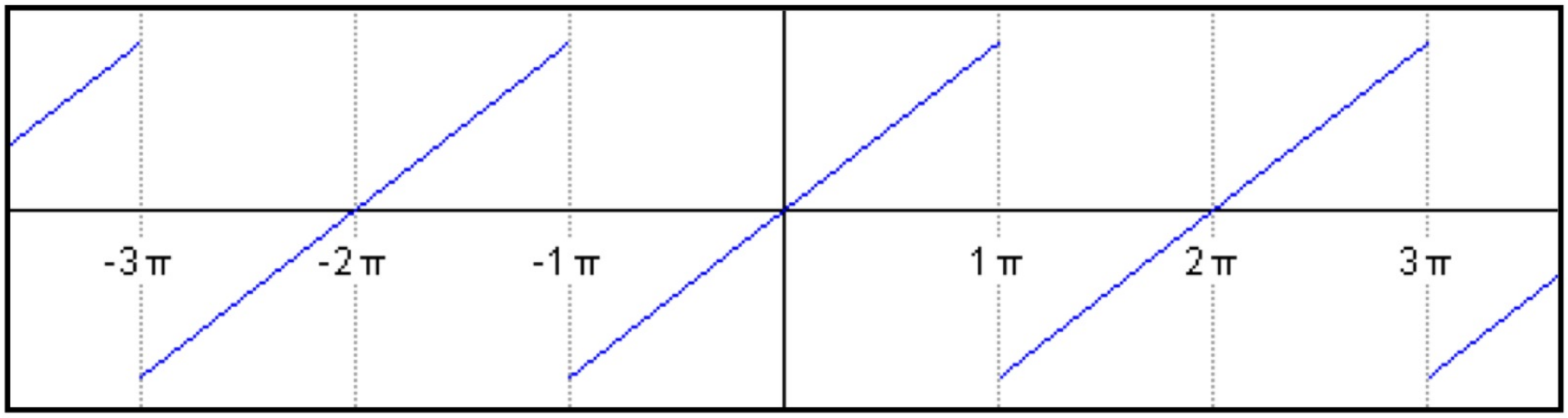
Sawtooth-wave function $\begin{cases} f(t) = t/2\,, & -\pi < t < +\pi \\ f(t \pm 2n\pi) = f(t) \end{cases}$

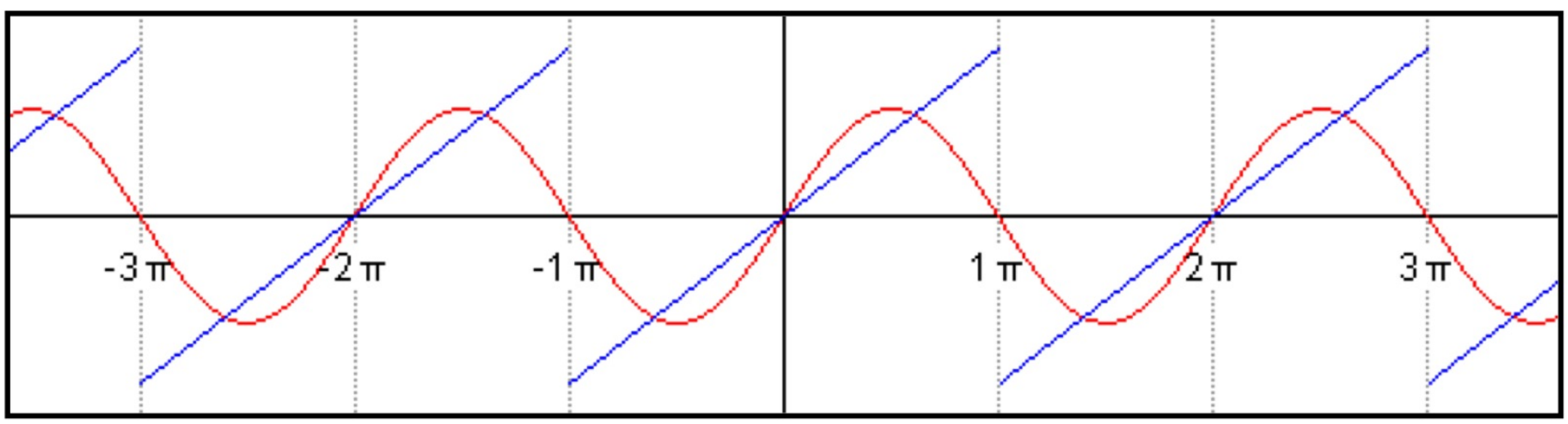


Fourier series representation $f(t) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{\sin(nt)}{n}$

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

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

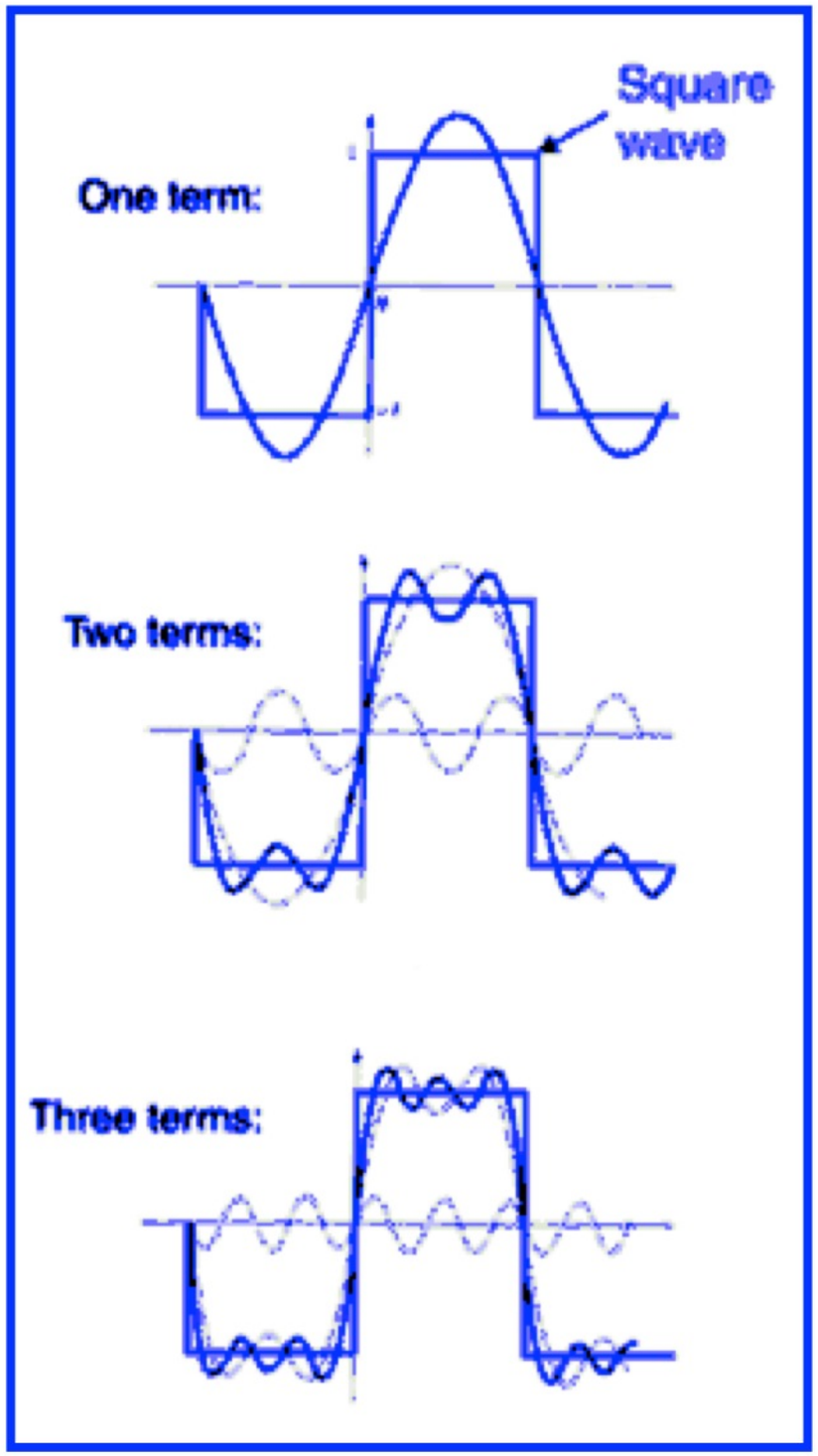




Fourier series representation $f(x) = 2\sum_{n=1}^{\infty} (-1)^{n+1} \frac{\sin(nx)}{n}$

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

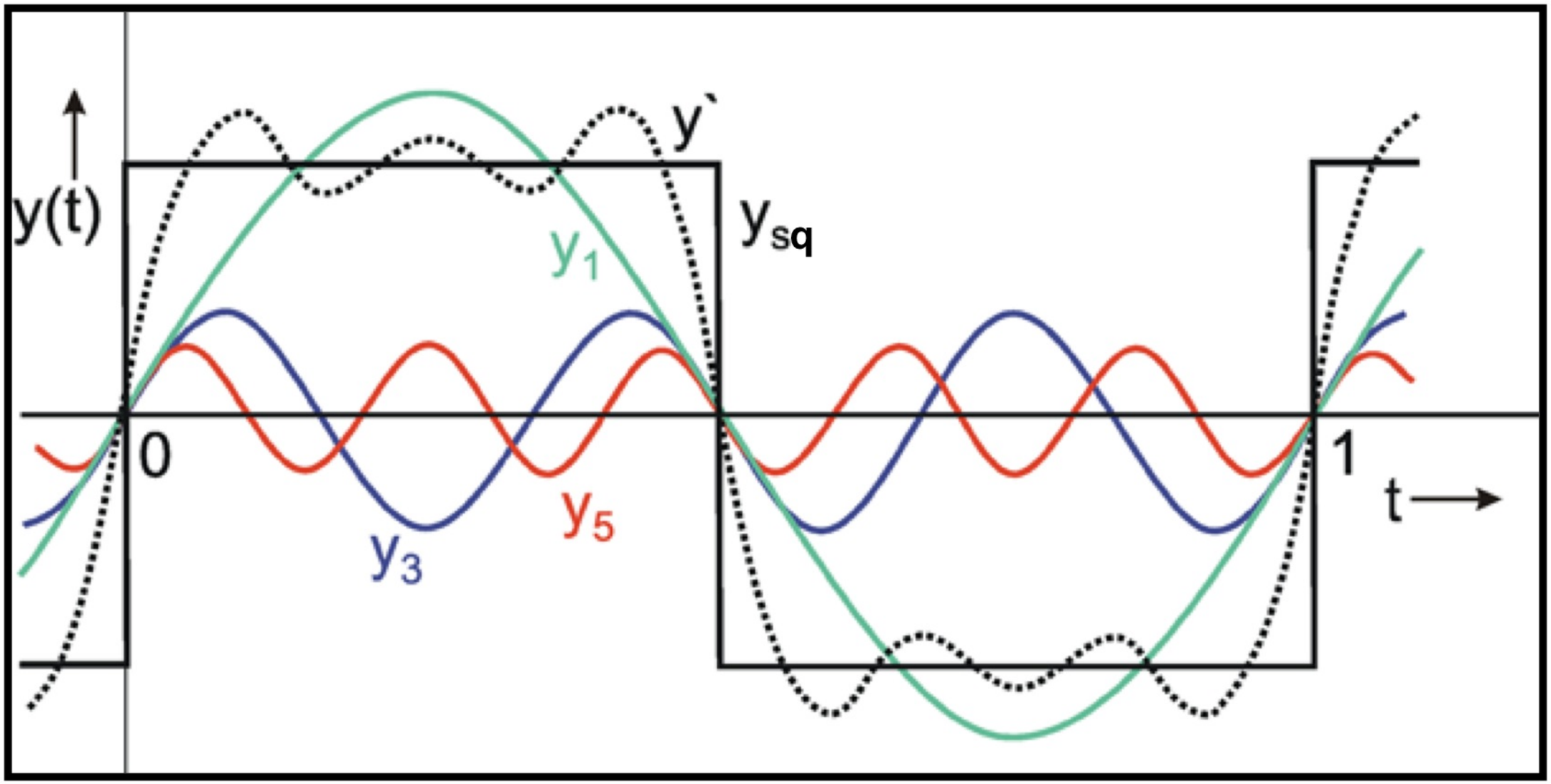


$$y_1 = \sin x$$

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

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

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

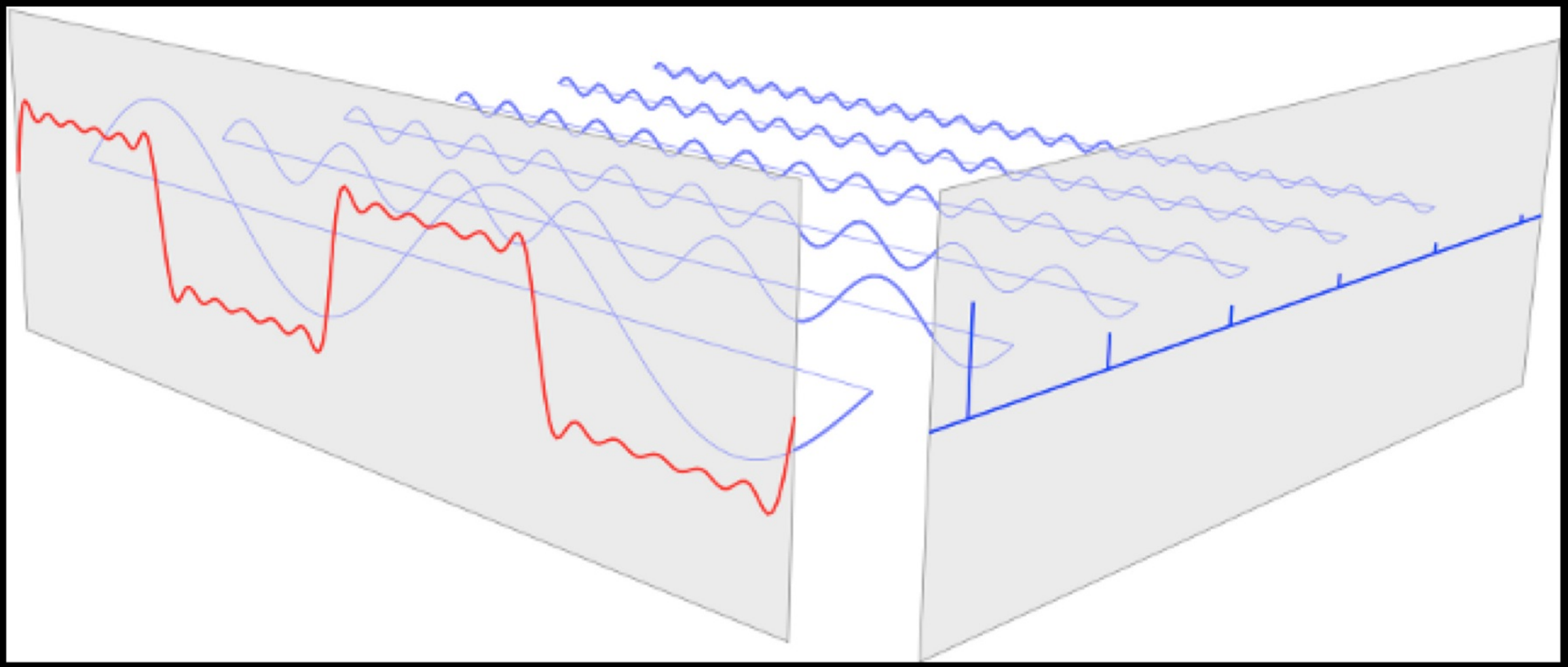


$$y_{\text{sq}} \approx y' = y_1 + y_3 + y_5 = \sin\left(2\pi t\right) + \frac{1}{3}\sin\left[3\left(2\pi t\right)\right] + \frac{1}{5}\sin\left[5\left(2\pi t\right)\right]$$

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

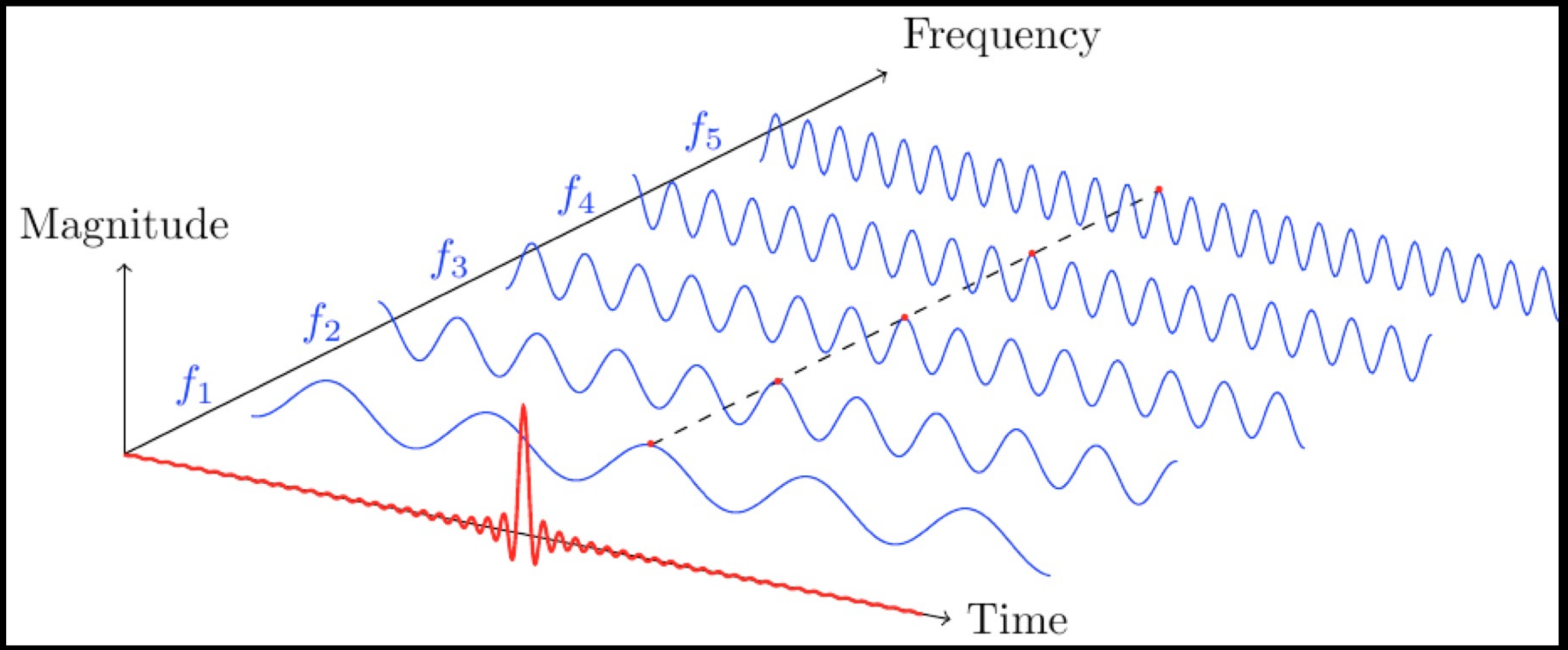
$$\mathrm{FT}\left[f(t) \right] = \hat{f}(\omega)$$

http://tex.stackexchange.com/questions/127375/replicate-the-fourier-transform-time-frequency-domains-correspondence-illustrati
http://i.stack.imgur.com/27HVo.gif



http://i.stack.imgur.com/BC9yQ.png

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



http://i.stack.imgur.com/BC9yQ.png

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,

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

where the $\left|F_{hkl}\right|$ 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

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

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

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

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

The “fundamental theorem” of structural crystallography

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

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

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

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

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

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

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

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

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

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

$$
\begin{aligned}
F_{\mathbf{h}} &= \sum_{a=1}^{N} f_a(\mathbf{h}) \exp\left(2\pi i \mathbf{h}\bullet\mathbf{r}_a\right) \\
&= \sum_{a=1}^{N} f_a(\mathbf{h}) \left[\cos\left(2\pi\mathbf{h}\bullet\mathbf{r}_a\right) + i\sin\left(2\pi\mathbf{h}\bullet\mathbf{r}_a\right)\right] \\
&= A_{\mathbf{h}} + iB_{\mathbf{h}}
\end{aligned}
$$

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

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

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

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

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

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

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

$$\begin{cases} \rho(\mathbf{r}) = \dfrac{1}{V_{\text{cell}}} \sum\limits_{\mathbf{h}=-\infty}^{+\infty} F_{\mathbf{h}} \exp(-2\pi i \mathbf{h}\bullet\mathbf{r}) \\ F_{\mathbf{h}} = \int_{V_{\text{cell}}} \rho(\mathbf{r}) \exp(+2\pi i \mathbf{h}\bullet\mathbf{r}) \, \mathrm{d}^3\mathbf{r} \end{cases}$$

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

Continuous and discrete Fourier synthesis

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

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

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

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

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

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

Fourier transformations by numerical grid summations

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

Fourier Synthesis

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

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

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

Fourier Analysis

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

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

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

Fourier Analysis

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

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

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

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

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

Shannon sampling

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

n points in **h**-space $\Leftrightarrow$ 2*n* 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

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

Basic principle of the FFT

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

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

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 $e^{i\theta}$ 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
⋮			
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}	$1{,}073{,}741{,}824 \approx 10^9$	$491{,}520 \approx 0.5\times10^6$
⋮	⋮	⋮	⋮

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

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

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

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

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

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

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

The Kronecker Delta

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

The Dirac Delta Function

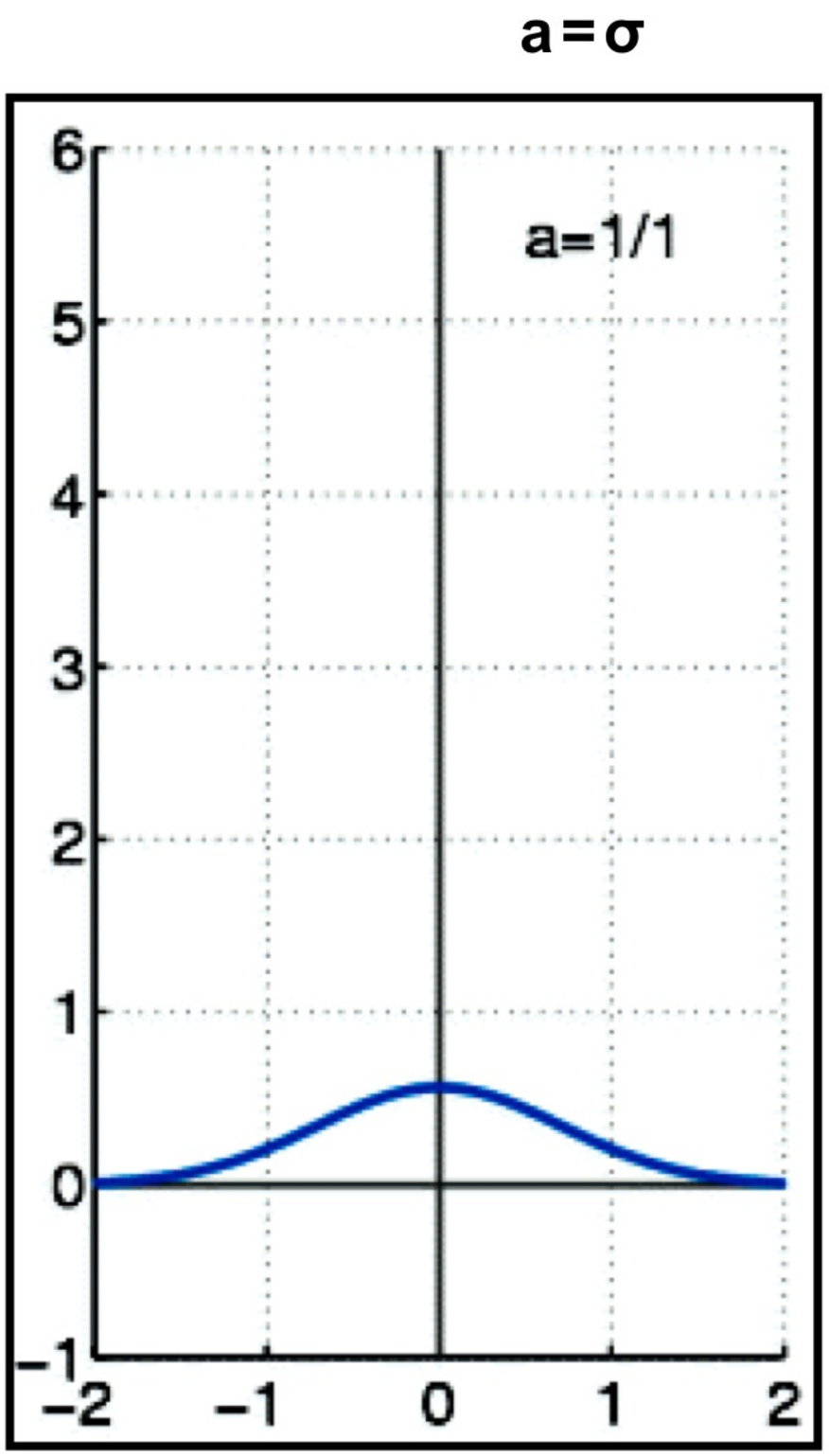
$$\delta\left(x - x_0\right) = 0\,, \quad \forall x \neq x_0$$

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

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

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

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



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

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 $\Rightarrow$ Phase shift

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

"Dirac comb" a linear array of delta functions

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

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

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

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

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

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

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

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

Reciprocal space

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

Space Lattice

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

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

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

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.

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

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

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

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

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

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

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

while by Friedel's law,

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

Thus,

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

and

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

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.