

Crystallographic Fourier Analysis

Crystallographic Diffraction

Laue diffraction by a three-dimensional abc lattice grating

$$\boxed{a(\cos \nu_1 - \cos \mu_1) = \mathbf{a} \cdot (\hat{\mathbf{s}} - \hat{\mathbf{s}}_0) = h\lambda \\ b(\cos \nu_2 - \cos \mu_2) = \mathbf{b} \cdot (\hat{\mathbf{s}} - \hat{\mathbf{s}}_0) = k\lambda \\ c(\cos \nu_3 - \cos \mu_3) = \mathbf{c} \cdot (\hat{\mathbf{s}} - \hat{\mathbf{s}}_0) = l\lambda}$$

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

Bragg reflection from families of parallel hkl lattice planes

$$\boxed{2d_{hkl} \sin \theta = n\lambda, \quad 2\left(\frac{d_{hkl}}{n}\right) \sin \theta = \lambda, \quad 2d_{nhnknl} \sin \theta = \lambda}$$

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

Integrated Bragg reflections

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

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 Lecture¹ 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 intensity² 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 the intensity but rather the amplitude,

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).

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

$$\text{If } f(x) = f(x \pm 2n\pi),$$

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

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

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

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

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



Il ne reste plus que les coefficients 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

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

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

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

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

$$\int \cos \frac{2i+1}{2} \pi y \cdot \cos \frac{2i+1}{2} \pi y \cdot dy$$

prise depuis $y = +\infty$ jusqu'à $y = -\infty$, 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°. 6, Paris (Bernard), March 1808, pp. 112-116.

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

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

$$(2) \quad \varphi(y) = a \cos \frac{\pi y}{2} + a' \cos 3 \frac{\pi y}{2} + a'' \cos 5 \frac{\pi y}{2} + \dots$$

Multippliant 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

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

prise depuis $y = -1$ jusqu'à $y = +1$, est nulle, excepté dans le cas de $i = j$, 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 .

Fourier (1807) translated...

“... one has

$$\varphi(y) = a \cos\left(\frac{1}{2}\pi y\right) + a' \cos\left(\frac{3}{2}\pi y\right) + a'' \cos\left(\frac{5}{2}\pi y\right) + \dots$$

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

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

since it is easy to show that the integral

$$\int_{-1}^{+1} \cos\left(\frac{2i+1}{2}\pi y\right) \cos\left(\frac{2i'+1}{2}\pi y\right) dy$$

is equal to zero, except in the case $i' = i$ where it equals π .”

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.

The “fundamental theorem” of structural crystallography

The fundamental theorem of arithmetic

Every integer has a unique expression as a product of primes.

The fundamental theorem of algebra

Every univariate polynomial of degree n has exactly n zeros.

The fundamental theorem of the calculus

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

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

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,

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

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

The “fundamental theorem” of structural crystallography

$$F_{hkl} = |F_{hkl}| e^{i\varphi_{hkl}} \begin{array}{c} \xrightarrow{\mathcal{F}} \\ \xleftarrow{\mathcal{F}^{-1}} \end{array} \rho(x,y,z) \quad \left\{ \begin{array}{l} \rho(x,y,z) = \mathcal{F}[F_{hkl}] \quad \text{Fourier synthesis} \\ F_{hkl} = \mathcal{F}^{-1}[\rho(x,y,z)] \quad \text{Fourier analysis} \end{array} \right.$$

$$\left\{ \begin{array}{l} \rho(x,y,z) = \frac{1}{V_{\text{cell}}} \sum_{h=-\infty}^{+\infty} \sum_{k=-\infty}^{+\infty} \sum_{l=-\infty}^{+\infty} F_{hkl} \exp[-2\pi i(hx + ky + lz)] \\ F_{hkl} = V_{\text{cell}} \int_0^1 \int_0^1 \int_0^1 \rho(x,y,z) \exp[+2\pi i(hx + ky + lz)] dx dy dz \end{array} \right.$$

$$\left\{ \begin{array}{l} F_{hkl} = \sum_{a=1}^N f_a(S_{hkl}) \exp[2\pi i(hx_a + ky_a + lz_a)] = |F_{hkl}| e^{i\varphi_{hkl}} \\ \rho(x,y,z) = \frac{1}{V_{\text{cell}}} \sum_{h=-\infty}^{+\infty} \sum_{k=-\infty}^{+\infty} \sum_{l=-\infty}^{+\infty} |F_{hkl}| \cos[\varphi_{hkl} - 2\pi(hx + ky + lz)] \\ S_{hkl} = \frac{1}{d_{hkl}} = 2 \left(\frac{\sin \theta_{hkl}}{\lambda} \right) \quad \text{and} \quad \left\{ \begin{array}{l} |F_{\bar{h}\bar{k}\bar{l}}| = |F_{hkl}| \\ \varphi_{\bar{h}\bar{k}\bar{l}} = -\varphi_{hkl} \end{array} \right. \end{array} \right.$$

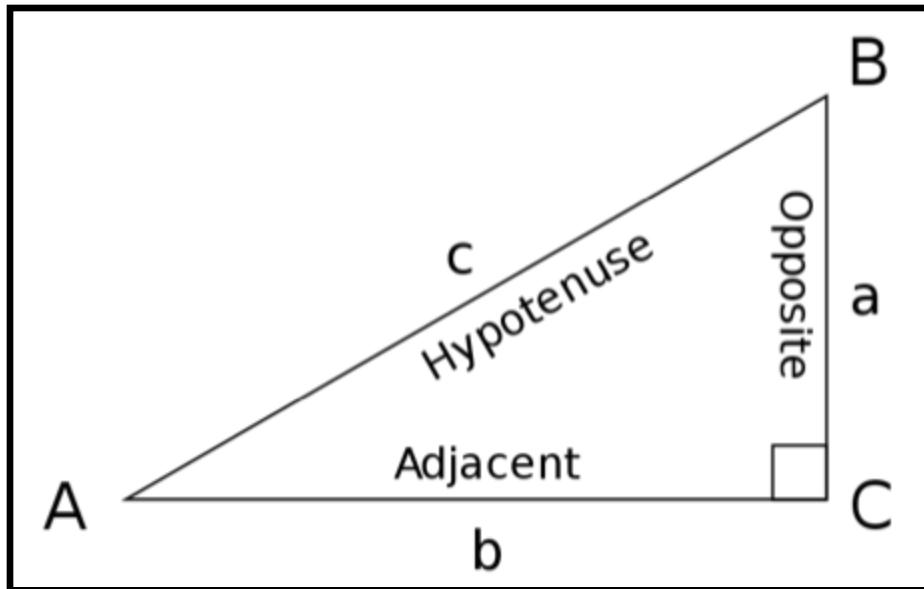
Sines and Cosines

**Sinusoids,
Sinusoidal Properties,
and
Sinusoid Superpositions**

The Euler Relationship

$$e^{ix} = \cos x + i \sin x$$

Trigonometric functions defined on a right triangle



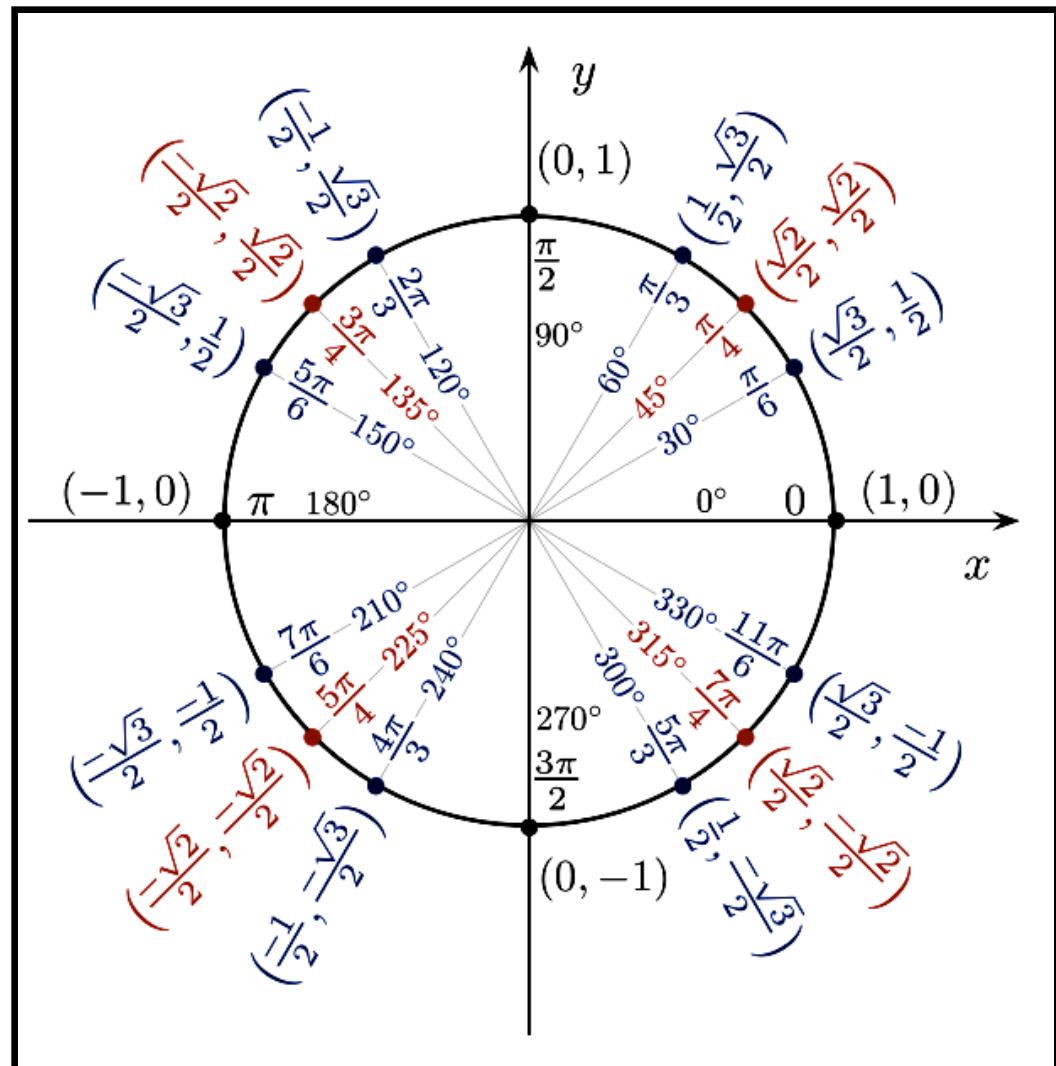
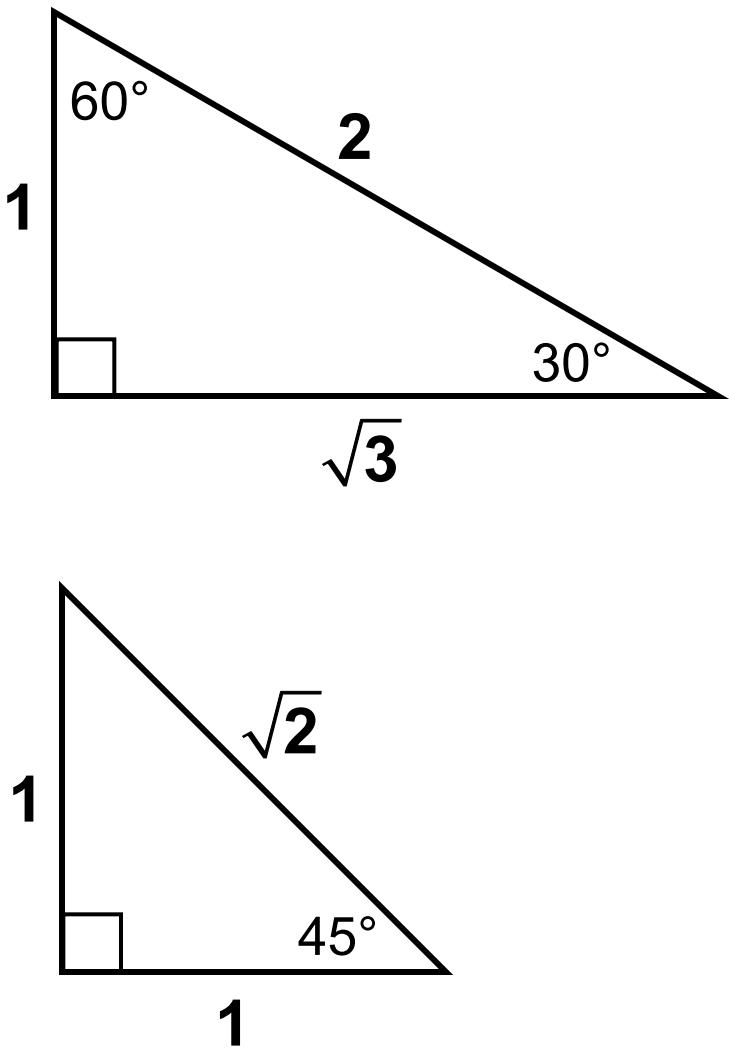
$$\sin A = \frac{\text{Opposite}}{\text{Hypotenuse}} = \frac{a}{c}$$

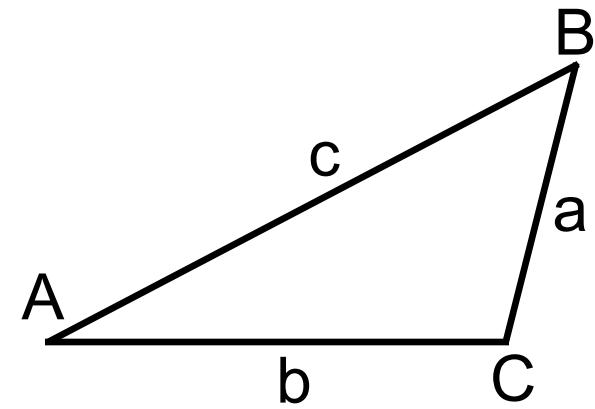
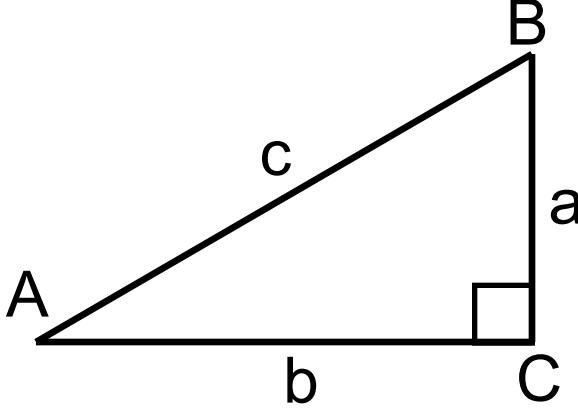
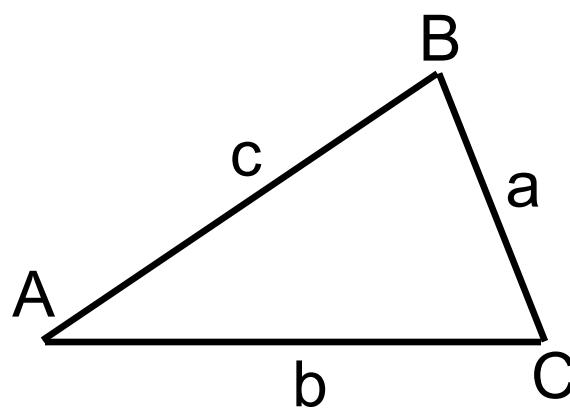
$$\cos A = \frac{\text{Adjacent}}{\text{Hypotenuse}} = \frac{b}{c}$$

$$\tan A = \frac{\text{Opposite}}{\text{Adjacent}} = \frac{a}{b} = \frac{\sin A}{\cos A}$$

"soh - cah - toa"

Special angles and their sines and cosines in 30° , 60° , 90° ($1, 2, \sqrt{3}$) and 45° ($1, 1, \sqrt{2}$) right triangles





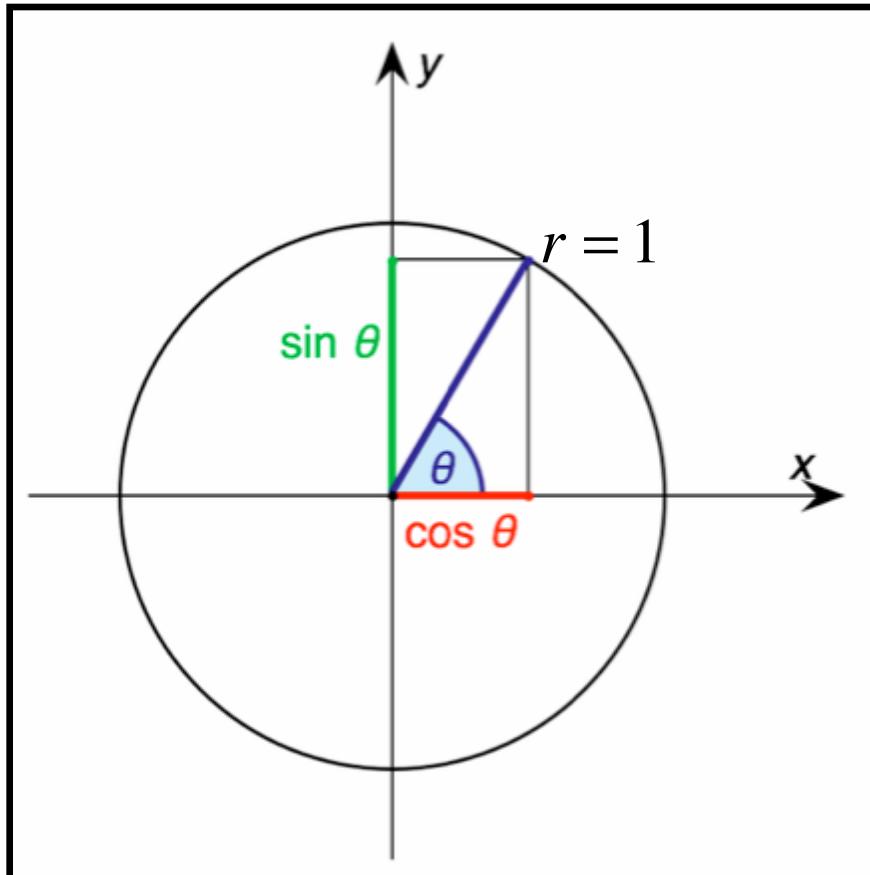
The law of cosines

$$c^2 = a^2 + b^2 - 2ab \cos \angle a, b$$

The law of sines

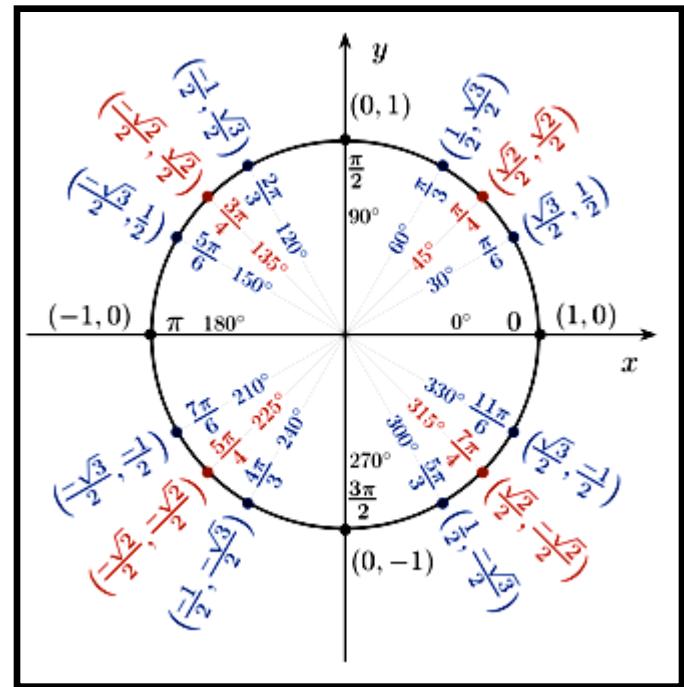
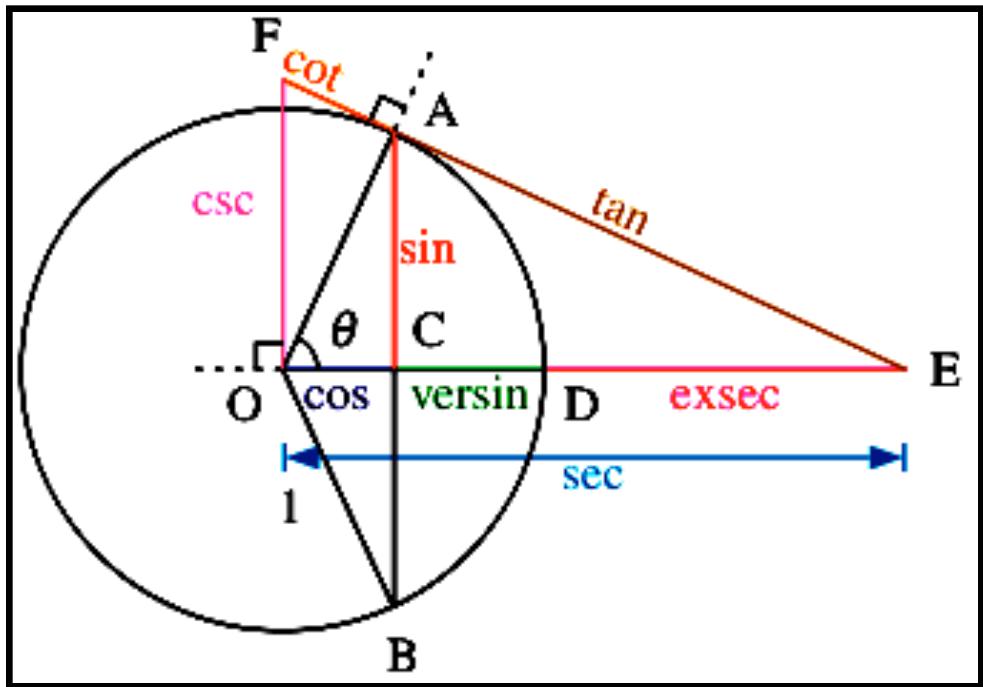
$$\frac{a}{\sin A} = \frac{b}{\sin B} = \frac{c}{\sin C}$$

Trigonometric functions defined on the unit circle



$$\sin \theta = \frac{y}{r}, \quad \cos \theta = \frac{x}{r}, \quad \tan \theta = \frac{y}{x} = \frac{\sin \theta}{\cos \theta}$$

The trigonometric functions on the unit circle



$$\sin \theta = \frac{y}{r},$$

$$\cos \theta = \frac{x}{r},$$

$$\tan \theta = \frac{y}{x} = \frac{\sin \theta}{\cos \theta}$$

The cosine and sine functions on the unit circle

$$\cos \theta = x/r$$

$$\sin \theta = y/r$$

$$r = 1$$

$$x = \cos \theta$$

$$y = \sin \theta$$

$$x^2 + y^2 = r^2$$

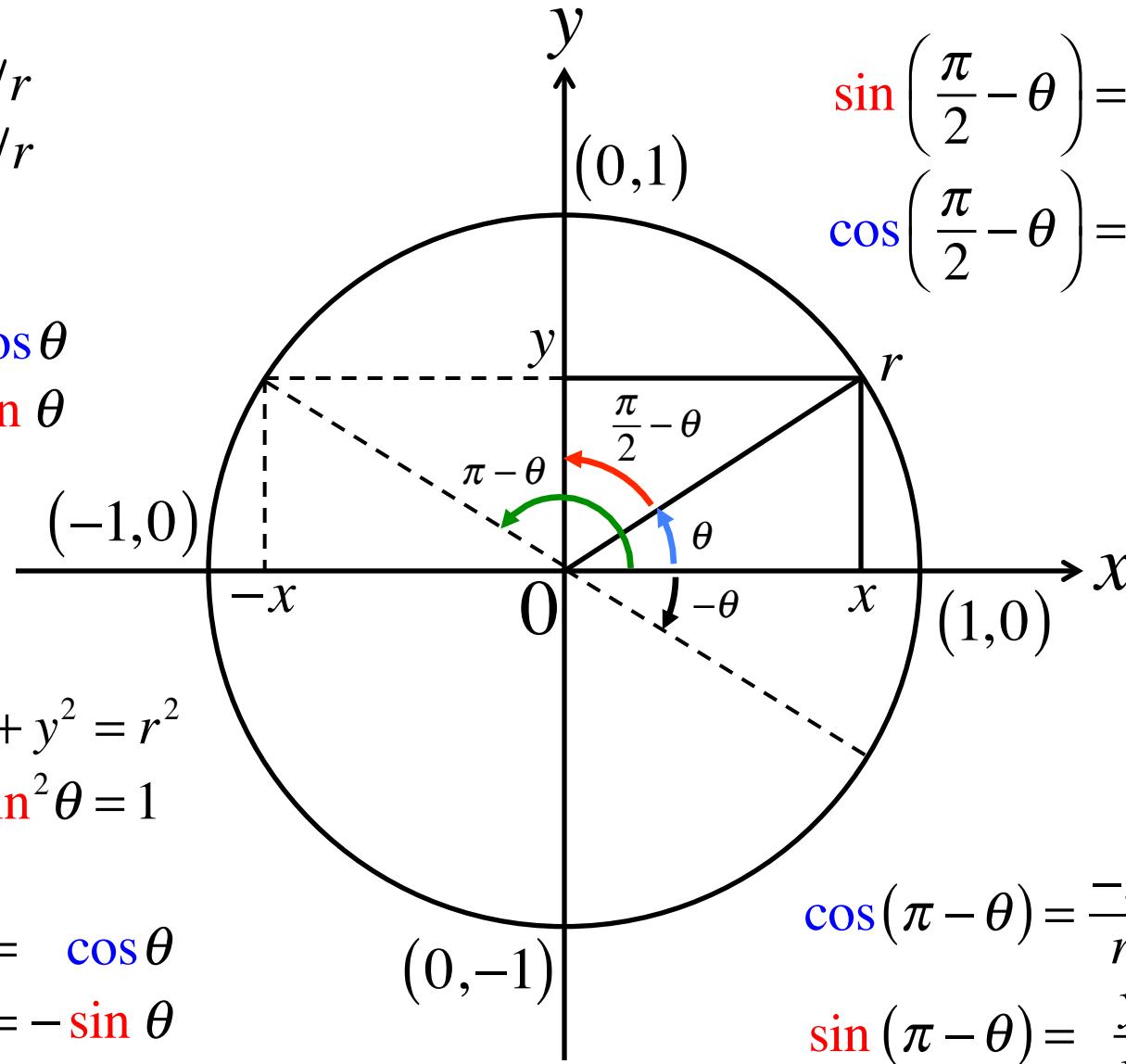
$$\cos^2 \theta + \sin^2 \theta = 1$$

$$\cos(-\theta) = \cos \theta$$

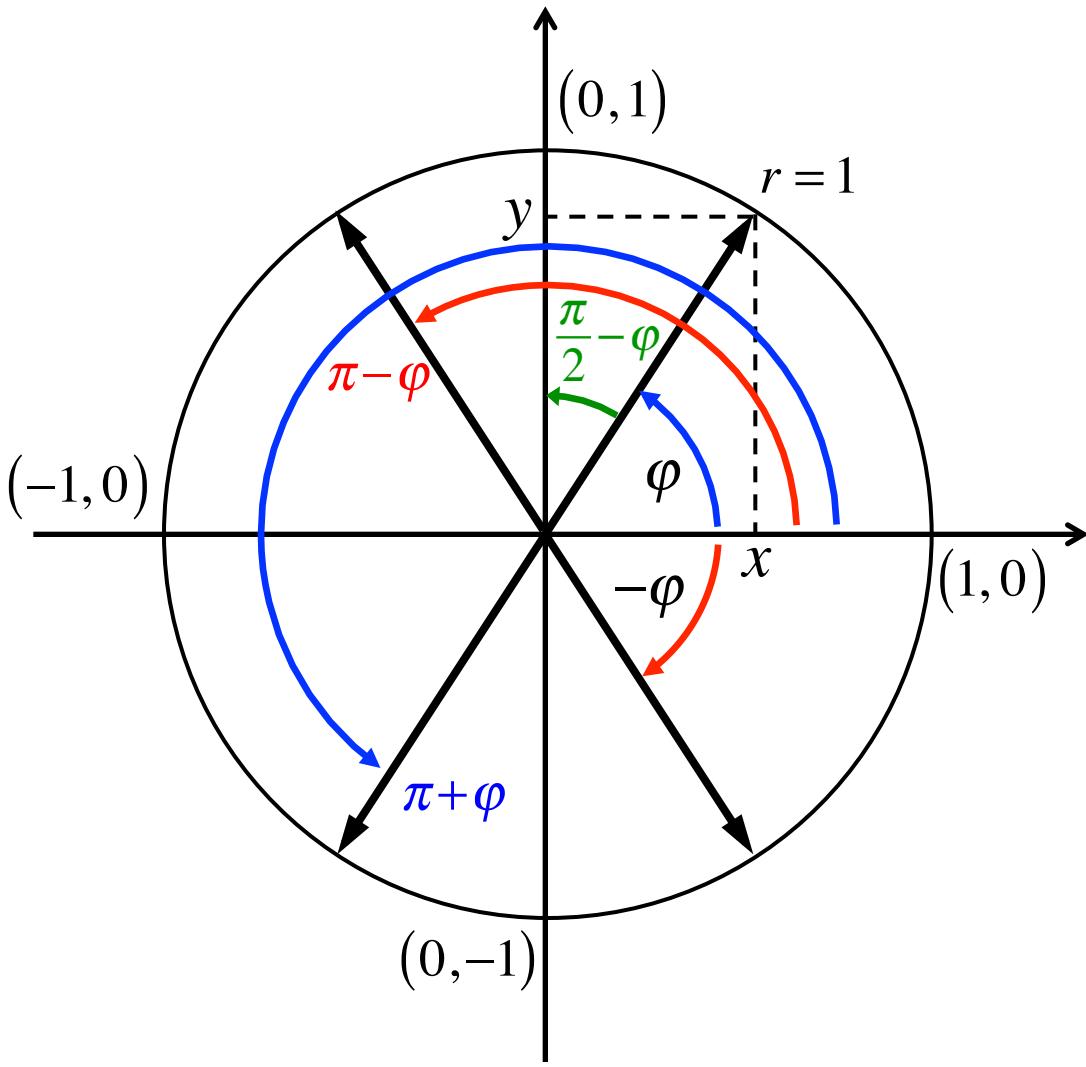
$$\sin(-\theta) = -\sin \theta$$

$$\sin\left(\frac{\pi}{2} - \theta\right) = \frac{x}{r} = \cos \theta$$

$$\cos\left(\frac{\pi}{2} - \theta\right) = \frac{y}{r} = \sin \theta$$



Sinusoidal identities on the unit circle



$$r = 1$$

$$\cos \varphi = x/r = x$$

$$\sin \varphi = y/r = y$$

$$\cos^2 \varphi + \sin^2 \varphi = 1$$

$$\cos(-\varphi) = \cos \varphi$$

$$\sin(-\varphi) = -\sin \varphi$$

$$\cos\left(\frac{\pi}{2} - \varphi\right) = \sin \varphi$$

$$\sin\left(\frac{\pi}{2} - \varphi\right) = \cos \varphi$$

$$\cos(\pi - \varphi) = -\cos \varphi$$

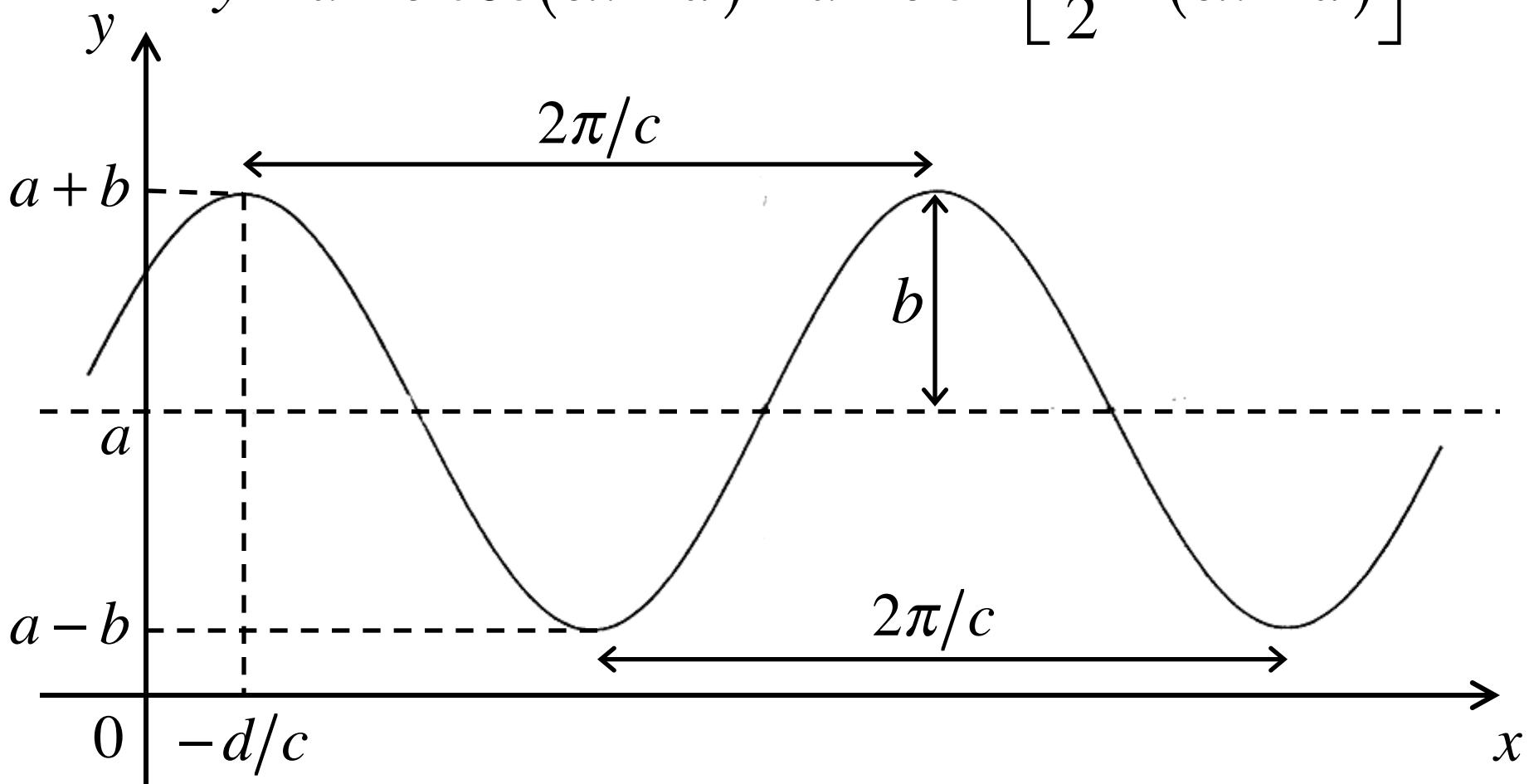
$$\cos(\pi + \varphi) = -\cos \varphi$$

$$\sin(\pi - \varphi) = \sin \varphi$$

$$\sin(\pi + \varphi) = -\sin \varphi$$

Sinusoid function

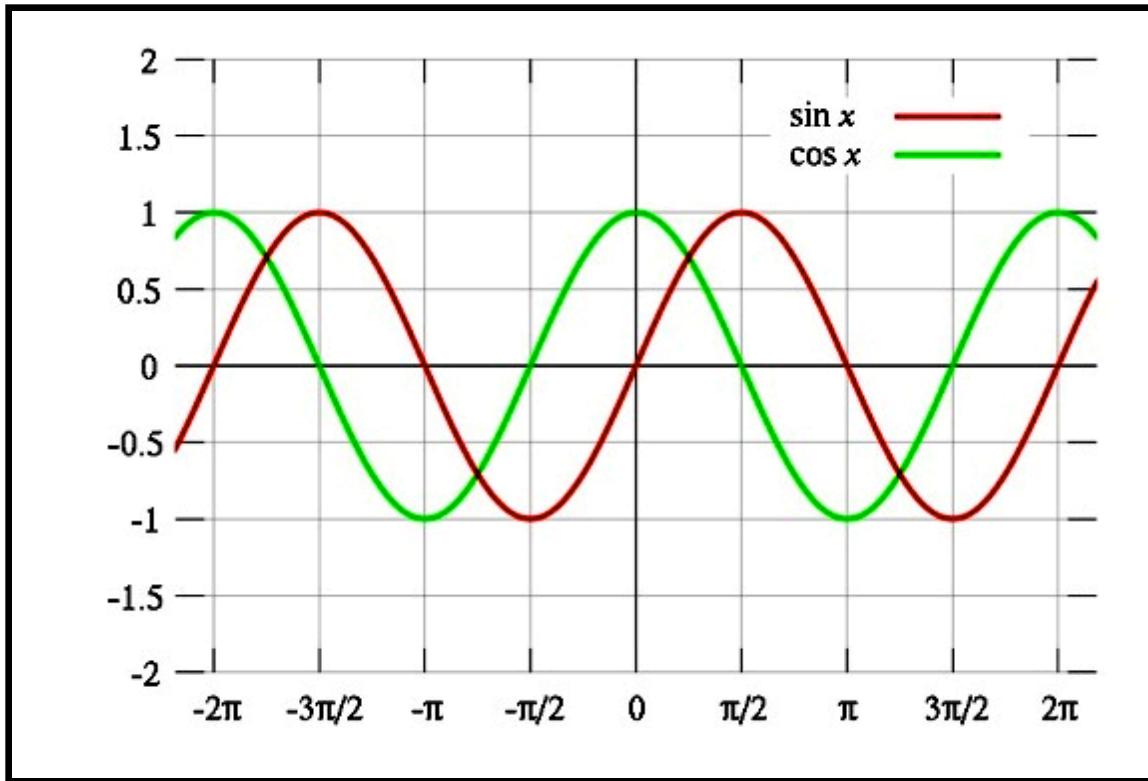
$$y = a + b \cos(cx + d) = a + b \sin\left[\frac{\pi}{2} - (cx + d)\right]$$



$$\begin{aligned} c(x + \lambda) + d &= cx + d + 2\pi \\ \lambda &= 2\pi/c \end{aligned}$$

baseline	a	wavelength	$2\pi/c$
amplitude	b	frequency	c
phase	d	phase shift	$-d/c$
frequency	c	phase shift	$-d/c$

The cosine and sine functions



The cosine is an even function, and the sine an odd function.

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

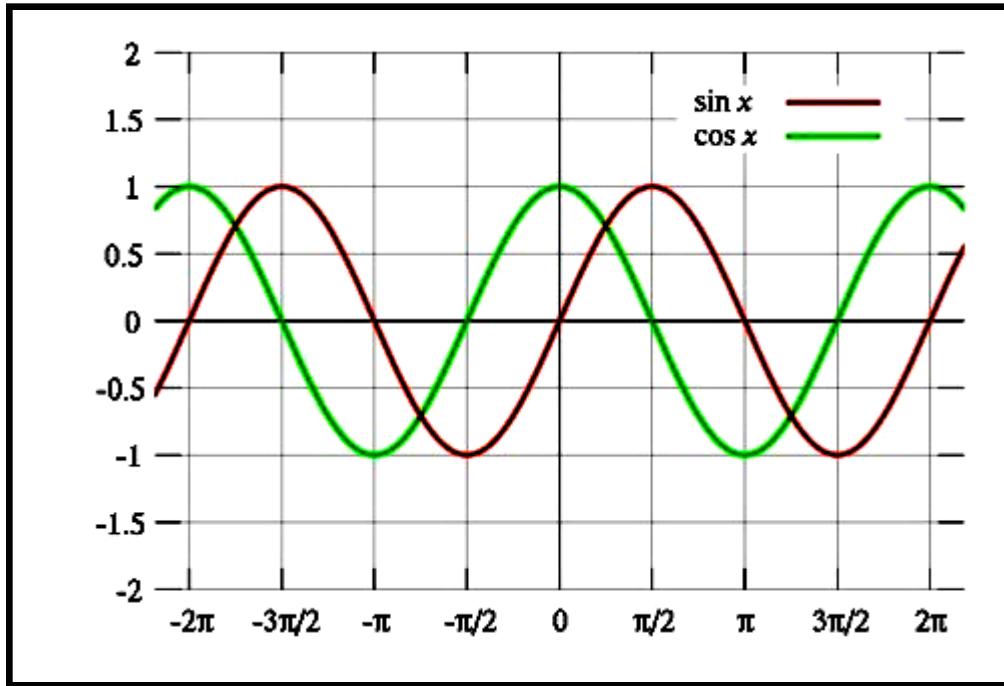
$$\sin(-x) = -\sin x$$

The cosine function is a phase-shifted sine function, and vice versa.

$$\cos x \equiv \sin\left(\frac{\pi}{2} - x\right)$$

$$\sin x \equiv \cos\left(\frac{\pi}{2} - x\right)$$

The sine and cosine functions and their derivatives and integrals



$$\frac{d}{dx} \sin x = \cos x$$

$$\frac{d}{dx} \cos x = -\sin x$$

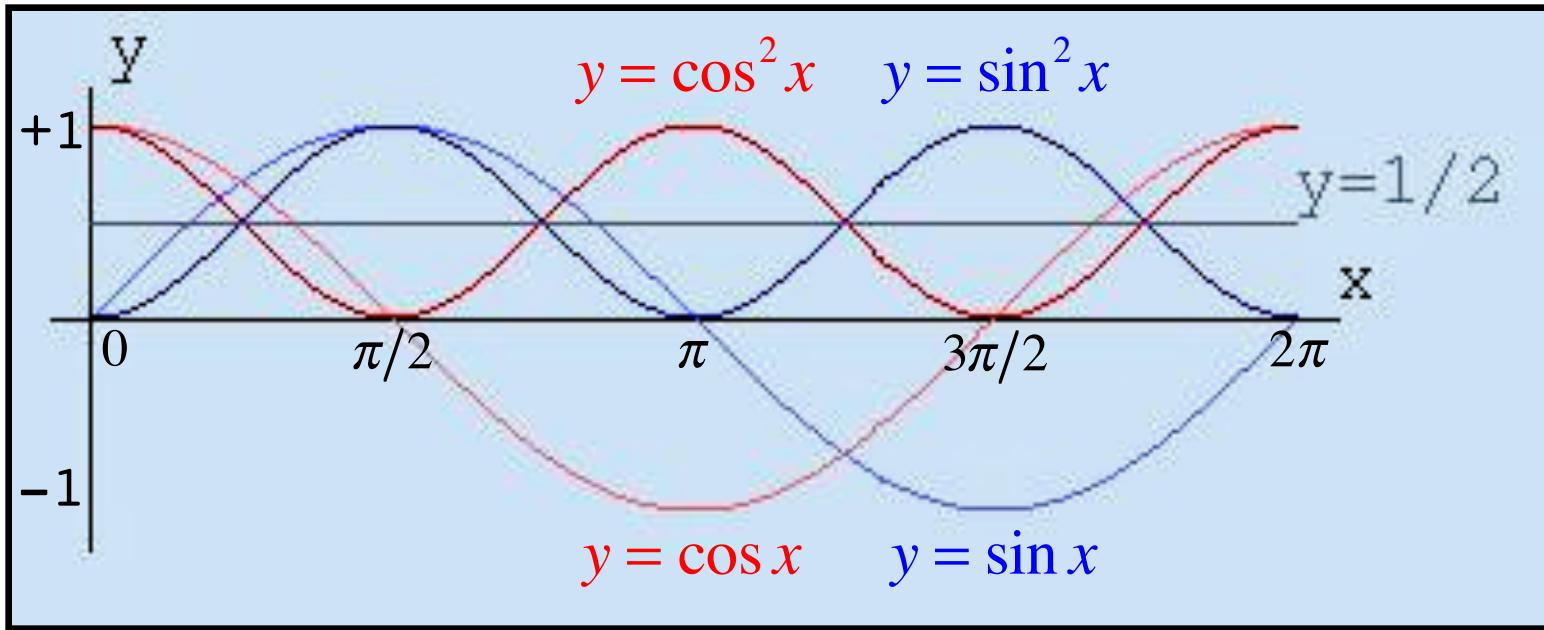
$$\int \sin x \, dx = \cos x + C$$

$$\int \cos x \, dx = -\sin x + C$$

$$\int_0^{2\pi} \cos x \, dx = \int_0^{2\pi} \sin x \, dx = 0$$

$$\int_0^{2\pi} \cos^2 x \, dx = \int_0^{2\pi} \sin^2 x \, dx = \frac{1}{2}$$

The sine and cosine functions and their squares

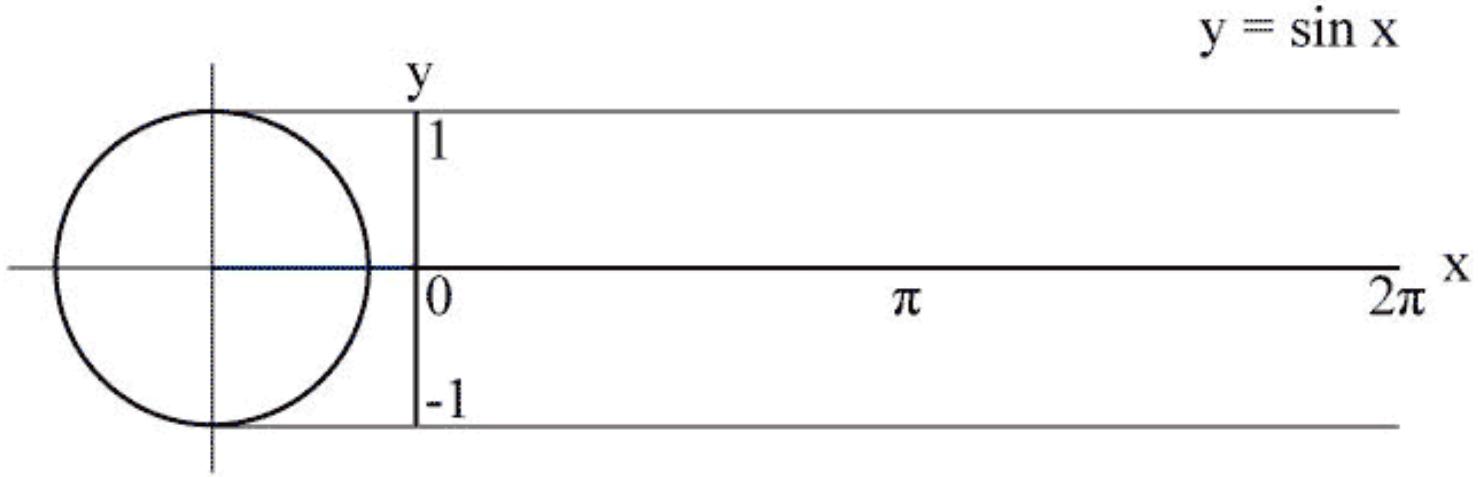


$$\langle \cos x \rangle_{0 \leq x < 2\pi} = \langle \sin x \rangle_{0 \leq x < 2\pi} = 0$$

$$\langle \cos^2 x \rangle_{0 \leq x < 2\pi} = \langle \sin^2 x \rangle_{0 \leq x < 2\pi} = \frac{1}{2}$$

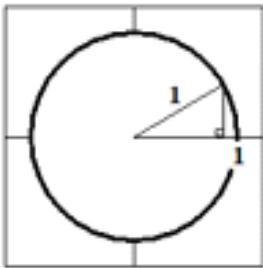
$$\cos^2 x + \sin^2 x = 1$$

The sine function on the unit circle



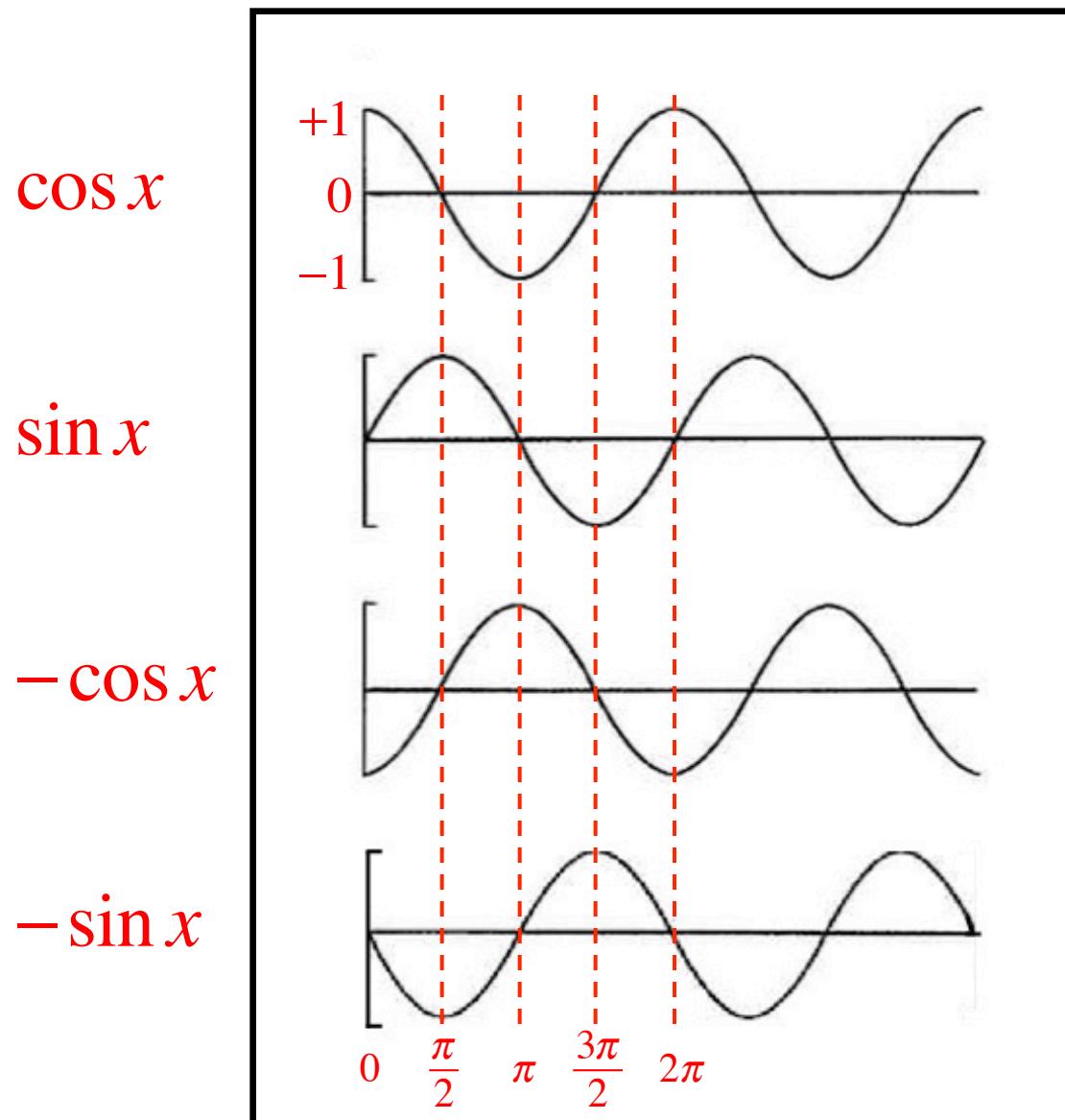
http://upload.wikimedia.org/wikipedia/commons/7/7d/Sin_drawing_process.gif

Relationships of the sine and cosine functions to the unit circle and helix



Unit Circle

Sine and cosine phase differences



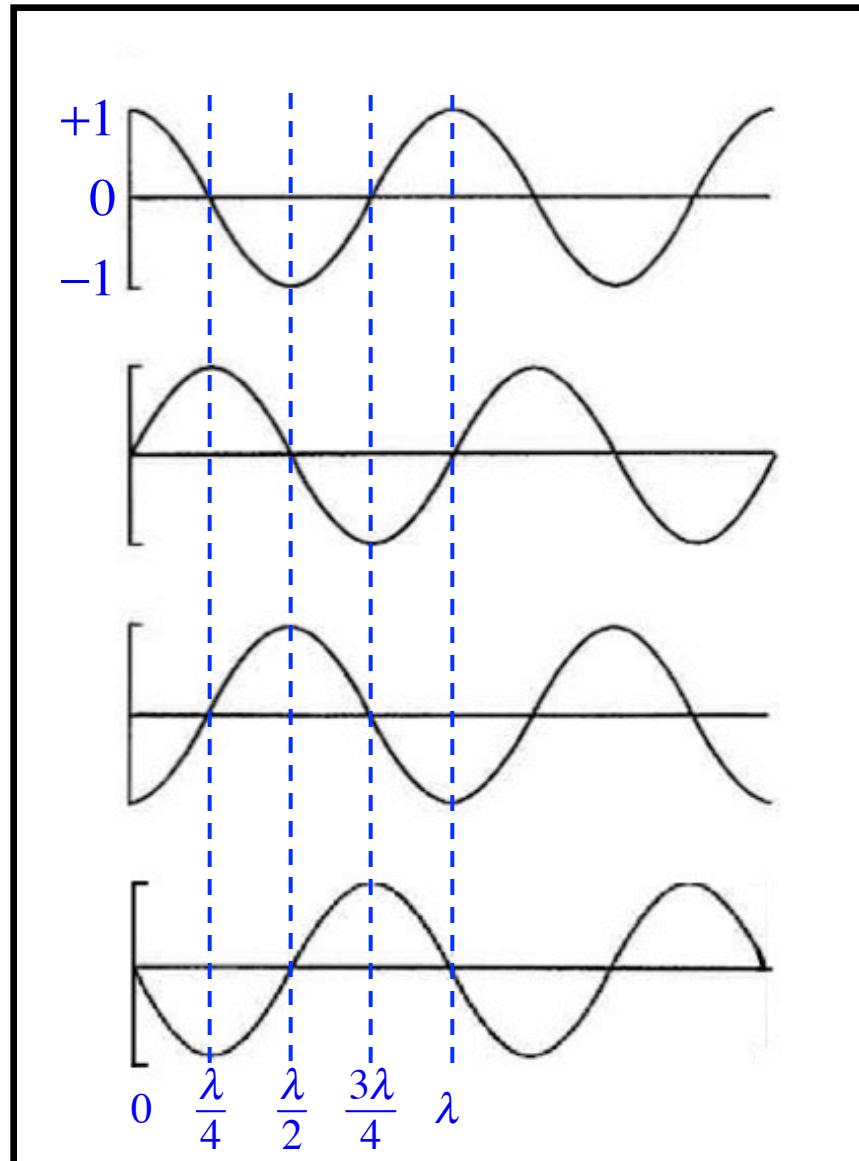
Sine and cosine phase differences

$$\cos(2\pi x/\lambda)$$

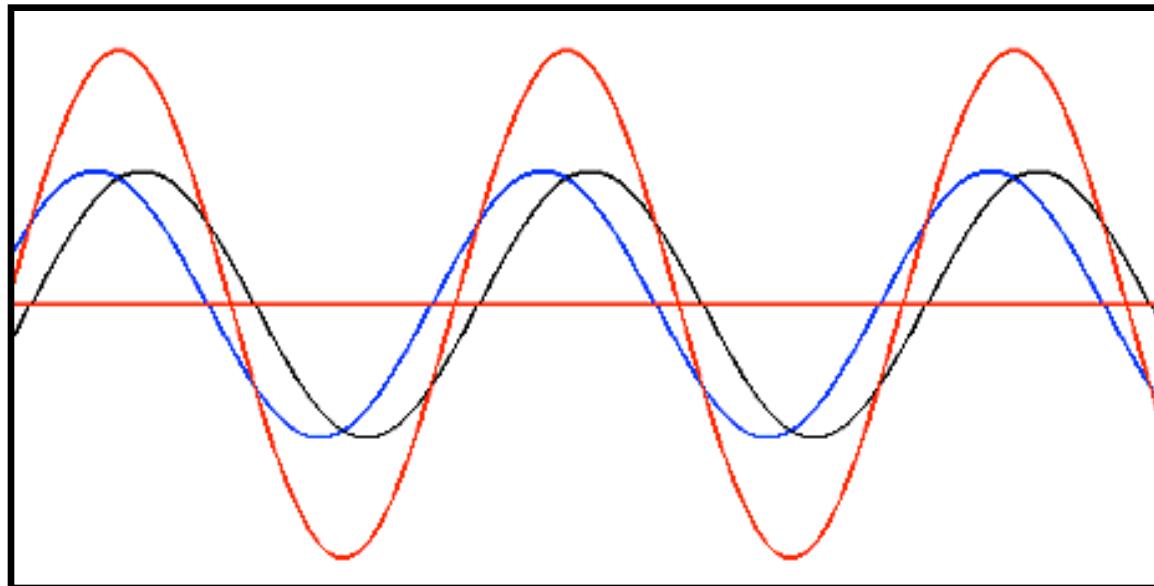
$$\sin(2\pi x/\lambda)$$

$$-\cos(2\pi x/\lambda)$$

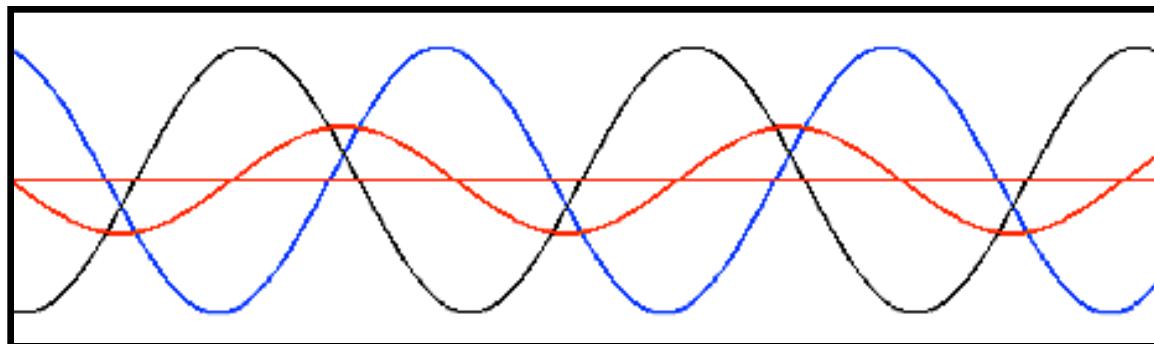
$$-\sin(2\pi x/\lambda)$$



Superposition of two equal-frequency, equal-amplitude waves



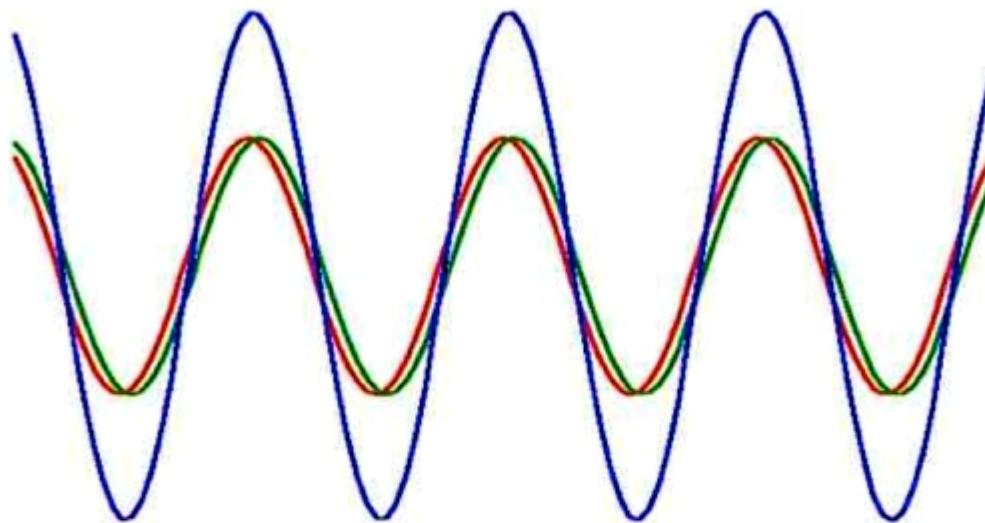
Constructive interference of waves almost in phase



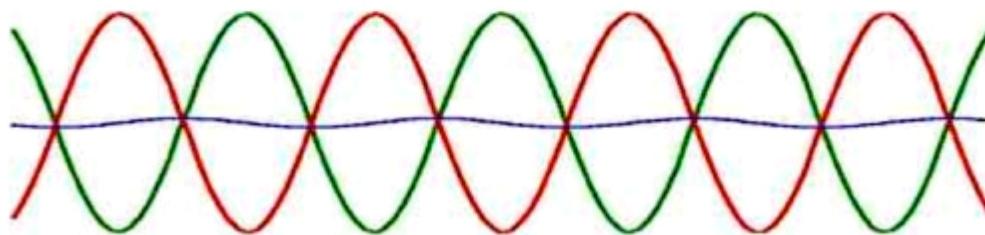
Destructive interference of waves almost 180° out of phase

Superposition of two equal-frequency, equal-amplitude waves

Wave superposition and interference

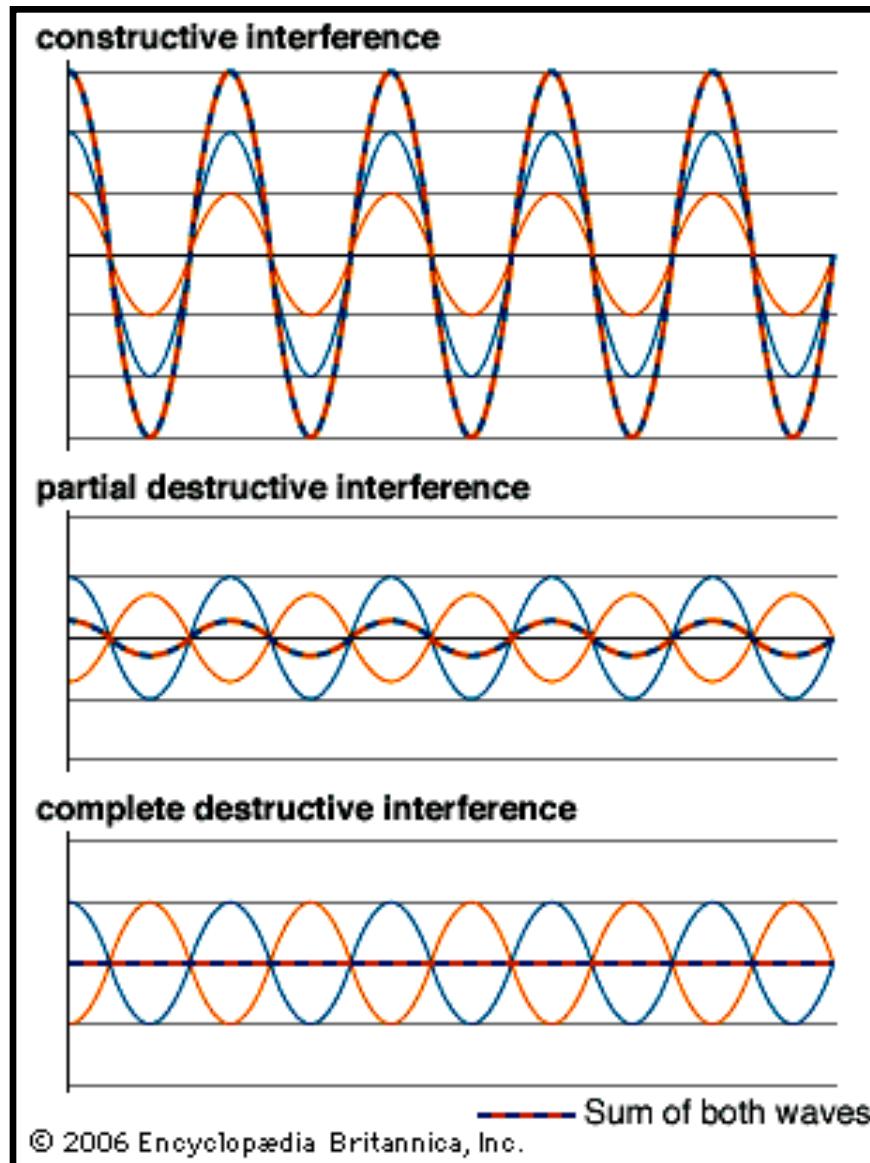


Equal-wavelength, equal-amplitude waves nearly in phase.
Constructive interference



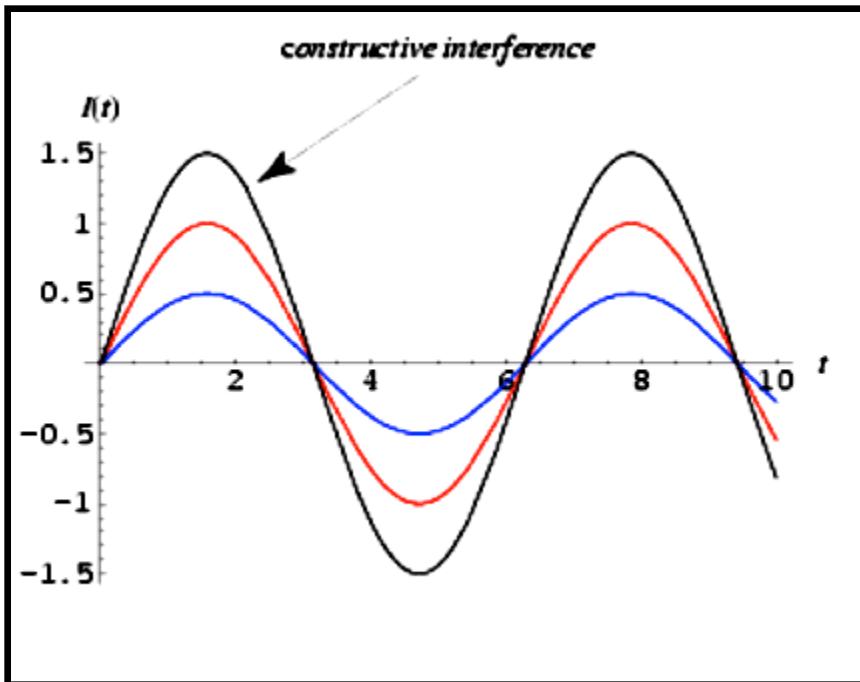
Equal-wavelength, equal-amplitude waves nearly 180° out of phase.
Destructive interference

Sinusoidal wave superposition and interference

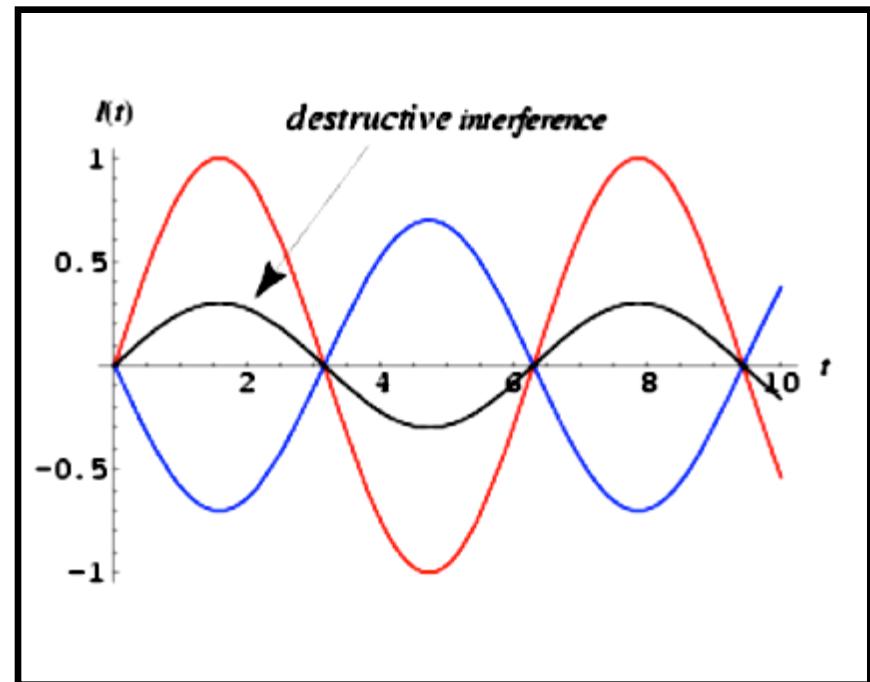


<http://media-2.web.britannica.com/eb-media/95/96595-004-16C2DCAD.gif>

Superposition of two waves with equal frequencies but unequal amplitudes



in phase
crest on crest
and
trough on trough



180° out of phase
crest on trough
and
trough on crest

Superposition of any number of equal-wavelength sinusoidal (sine and/or cosine) waves gives a sinusoidal resultant wave.

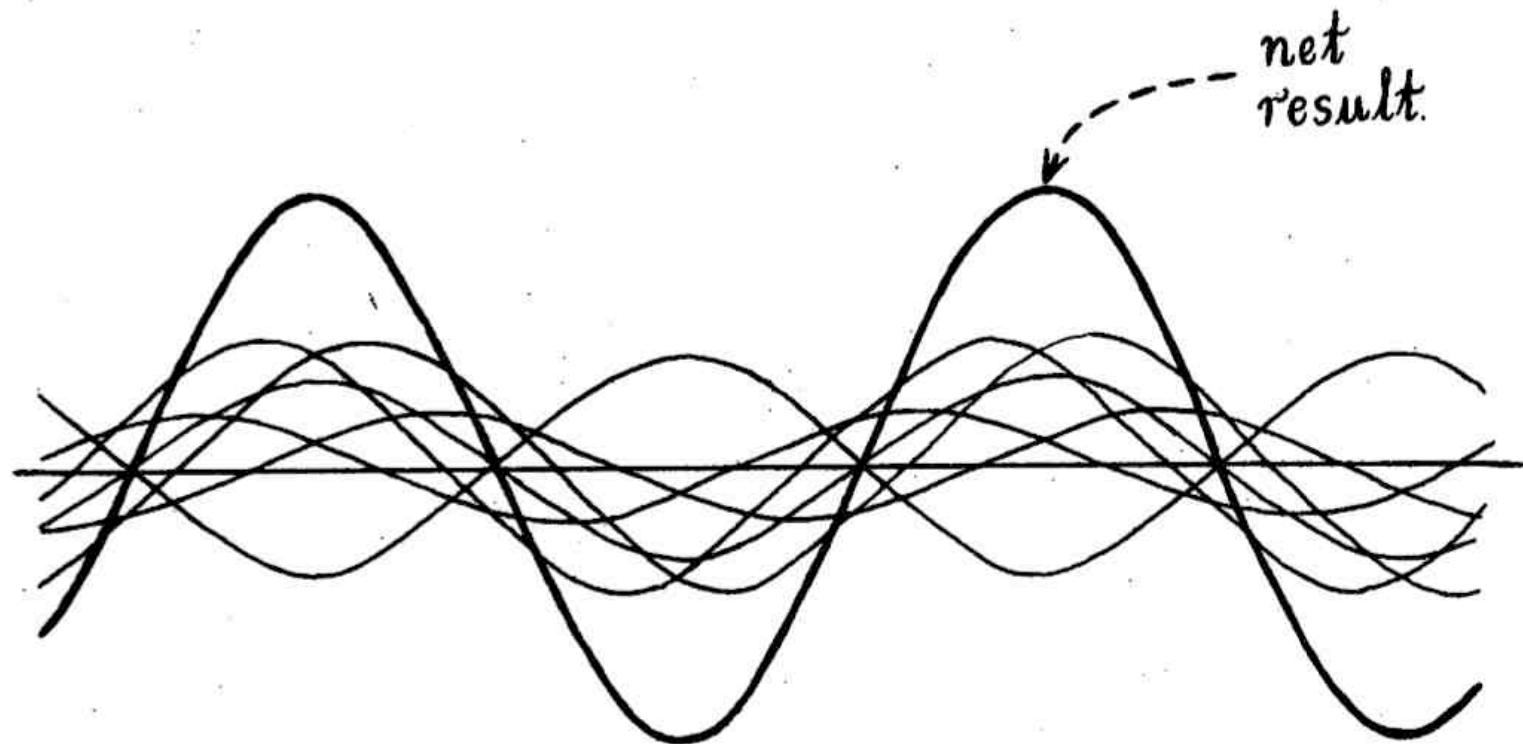
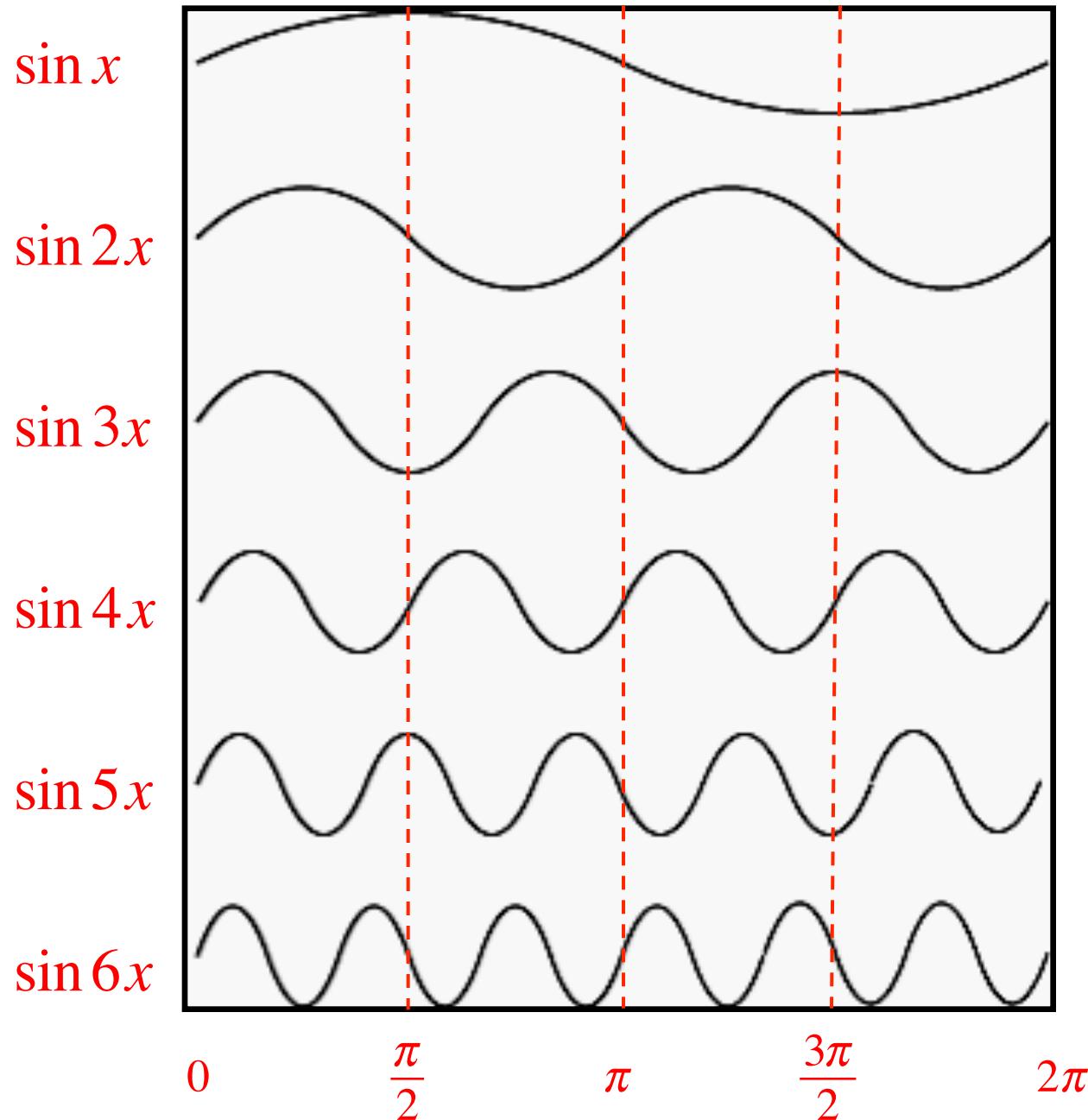
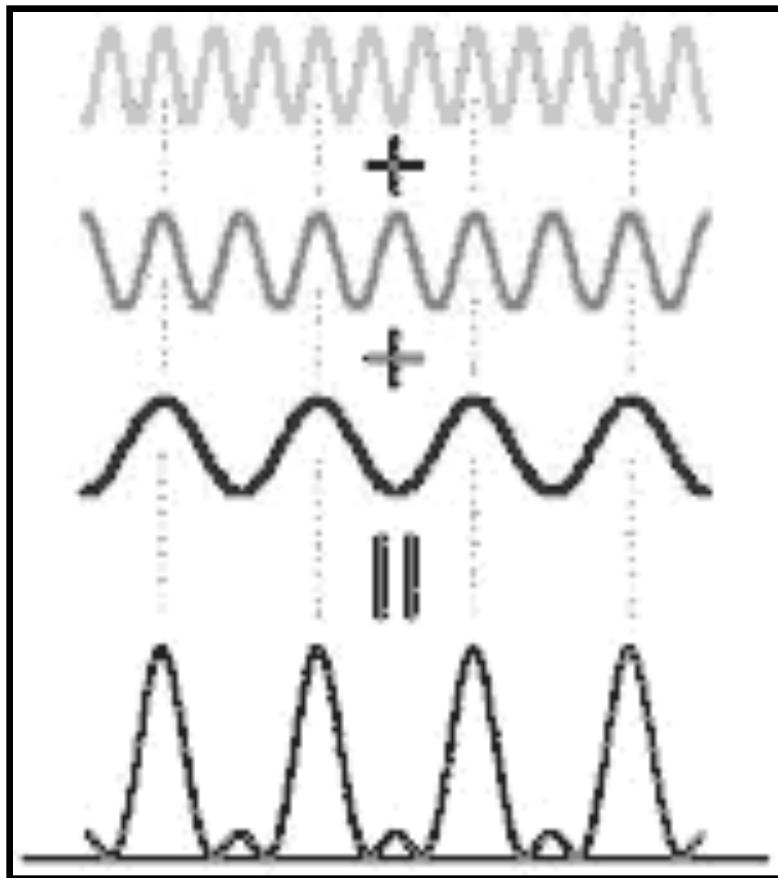


FIG. 115. For complex crystals, the net wave for any particular reflection is the result of a combination of a number of waves out of step by different amounts.

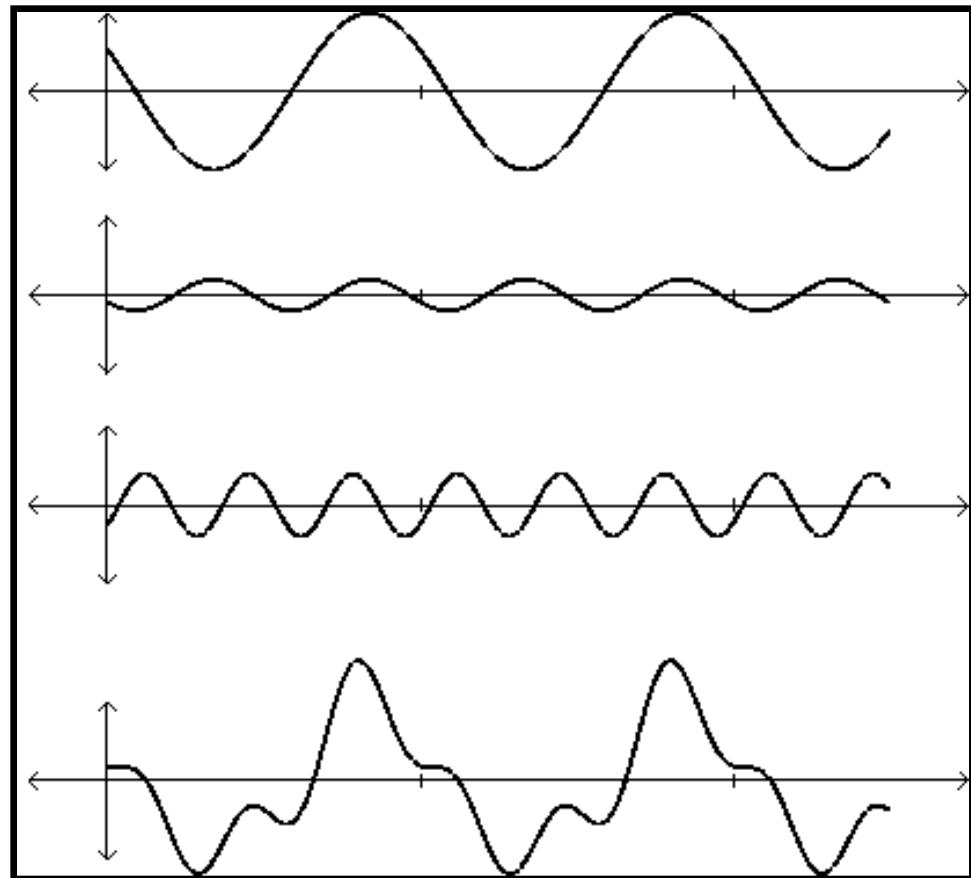
Sine function harmonics, $\sin nx$, $\lambda = 2\pi/n$



Two examples of harmonic sums of sinusoidal components

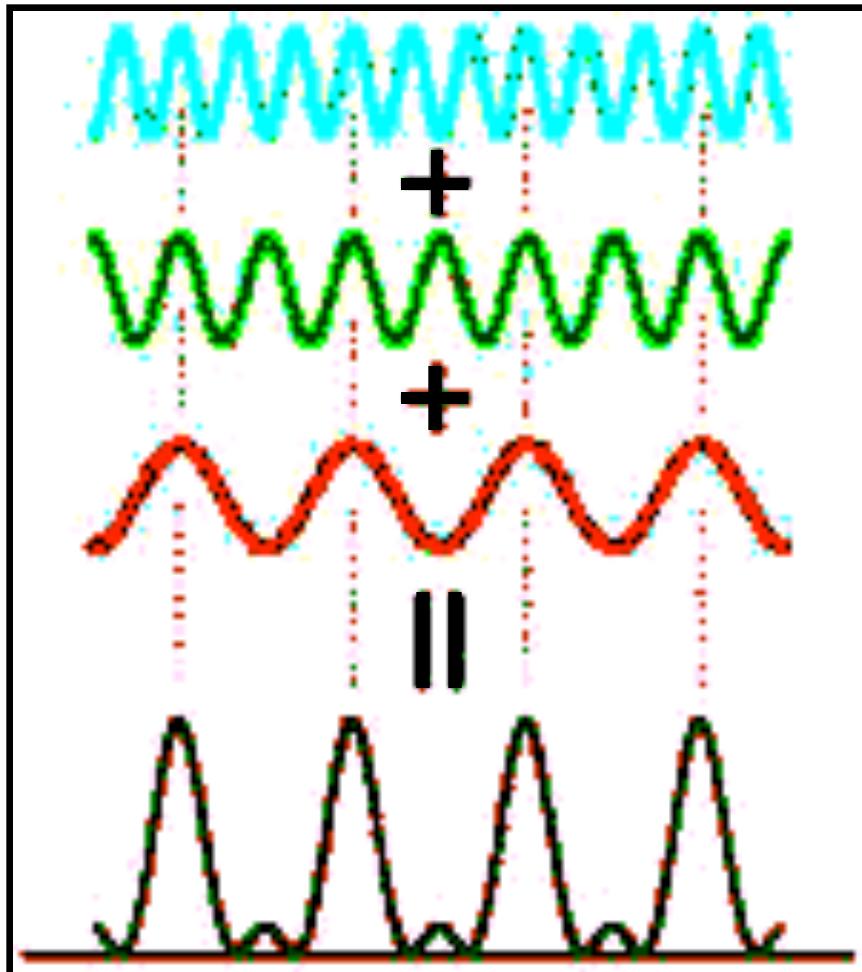


**Equal phases
and
equal amplitudes**



**Unequal phases
and
unequal amplitudes**

A sum of equal-amplitude, in-phase cosine harmonics



$$y_3 = \cos 3x$$

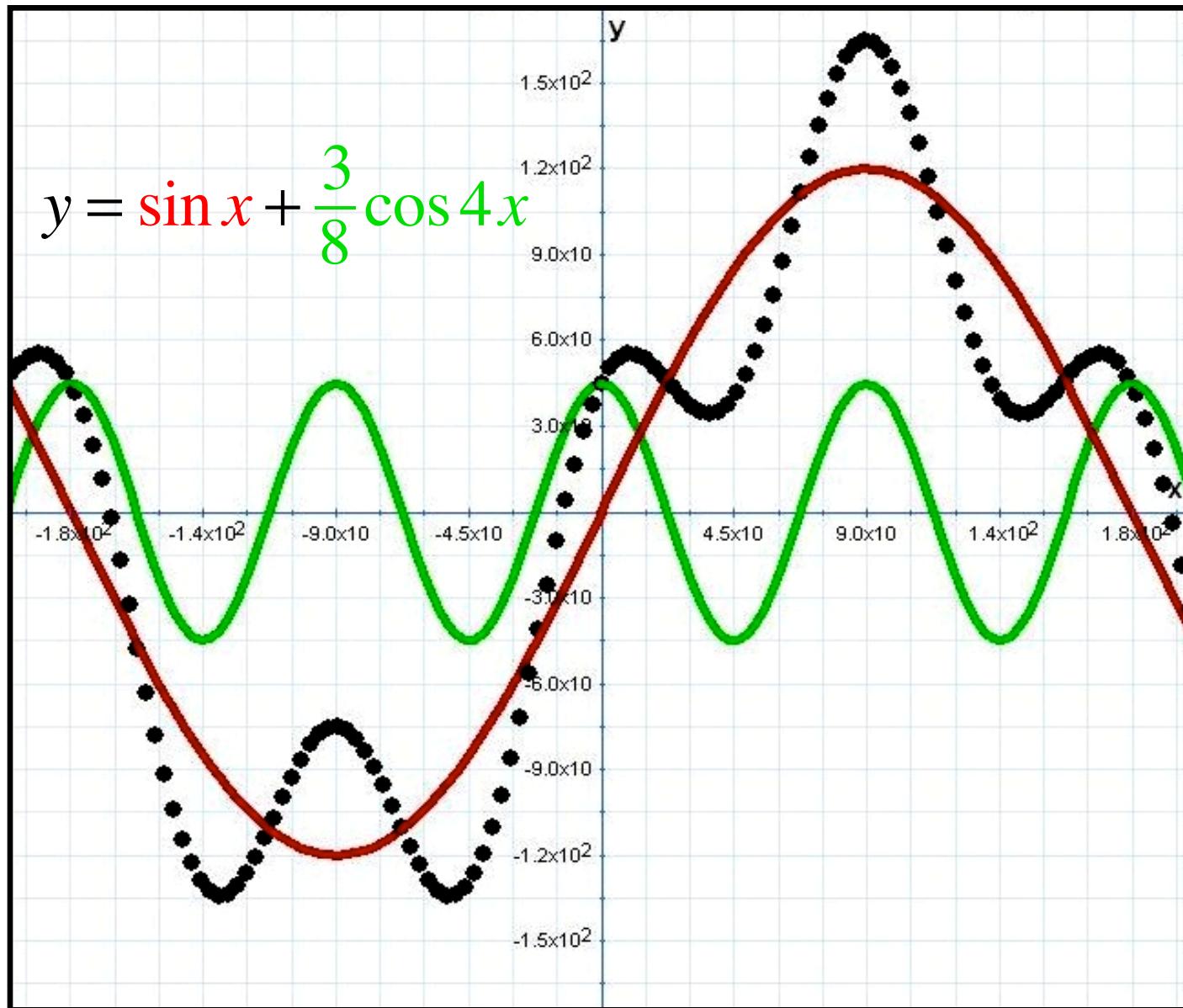
$$y_2 = \cos 2x$$

$$y_1 = \cos x$$

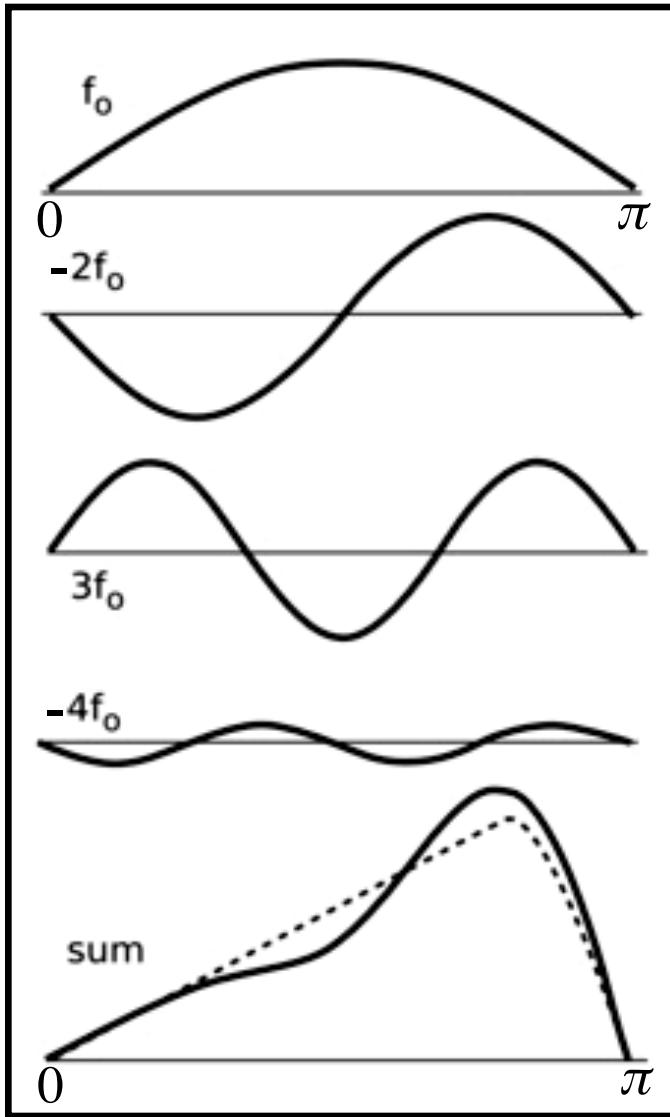
$$y = y_1 + y_2 + y_3$$

$$= \cos x + \cos 2x + \cos 3x$$

A superposition of unequal frequency, unequal amplitude sinusoids



A superposition sum of sine wave harmonics

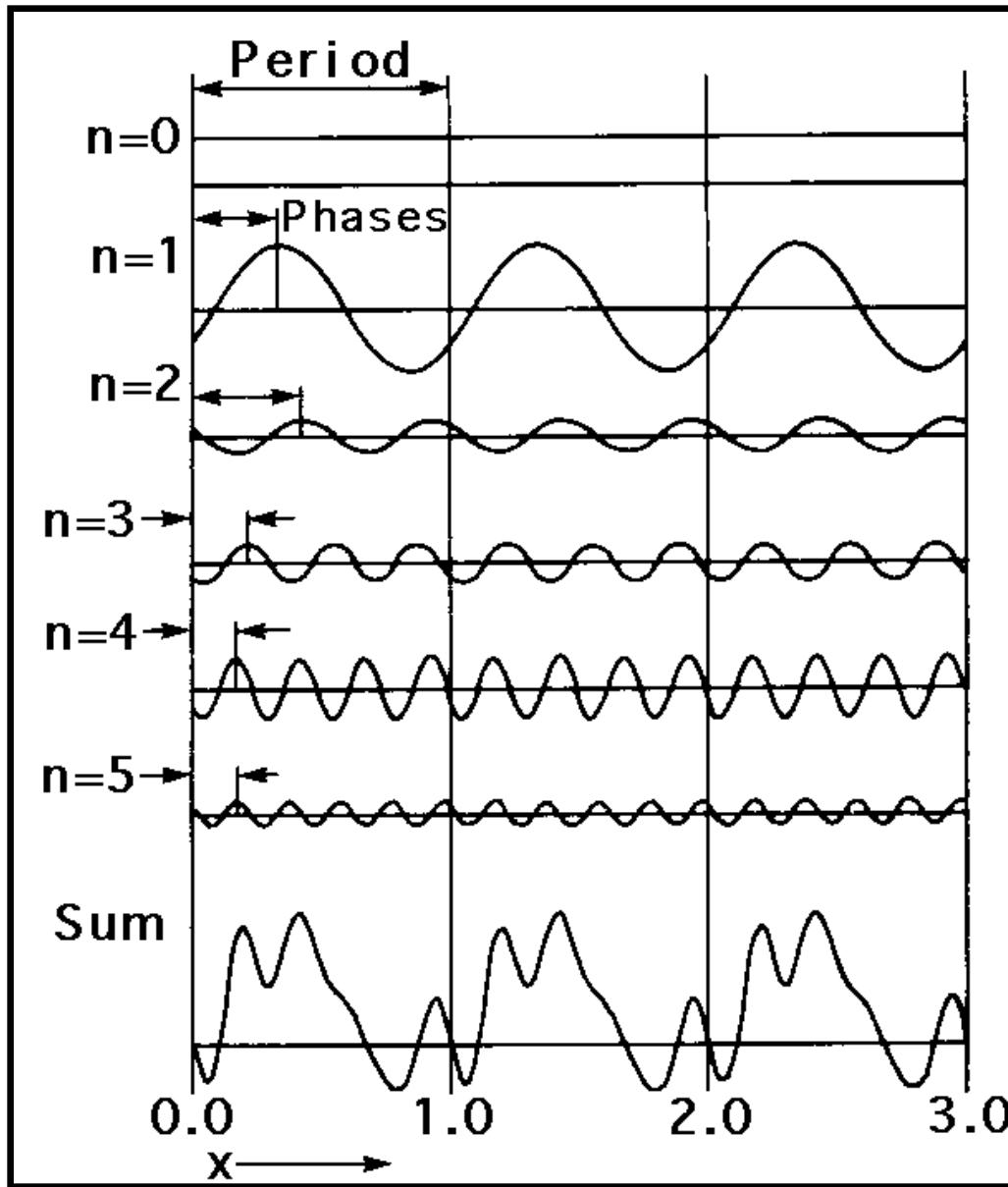


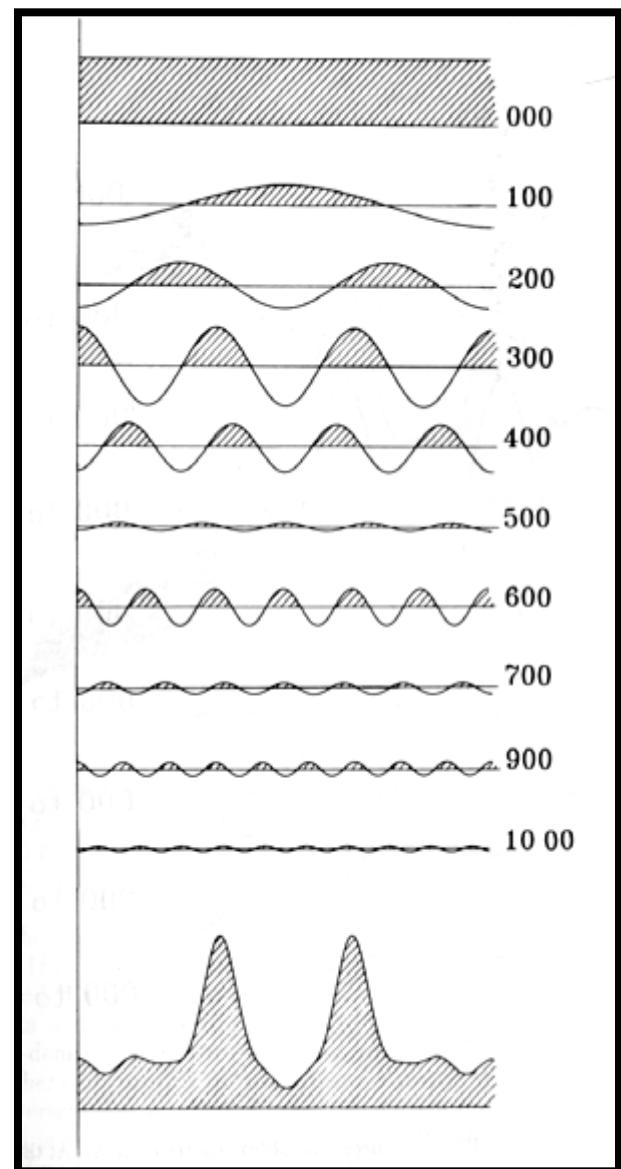
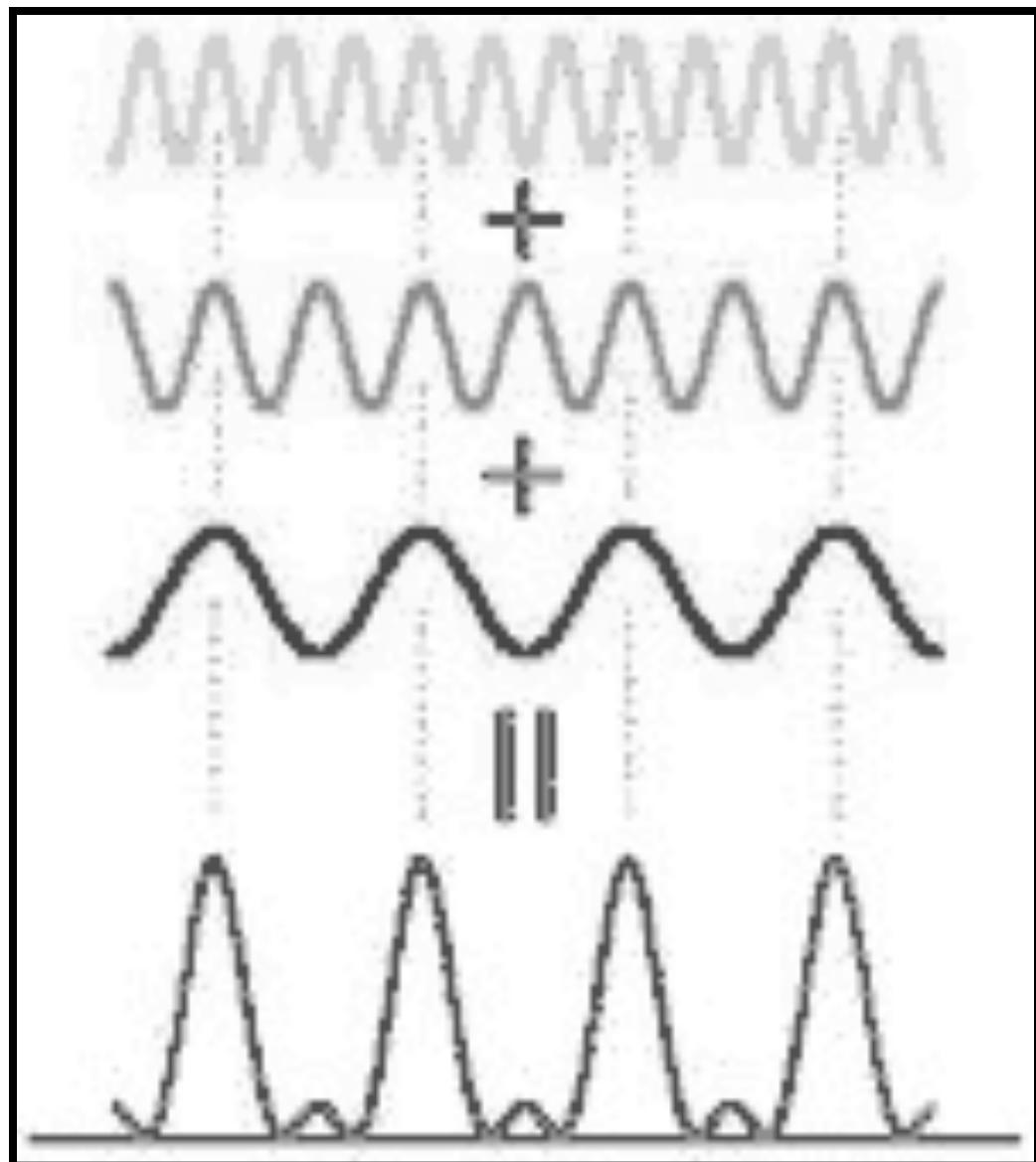
$$\sin nx, \quad 0 \leq x \leq \pi$$

$$-\sin nx = \sin(-nx)$$

$$-\sin nx = \sin(-nx)$$

Sum of sinusoidal harmonic components with different phases and different amplitudes





Both the crystal structure factor

$$F_{hkl} = V_{\text{cell}} \int_0^1 \int_0^1 \int_0^1 \rho(x, y, z) \exp[+2\pi i(hx + ky + lz)] dx dy dz$$

$$F_{hkl} = \sum_{a=1}^N f_a(S_{hkl}) \exp[2\pi i(hx_a + ky_a + lz_a)]$$

$$F_{hkl} = |F_{hkl}| e^{i\varphi_{hkl}} = |F_{hkl}| (\cos \varphi_{hkl} + i \sin \varphi_{hkl})$$

$$S_{hkl} = \frac{1}{d_{hkl}} = 2 \left(\frac{\sin \theta_{hkl}}{\lambda} \right), \quad |F_{\bar{h}\bar{k}\bar{l}}| = |F_{hkl}|, \quad \varphi_{\bar{h}\bar{k}\bar{l}} = -\varphi_{hkl}$$

and the unit-cell electron density distribution

$$\rho(x, y, z) = \frac{1}{V_{\text{cell}}} \sum_{h_{\min}}^{h_{\max}} \sum_{k_{\min}}^{k_{\max}} \sum_{l_{\min}}^{l_{\max}} |F_{hkl}| \cos[\varphi_{hkl} - 2\pi(hx + ky + lz)]$$

are sinusoidal wave superpositions.

F_{hkl} is a superposition of sinusoidal waves with different amplitudes and phases but the same frequency.

$\rho(x, y, z)$ is a superposition of sinusoidal waves with different amplitudes and phases and *different* harmonic frequencies.

Both the crystal structure factor

$$F_{hkl} = V_{\text{cell}} \int_0^1 \int_0^1 \int_0^1 \rho(x, y, z) \exp[+2\pi i(hx + ky + lz)] dx dy dz$$

$$F_{hkl} = \sum_{a=1}^N f_a(S_{hkl}) \exp[2\pi i(hx_a + ky_a + lz_a)]$$

$$F_{hkl} = |F_{hkl}| e^{i\varphi_{hkl}} = |F_{hkl}| (\cos \varphi_{hkl} + i \sin \varphi_{hkl})$$

$$S_{hkl} = \frac{1}{d_{hkl}} = 2 \left(\frac{\sin \theta_{hkl}}{\lambda} \right), \quad |F_{\bar{h}\bar{k}\bar{l}}| = |F_{hkl}|, \quad \varphi_{\bar{h}\bar{k}\bar{l}} = -\varphi_{hkl}$$

and the unit-cell electron density distribution

$$\rho(x, y, z) = \frac{1}{V_{\text{cell}}} \sum_{h_{\min}}^{h_{\max}} \sum_{k_{\min}}^{k_{\max}} \sum_{l_{\min}}^{l_{\max}} |F_{hkl}| \cos[\varphi_{hkl} - 2\pi(hx + ky + lz)]$$

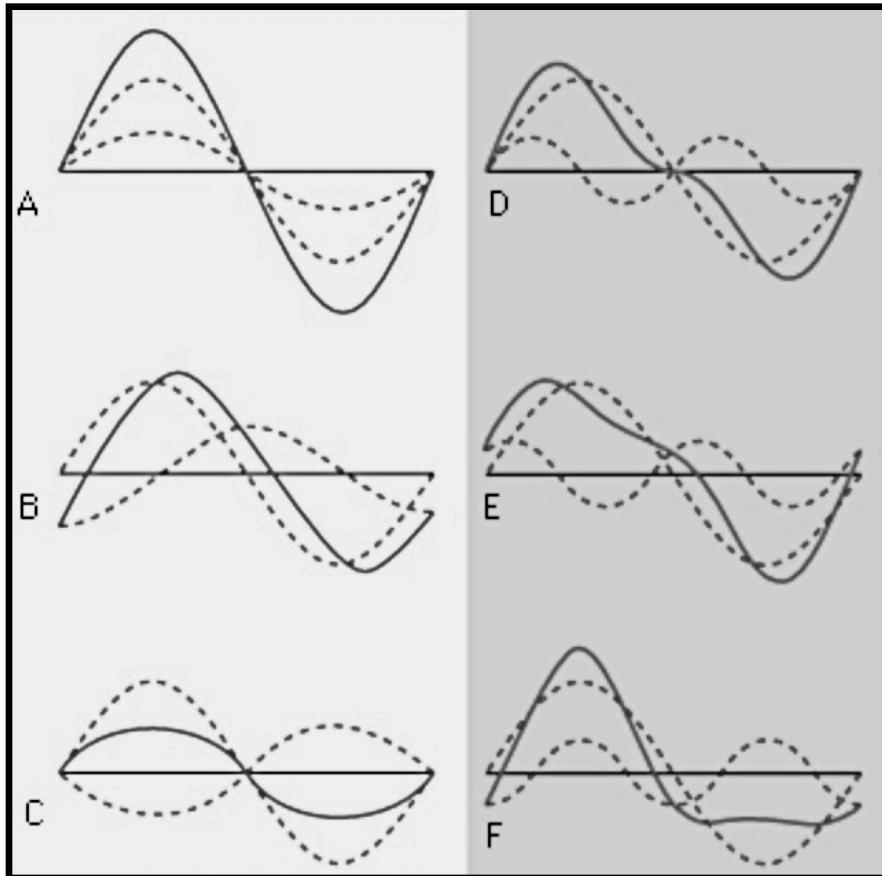
are sinusoidal wave superpositions.

F_{hkl} is a superposition of sinusoidal waves with different amplitudes and phases but the same frequency.

$\rho(x, y, z)$ is a superposition of sinusoidal waves with different amplitudes and phases and *different* harmonic frequencies.

Equal frequency Unequal frequency
 F_{hkl} waves $\rho(x,y,z)$ waves

different
amplitudes
and phases
but
the same
frequency

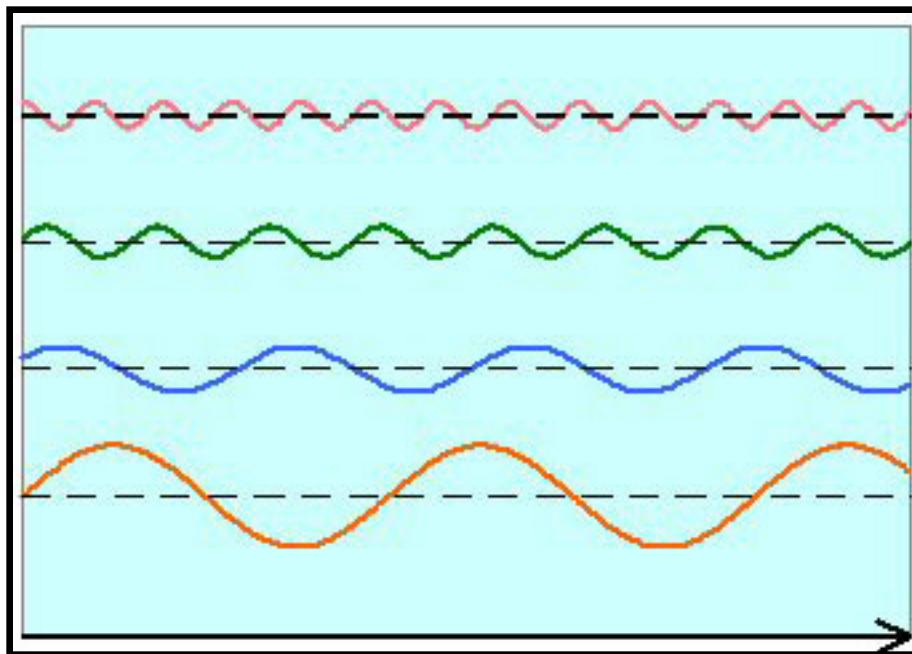


different
amplitudes
and phases
and
different
harmonic
frequencies

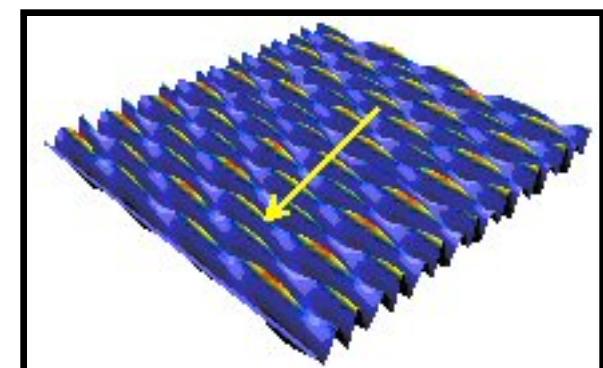
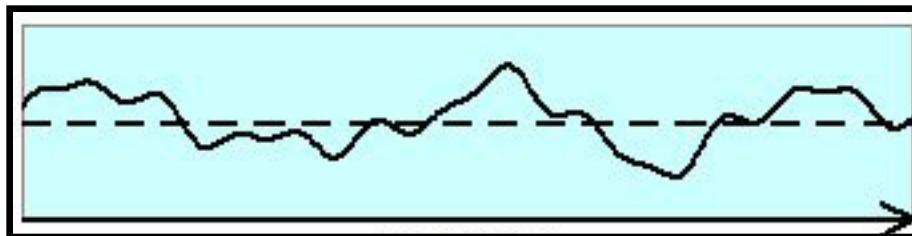
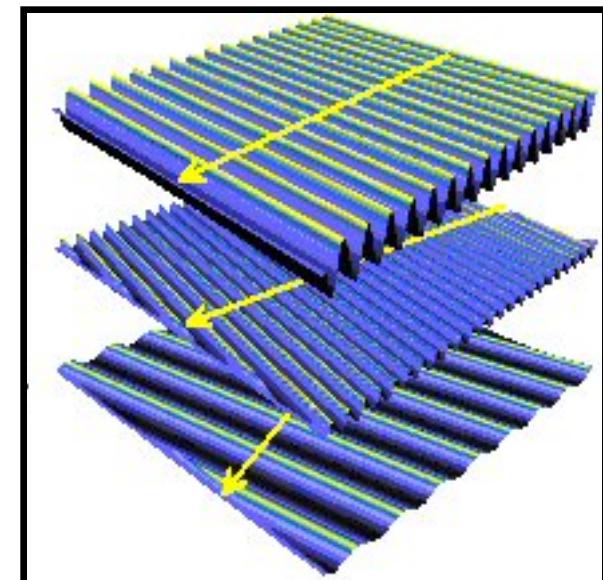
F_{hkl} is a superposition of sinusoidal waves with *different amplitudes and phases but the same frequency*.

$\rho(x,y,z)$ is a superposition of sinusoidal waves with *different amplitudes and phases and different harmonic frequencies*.

Two examples of Fourier sums of sinusoidal harmonic components

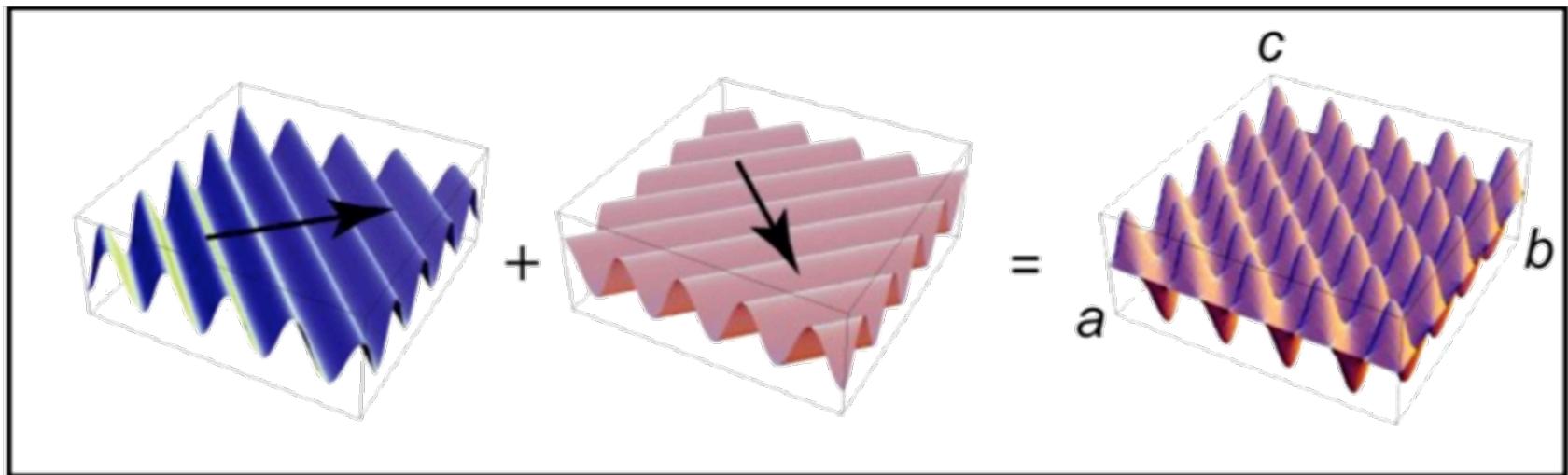


1-D



2-D

A superposition sum of density waves that produces density peaks



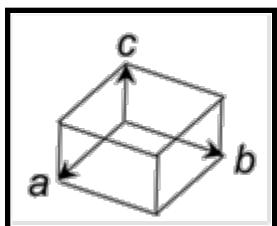
$$\rho_{5\bar{5}0} = \mathcal{F}[F_{5\bar{5}0}]$$

Fourier component
density waves

$$\rho_{550} = \mathcal{F}[F_{550}]$$

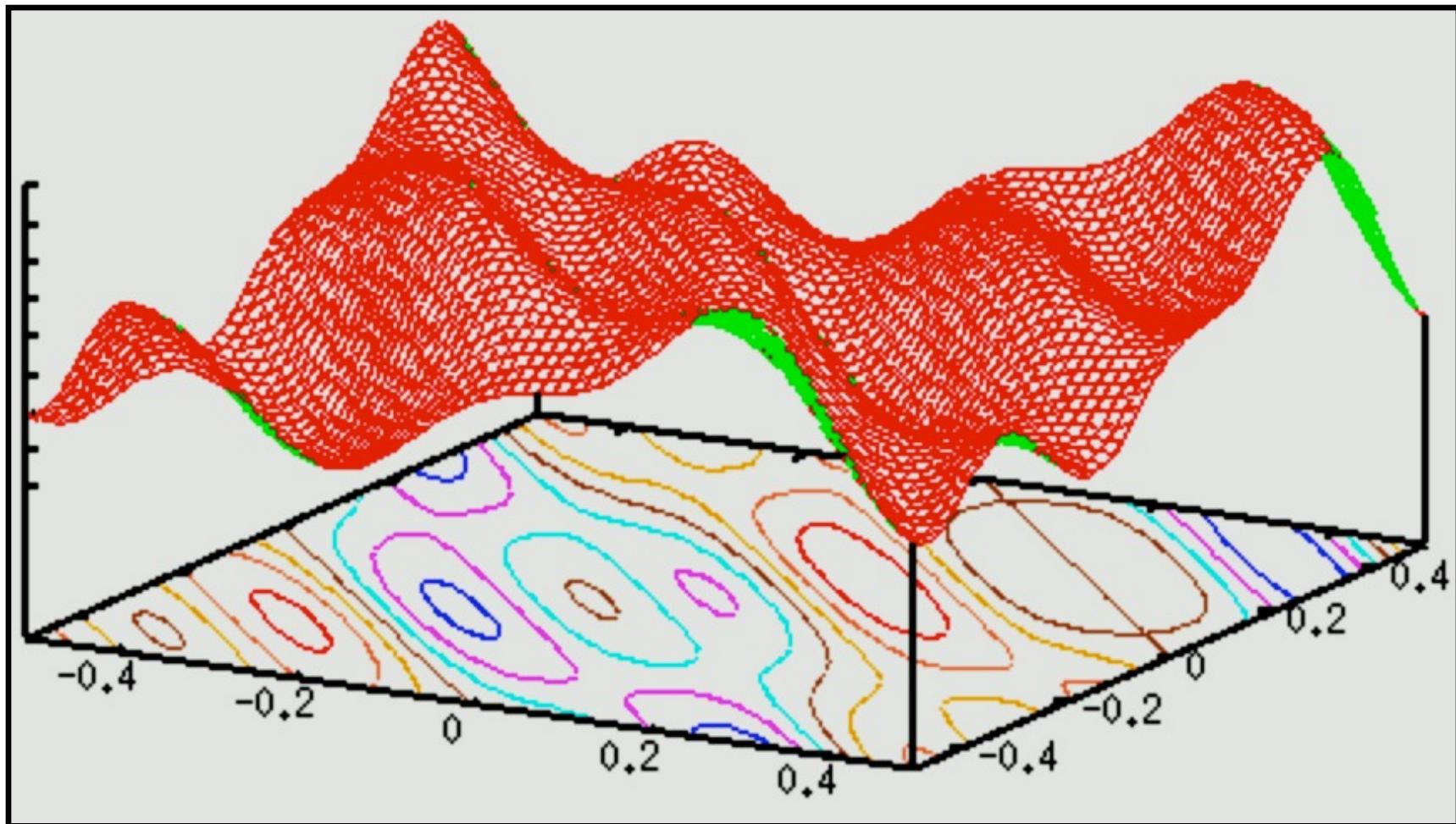
$$\rho(x, y, 0) = \rho_{5\bar{5}0} + \rho_{550}$$

Fourier sum
density peaks



3-D relief and 2-D contour plots of a sum of sinusoidal terms

$$z = \sum_{i=1}^n A_i \cos(a_i x + b_i y) + B_i \sin(c_i x + d_i y)$$



3-D relief map and 2-D isocontour map

Complex numbers

imaginary unit, i

$$i^2 = -1, \quad i^{-1} = -i, \quad i(-i) = -i^2 = 1$$

complex number

Cartesian form

$$z = x + iy$$

polar form

$$= |z| e^{i\varphi}$$

trigonometric form

$$= |z| (\cos \varphi + i \sin \varphi)$$

magnitude (or modulus)

$$|z| = \sqrt{x^2 + y^2}$$

phase (or argument)

$$\varphi = \tan^{-1} \left(\frac{\sin \varphi}{\cos \varphi} \right) = \tan^{-1} \left(\frac{y}{x} \right)$$

real part

$$\operatorname{Re}(z) = x = |z| \cos \varphi$$

imaginary part

$$\operatorname{Im}(z) = y = |z| \sin \varphi$$

conjugation

$$\begin{cases} z = x + iy \rightarrow z^* = x - iy \\ \text{Replace } i \text{ with } -i. \end{cases}$$

complex conjugate

Cartesian form

$$z^* = x - iy$$

polar form

$$= |z| e^{-i\varphi}$$

trigonometric form

$$= |z| (\cos \varphi - i \sin \varphi)$$

squared magnitude

$$|z|^2 = z^* z = z z^* = x^2 + y^2$$

equality

$$z_1 = z_2 \Leftrightarrow (x_1 = x_2) \wedge (y_1 = y_2) \Leftrightarrow (|z_1| = |z_2|) \wedge (\varphi_1 = \varphi_2)$$

addition or

$$z_1 \pm z_2 = (x_1 + iy_1) \pm (x_2 + iy_2) = (x_1 \pm x_2) + i(y_1 \pm y_2)$$

subtraction

multiplication

$$z_1 z_2 = (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + x_2 y_1)$$

$$= |z_1| |z_2| \exp[i(\varphi_1 + \varphi_2)]$$

division

$$\frac{z_1}{z_2} = \frac{x_1 + iy_1}{x_2 + iy_2} = \frac{z_1 z_2^*}{z_2 z_2^*} = \frac{(x_1 + iy_1)(x_2 - iy_2)}{x_2^2 + y_2^2}$$

$$= \frac{|z_1|}{|z_2|} \exp[i(\varphi_1 - \varphi_2)]$$

The Euler formula

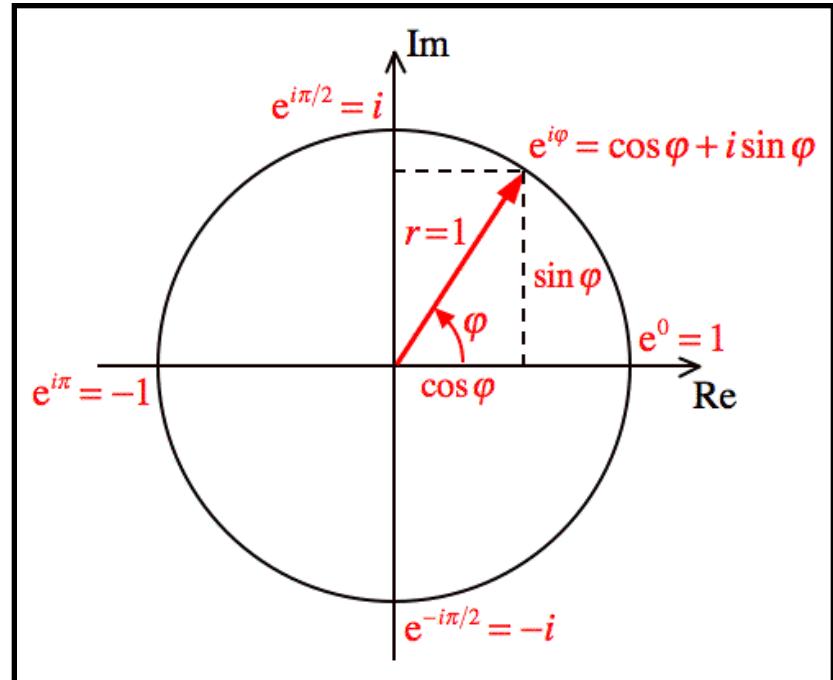
$$e^{i\varphi} = \cos \varphi + i \sin \varphi$$

Feynman called this “... the most remarkable formula in mathematics..., our jewel”.

The Euler identity

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

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.

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

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

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

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

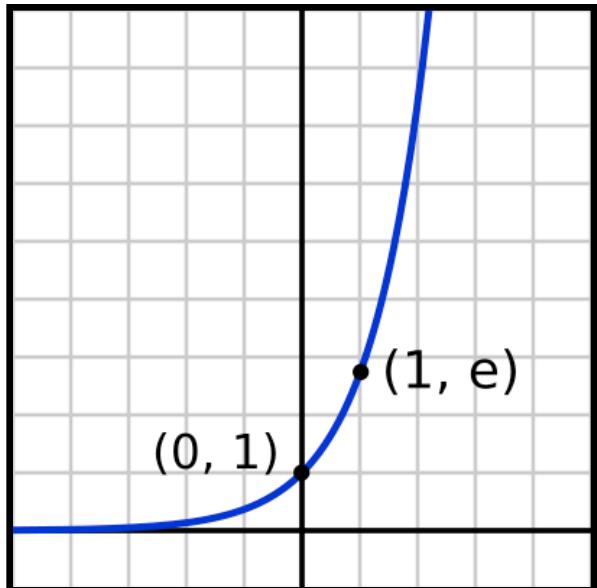
The Euler identity is a thing of *great mathematical beauty*. It links the real numbers 0 and -1, the transcendental numbers π and e , and the imaginary unit i .

Euler's number e and the exponential function $y = f(x) = e^x$

$$e = \sum_{n=0}^{\infty} \frac{1}{n!} = \lim_{n \rightarrow \infty} \left(1 + \frac{1}{n}\right)^n, \quad \begin{cases} e \in \mathbb{R} \\ e \notin \mathbb{Q} \\ e \notin \mathbb{A} \end{cases}$$

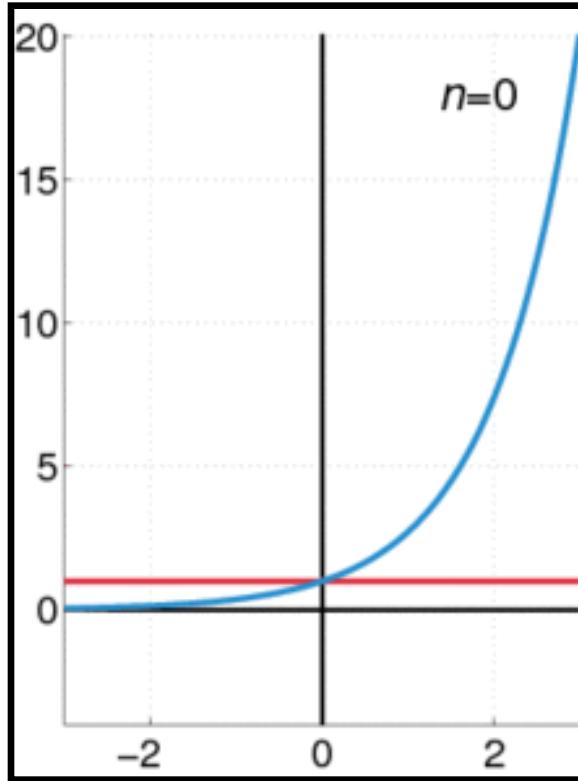
$$y = f(x) = e^x, \quad \frac{dy}{dx} = \frac{d}{dx} f(x) = \frac{d}{dx} e^x = e^x$$

$e \approx 2.71828\dots$

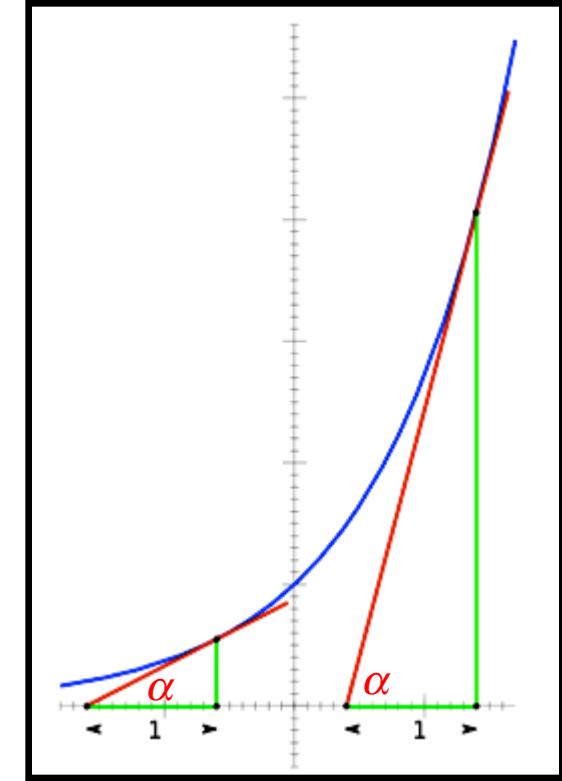


$$y = e^x, \quad \frac{dy}{dx} = e^x$$

$$\left. \frac{dy}{dx} \right|_{x=0} = 1$$



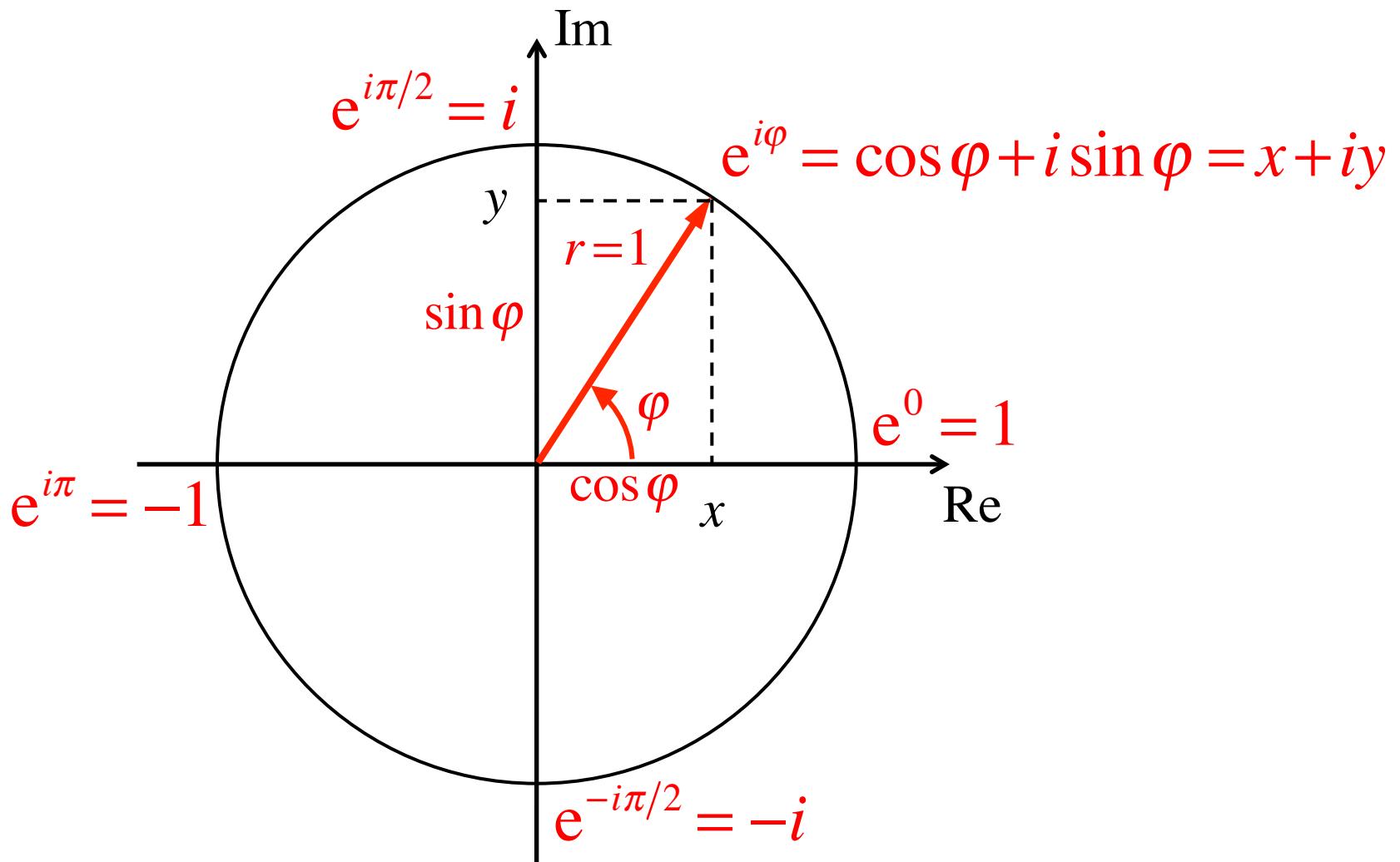
$$y = e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = \lim_{n \rightarrow \infty} \left(1 + \frac{x}{n}\right)^n$$



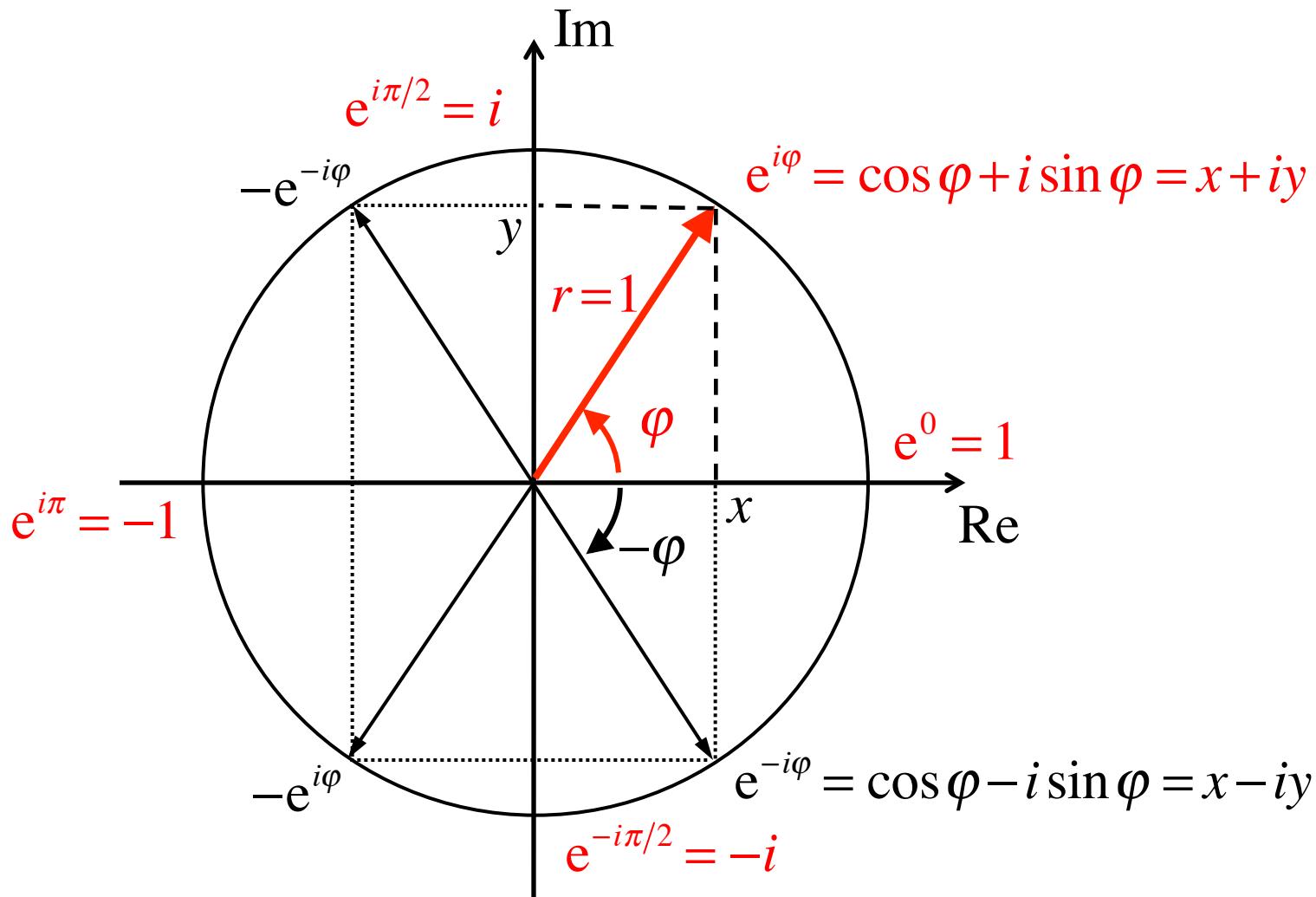
$$y = e^x, \quad \frac{dy}{dx} = \tan \alpha = \frac{y}{1}$$

$$\frac{d}{dx} e^x = e^x$$

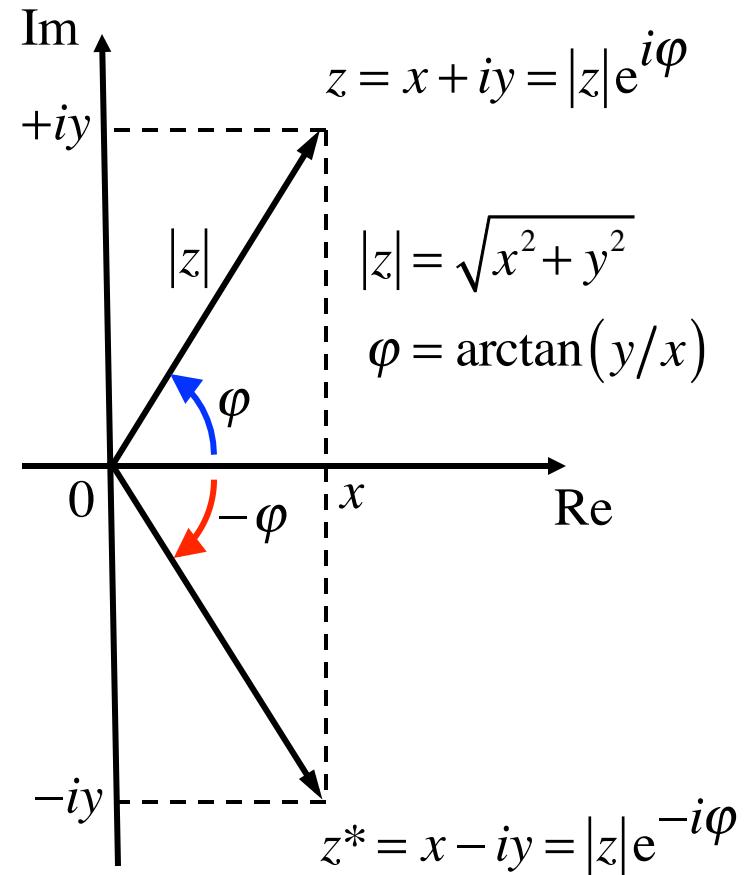
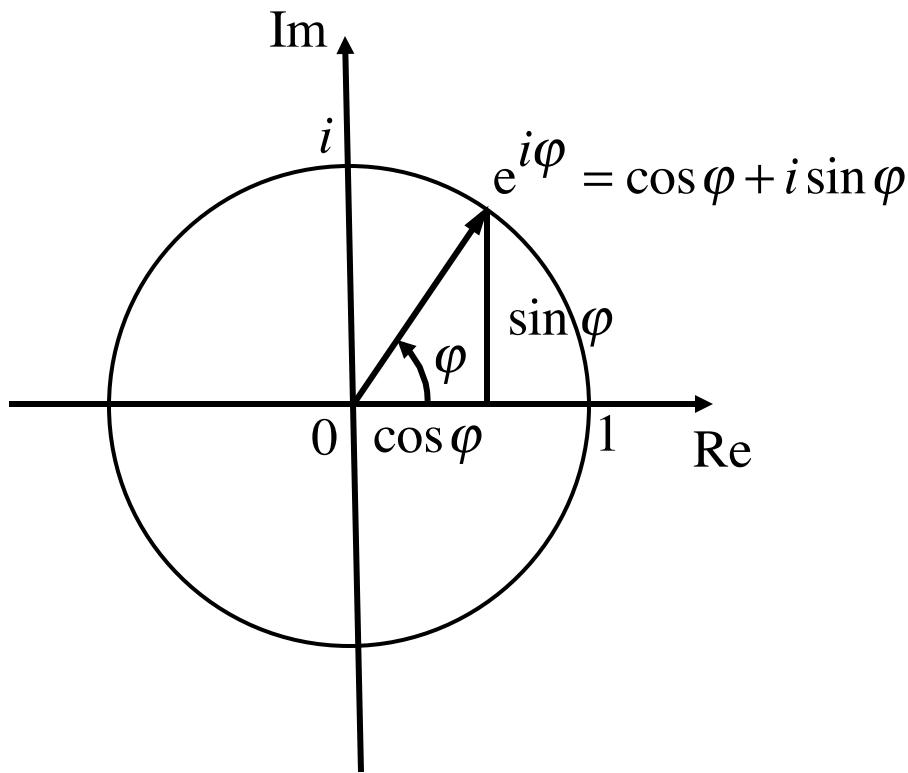
The Euler relationship on an Argand diagram of the unit circle on the complex plane



The Euler relationship on an Argand diagram of the unit circle on the complex plane



The Euler relationship and a conjugate pair of complex numbers illustrated as Argand diagrams on the complex plane

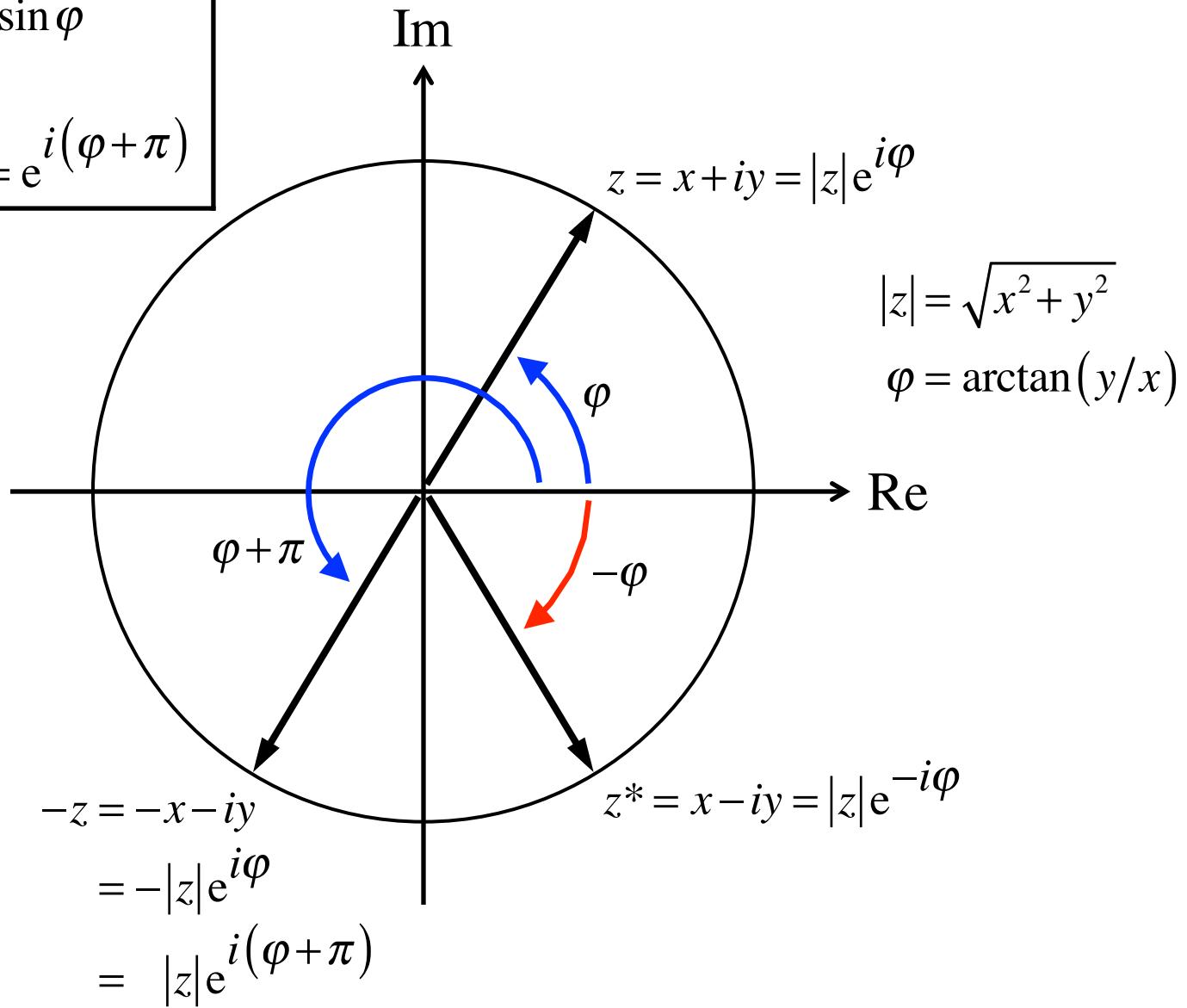


Conjugate versus negative complex numbers

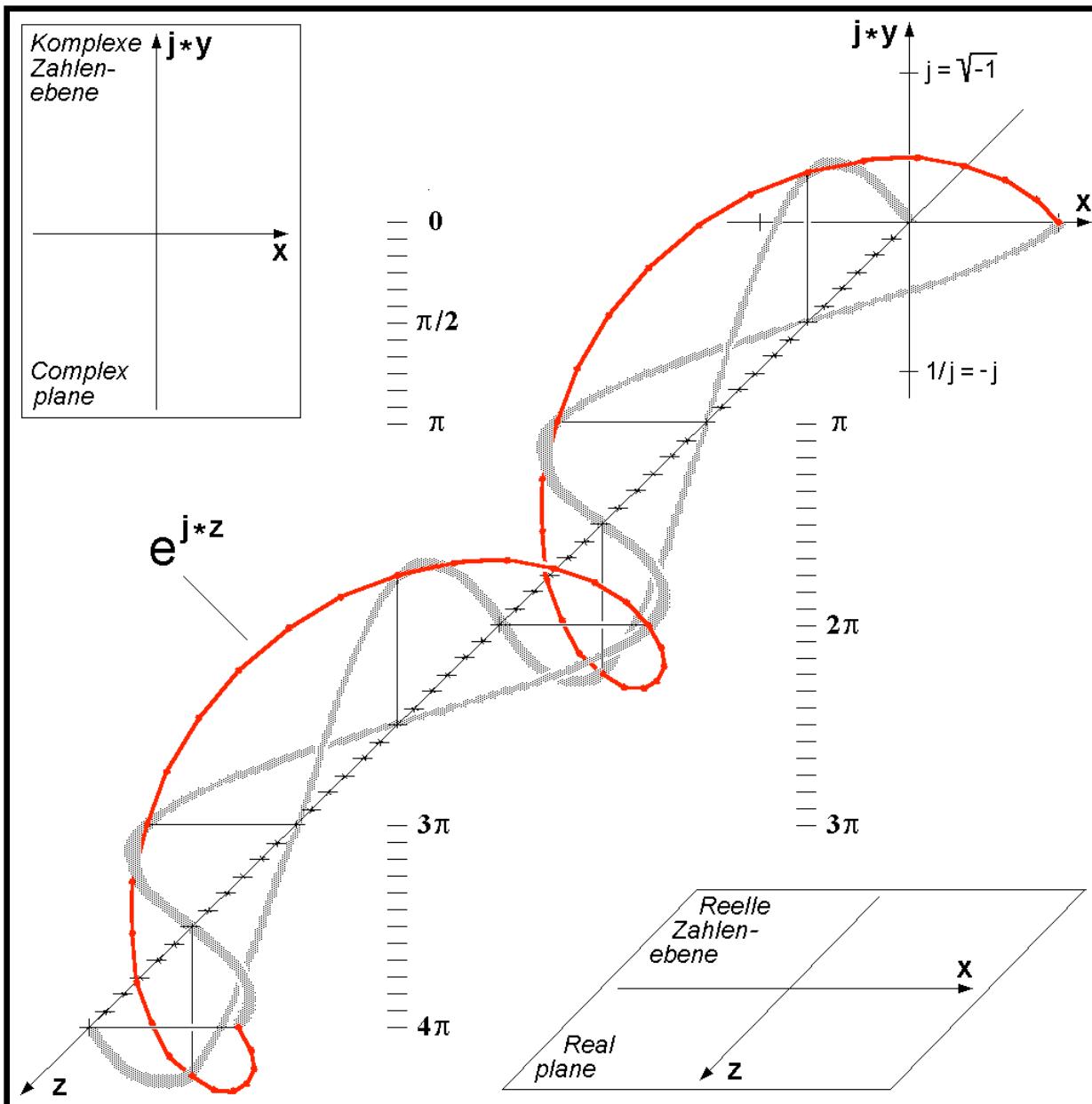
$$e^{i\varphi} = \cos \varphi + i \sin \varphi$$

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

$$-e^{i\varphi} = e^{i\pi} e^{i\varphi} = e^{i(\varphi+\pi)}$$



The Euler Relationship in 3-D



http://upload.wikimedia.org/wikipedia/commons/e/e3/Euler%27s_Formula_c.png

Taylor Series

Infinite series expansion of $f(x)$ about $x = x_0$

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2!} f''(x_0)(x - x_0)^2 + \frac{1}{3!} f'''(x_0)(x - x_0)^3 + \dots$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} f^{[n]}(x_0)(x - x_0)^n$$

$$f'(x_0) = \left. \frac{df}{dx} \right|_{x_0}, \quad f''(x_0) = \left. \frac{d^2 f}{dx^2} \right|_{x_0}, \quad f'''(x_0) = \left. \frac{d^3 f}{dx^3} \right|_{x_0}, \dots, \quad f^{[n]}(x_0) = \left. \frac{d^n f}{dx^n} \right|_{x_0}$$

Maclaurin Series

Taylor series expansion of $f(x)$ about $x = 0$

$$f(x) = f(0) + f'(0)x + \frac{1}{2!} f''(0)x^2 + \frac{1}{3!} f'''(0)x^3 + \dots$$

Series expansions of $\cos x$ and $\sin x$

$$f(x) = f(0) + f'(0)x + \frac{1}{2!}f''(0)x^2 + \frac{1}{3!}f'''(0)x^3 + \dots$$

$$\left\{ \begin{array}{ll} f(x) = \cos x & f(0) = 1 \\ f'(x) = -\sin x & f'(0) = 0 \\ f''(x) = -\cos x & f''(0) = -1 \\ f'''(x) = \sin x & f'''(0) = 0 \\ f^{[4]}(x) = \cos x & f^{[4]}(0) = 1 \end{array} \right.$$
$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots$$

$$\left\{ \begin{array}{ll} f(x) = \sin x & f(0) = 0 \\ f'(x) = \cos x & f'(0) = 1 \\ f''(x) = -\sin x & f''(0) = 0 \\ f'''(x) = -\cos x & f'''(0) = -1 \\ f^{[4]}(x) = \sin x & f^{[4]}(0) = 0 \end{array} \right.$$
$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots$$

Series expansions of e^x and e^{ix}

$$f(x) = f(0) + f'(0)x + \frac{1}{2!}f''(0)x^2 + \frac{1}{3!}f'''(0)x^3 + \dots$$

$$f(x) = e^x \quad f(0) = 1$$

$$f'(x) = e^x \quad f'(0) = 1$$

$$f''(x) = e^x \quad f''(0) = 1$$

$$f'''(x) = e^x \quad f'''(0) = 1$$

$$f^{[n]}(x) = e^x \quad f^{[n]}(0) = 1$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$$

$$e = 1 + 1 + \frac{1}{2!} + \frac{1}{3!} + \frac{1}{4!} + \dots = 2.71828\dots$$

$$e^{ix} = 1 + ix + \frac{(ix)^2}{2!} + \frac{(ix)^3}{3!} + \frac{(ix)^4}{4!} + \dots$$

$$= 1 + ix - \frac{x^2}{2!} - \frac{ix^3}{3!} + \frac{x^4}{4!} + \frac{ix^5}{5!} - \frac{x^6}{6!} - \frac{ix^7}{7!} + \dots$$

$$= \underbrace{1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots}_{\cos x} + i \underbrace{\left(x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots \right)}_{\sin x}$$

$$e^{ix} = \cos x + i \sin x$$

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

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

⋮

$$i^{-2} = -1$$

$$i^{-1} = -i$$

$$i^0 = 1$$

$$i^1 = i$$

$$i^2 = -1$$

$$i^3 = -i$$

$$i^4 = 1$$

$$i^5 = i$$

$$i^6 = -1$$

$$i^7 = -i$$

$$i^8 = 1$$

⋮

$$i^n = i^{n \bmod 4}$$

The Euler formula from Taylor series

$$\cos \varphi = 1 - \frac{\varphi^2}{2!} + \frac{\varphi^4}{4!} - \frac{\varphi^6}{6!} + \dots$$

$$\sin \varphi = \varphi - \frac{\varphi^3}{3!} + \frac{\varphi^5}{5!} - \frac{\varphi^7}{7!} + \dots$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$$

$$e = 1 + \frac{1}{1!} + \frac{1}{2!} + \frac{1}{3!} + \dots = 2.71828\dots$$

$$e^{i\varphi} = 1 + i\varphi + \frac{(i\varphi)^2}{2!} + \frac{(i\varphi)^3}{3!} + \frac{(i\varphi)^4}{4!} + \dots$$

$$= 1 + i\varphi - \frac{\varphi^2}{2!} - i \frac{\varphi^3}{3!} + \frac{\varphi^4}{4!} + i \frac{\varphi^5}{5!} - \frac{\varphi^6}{6!} - i \frac{\varphi^7}{7!} + \dots$$

$$= 1 + i\varphi - \frac{\varphi^2}{2!} - i \frac{\varphi^3}{3!} + \frac{\varphi^4}{4!} + i \frac{\varphi^5}{5!} - \frac{\varphi^6}{6!} - i \frac{\varphi^7}{7!} + \dots$$

$$= \left(1 - \frac{\varphi^2}{2!} + \frac{\varphi^4}{4!} - \frac{\varphi^6}{6!} + \dots \right) + i \left(\varphi - \frac{\varphi^3}{3!} + \frac{\varphi^5}{5!} - \frac{\varphi^7}{7!} + \dots \right)$$

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

⋮

$$i^{-2} = -1$$

$$i^{-1} = -i$$

$$i^0 = 1$$

$$i^1 = i$$

$$i^2 = -1$$

$$i^3 = -i$$

$$i^4 = 1$$

$$i^5 = i$$

$$i^6 = -1$$

$$i^7 = -i$$

$$i^8 = 1$$

⋮

$$i^n = i^{n \bmod 4}$$

The Euler formula from ordinary differential equations and boundary conditions

$$y = e^{ix}$$

$$\begin{aligned}\frac{dy}{dx} &= ie^{ix} \\ &= iy\end{aligned}$$

$$\frac{dy}{dx} - iy = 0$$

$$y(0) = 1$$

$$z = \cos x + i \sin x$$

$$\begin{aligned}\frac{dz}{dx} &= -\sin x + i \cos x \\ &= i^2 \sin x + i \cos x \\ &= i(\cos x + i \sin x) \\ &= iz\end{aligned}$$

$$\frac{dz}{dx} - iz = 0$$

$$z(0) = 1$$

The functions $y = e^{ix}$ and $z = \cos x + i \sin x$ are both solutions of the same differential equation, and both have the same value at $x = 0$.

Therefore, $y(x) = z(x)$, that is, $e^{ix} = \cos x + i \sin x$.

Sum of angles trigonometric identities from the Euler formula

$$e^{i(x+y)} = e^{ix} e^{iy}$$

$$\begin{aligned}\cos(x+y) + i \sin(x+y) &= (\cos x + i \sin x)(\cos y + i \sin y) \\&= \cos x \cos y + i \cos x \sin y + i \sin x \cos y - \sin x \sin y \\&= (\cos x \cos y - \sin x \sin y) + i(\cos x \sin y + \sin x \cos y)\end{aligned}$$

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

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

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

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

$$\cos x \cos y = \frac{1}{2} [\cos(x+y) + \cos(x-y)], \quad \cos^2 x = \frac{1}{2} (\cos 2x + 1)$$

$$\sin x \sin y = \frac{1}{2} [\cos(x-y) - \cos(x+y)], \quad \sin^2 x = \frac{1}{2} (1 - \cos 2x)$$

$$\cos x \sin y = \frac{1}{2} [\sin(x+y) - \sin(x-y)]$$

$$\sin x \cos y = \frac{1}{2} [\sin(x+y) + \sin(x-y)]$$

Sine and Cosine Sum of Angles Formulae by Plane Geometry

$$\begin{cases} \cos(\alpha \pm \beta) = \cos \alpha \cos \beta \mp \sin \alpha \sin \beta \\ \sin(\alpha \pm \beta) = \sin \alpha \cos \beta \pm \cos \alpha \sin \beta \end{cases}$$

$PB \perp OB$, $PQ \perp OQ$, $QR \perp PB$; $\therefore QR \parallel OA$

$$\angle RPQ = \frac{\pi}{2} - \angle PQR = \frac{\pi}{2} - \left(\frac{\pi}{2} - \angle OQR \right) = \angle OQR = \alpha$$

$$OP = 1$$

$$OQ = \cos \beta$$

$$PQ = \sin \beta$$

$$\frac{OA}{OQ} = \cos \alpha, \quad \therefore OA = \cos \alpha \cos \beta$$

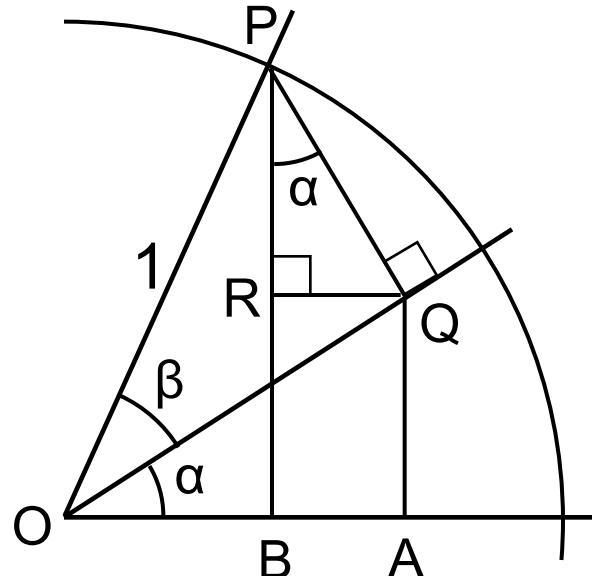
$$\frac{RQ}{PQ} = \sin \alpha, \quad \therefore RQ = \sin \alpha \sin \beta$$

$$\cos(\alpha + \beta) = OB = OA - BA = OA - RQ = \cos \alpha \cos \beta - \sin \alpha \sin \beta$$

$$\frac{AQ}{OQ} = \sin \alpha, \quad \therefore AQ = \sin \alpha \cos \beta$$

$$\frac{PR}{PQ} = \cos \alpha, \quad \therefore PR = \cos \alpha \sin \beta$$

$$\sin(\alpha + \beta) = PB = RB + PR = AQ + PR = \sin \alpha \cos \beta + \cos \alpha \sin \beta$$



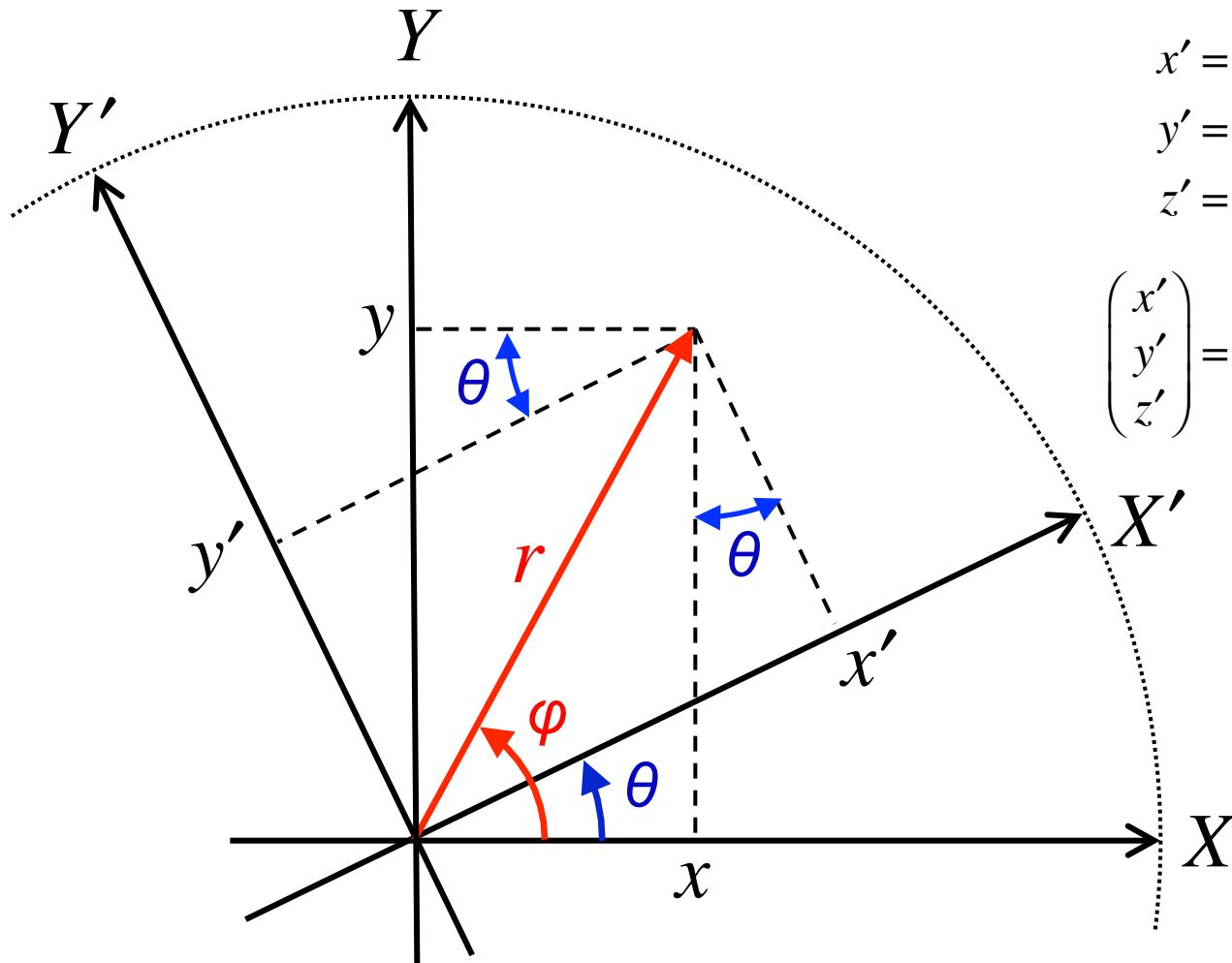
$$x = r \cos \theta$$

$$y = r \sin \theta$$

Rotation of Cartesian coordinate axes

$$x' = r \cos(\theta - \varphi) = r[\cos \theta \cos \varphi + \sin \theta \sin \varphi] = x \cos \varphi + y \sin \varphi$$

$$y' = r \sin(\theta - \varphi) = r[\sin \theta \cos \varphi - \cos \theta \sin \varphi] = y \cos \varphi - x \sin \varphi$$



$$x' = x \cos \varphi + y \sin \varphi$$

$$y' = -x \sin \varphi + y \cos \varphi$$

$$z' = z$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Rotation of a Cartesian vector

$$r^2 = x^2 + y^2 = x'^2 + y'^2$$

$$x = r \cos \alpha$$

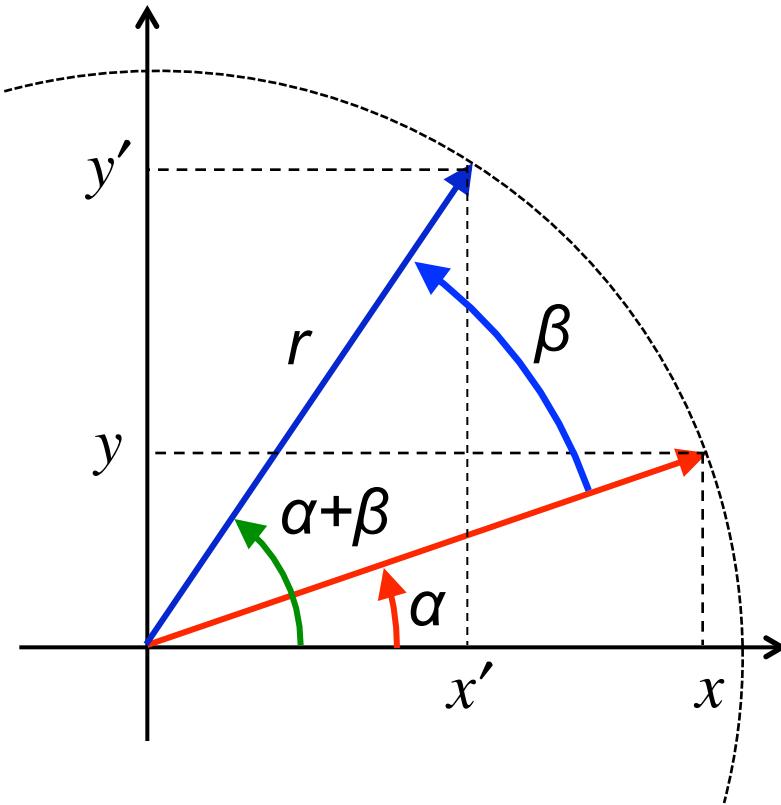
$$y = r \sin \alpha$$

$$x' = r \cos(\alpha + \beta) = r(\cos \alpha \cos \beta - \sin \alpha \sin \beta) = x \cos \beta - y \sin \beta$$

$$y' = r \sin(\alpha + \beta) = r(\sin \alpha \cos \beta + \cos \alpha \sin \beta) = y \cos \beta + x \sin \beta$$

$$z' = z$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos \beta & -\sin \beta & 0 \\ \sin \beta & \cos \beta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



Orthogonality of the sine and cosine functions

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

$$\int_{-\pi}^{+\pi} \cos(mx) \cos(nx) dx = \int_{-\pi}^{+\pi} \sin(mx) \sin(nx) dx = \pi \delta_{mn} = \begin{cases} 0 , & m \neq n \\ \pi , & m = n \end{cases}$$

$$\int_{-\pi}^{+\pi} \cos(mx) \sin(nx) dx = 0$$

Sine and cosine orthogonality integrals

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

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

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

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

$$\int_{-\pi}^{+\pi} \cos(mx) \cos(nx) dx = \frac{1}{2} \int_{-\pi}^{+\pi} [\cos((m+n)x) + \cos((m-n)x)] dx$$

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

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

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

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

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

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

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

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

Sine and Cosine Sum of Angles Formulae by Plane Geometry

$$\begin{cases} \cos(\alpha \pm \beta) = \cos \alpha \cos \beta \mp \sin \alpha \sin \beta \\ \sin(\alpha \pm \beta) = \sin \alpha \cos \beta \pm \cos \alpha \sin \beta \end{cases}$$

$PB \perp OB$, $PQ \perp OQ$, $QR \perp PB$; $\therefore QR \parallel OA$

$$\angle RPQ = \frac{\pi}{2} - \angle PQR = \frac{\pi}{2} - \left(\frac{\pi}{2} - \angle OQR \right) = \angle OQR = \alpha$$

$$OP = 1$$

$$OQ = \cos \beta$$

$$PQ = \sin \beta$$

$$\frac{OA}{OQ} = \cos \alpha, \therefore OA = \cos \alpha \cos \beta$$

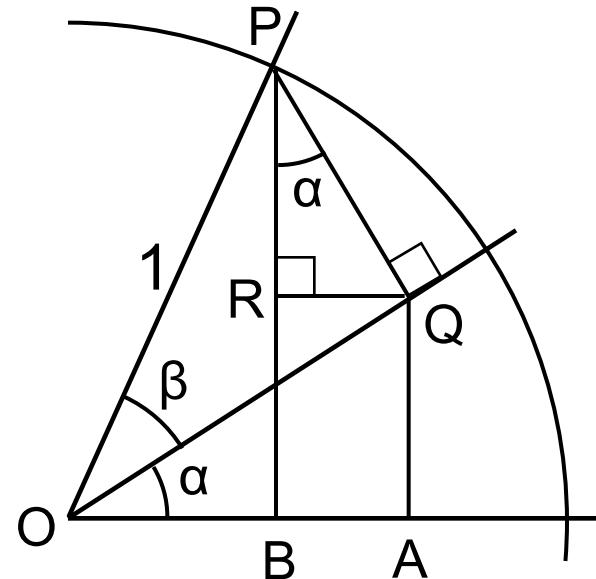
$$\frac{RQ}{PQ} = \sin \alpha, \therefore RQ = \sin \alpha \sin \beta$$

$$\cos(\alpha + \beta) = OB = OA - BA = OA - RQ = \cos \alpha \cos \beta - \sin \alpha \sin \beta$$

$$\frac{AQ}{OQ} = \sin \alpha, \therefore AQ = \sin \alpha \cos \beta$$

$$\frac{PR}{PQ} = \cos \alpha, \therefore PR = \cos \alpha \sin \beta$$

$$\sin(\alpha + \beta) = PB = RB + PR = AQ + PR = \sin \alpha \cos \beta + \cos \alpha \sin \beta$$



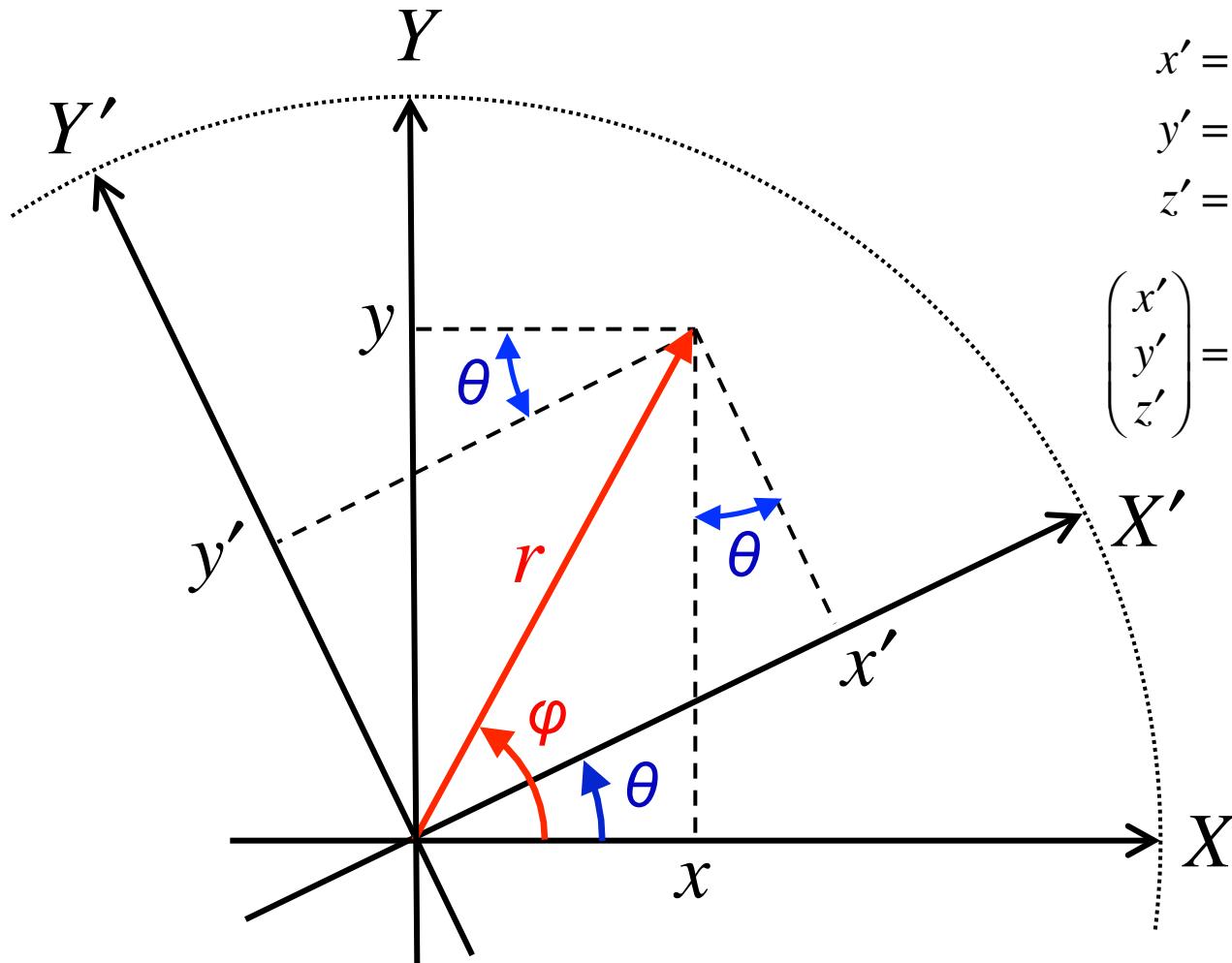
$$x = r \cos \theta$$

$$y = r \sin \theta$$

Rotation of Cartesian coordinate axes

$$x' = r \cos(\theta - \varphi) = r[\cos \theta \cos \varphi + \sin \theta \sin \varphi] = x \cos \varphi + y \sin \varphi$$

$$y' = r \sin(\theta - \varphi) = r[\sin \theta \cos \varphi - \cos \theta \sin \varphi] = y \cos \varphi - x \sin \varphi$$



$$x' = x \cos \varphi + y \sin \varphi$$

$$y' = -x \sin \varphi + y \cos \varphi$$

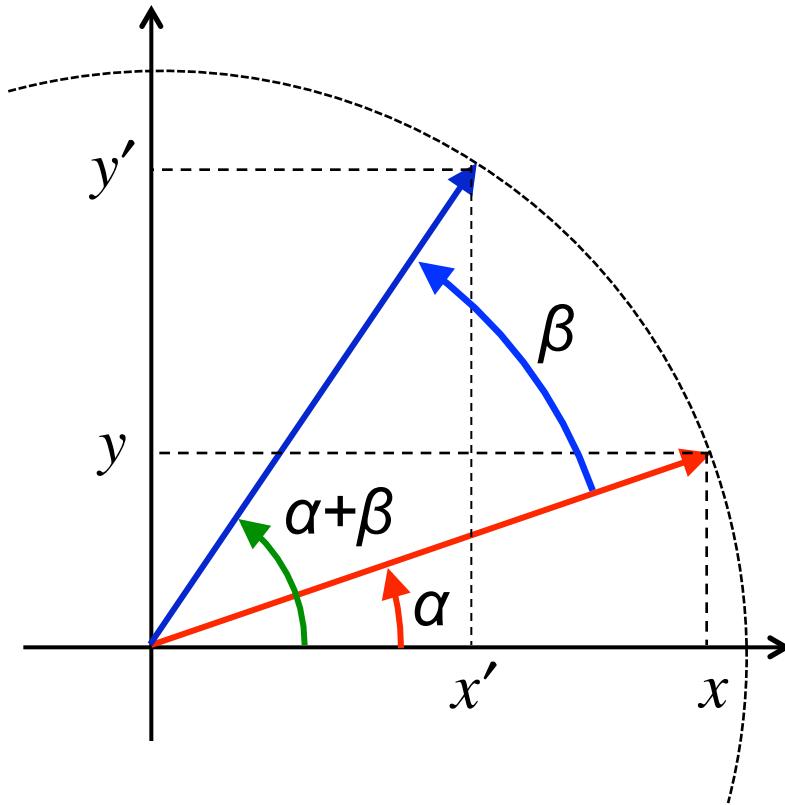
$$z' = z$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Rotation of a Cartesian vector

$$x = r \cos \alpha$$

$$y = r \sin \alpha$$

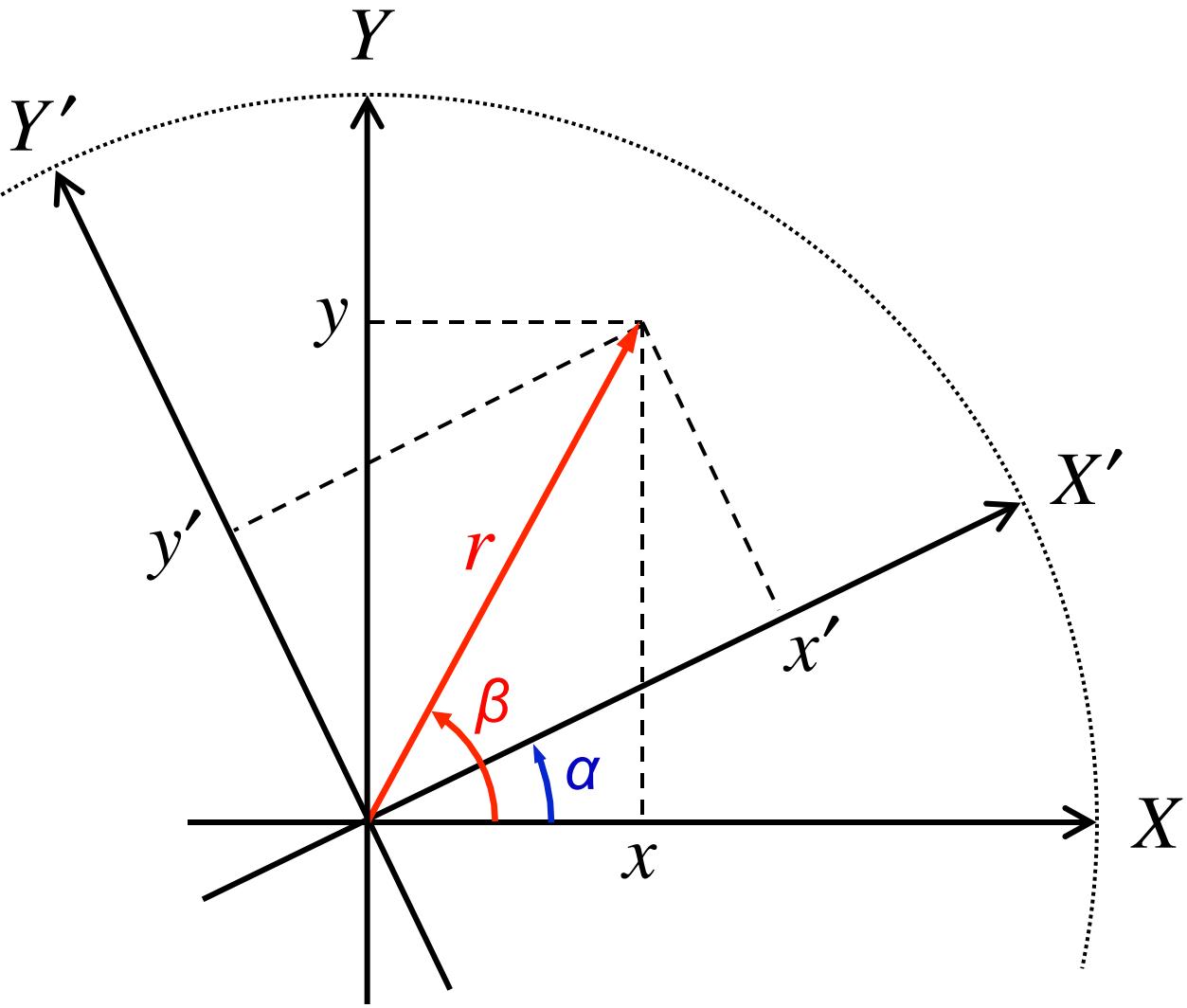


$$x' = r \cos(\alpha + \beta) = r(\cos \alpha \cos \beta - \sin \alpha \sin \beta) = x \cos \beta - y \sin \beta$$

$$y' = r \sin(\alpha + \beta) = r(\sin \alpha \cos \beta + \cos \alpha \sin \beta) = y \cos \beta + x \sin \beta$$

$$z' = z$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos \beta & -\sin \beta & 0 \\ \sin \beta & \cos \beta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



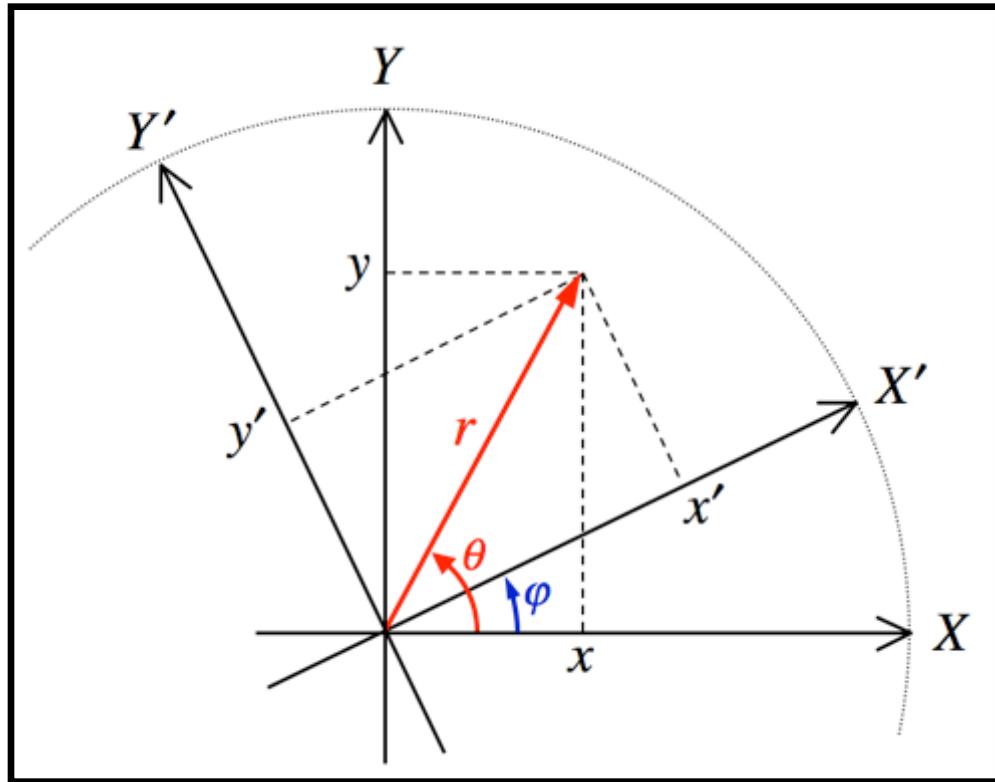
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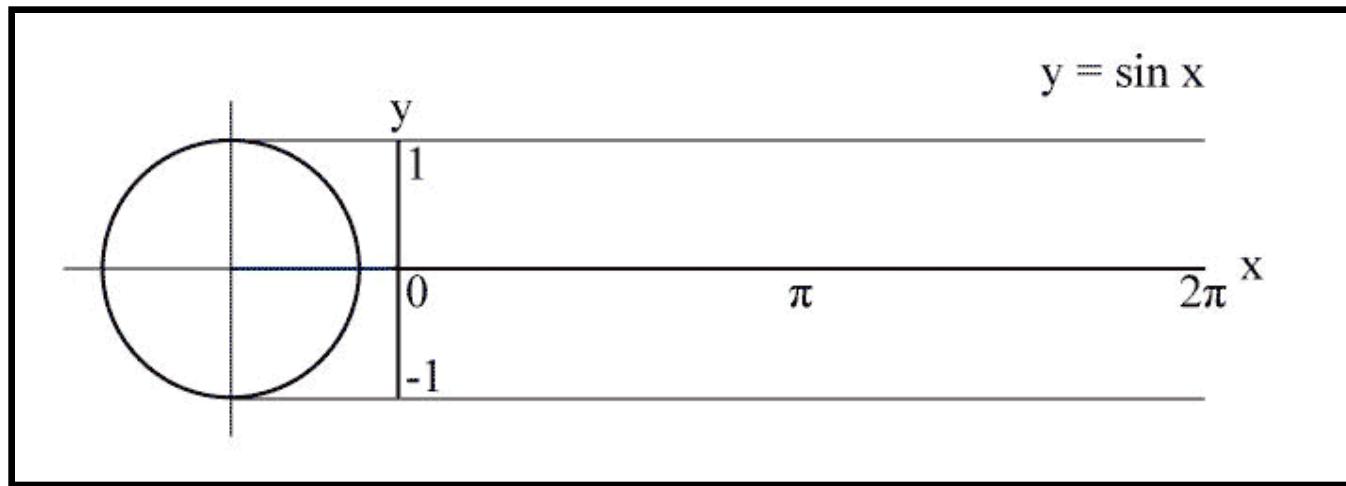
$$x' = x \cos \varphi + y \sin \varphi$$

$$y' = -x \sin \varphi + y \cos \varphi$$

$$z' = z$$

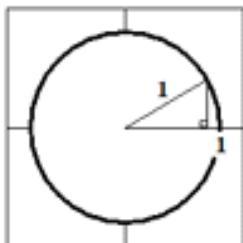
$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

The sine function on the unit circle



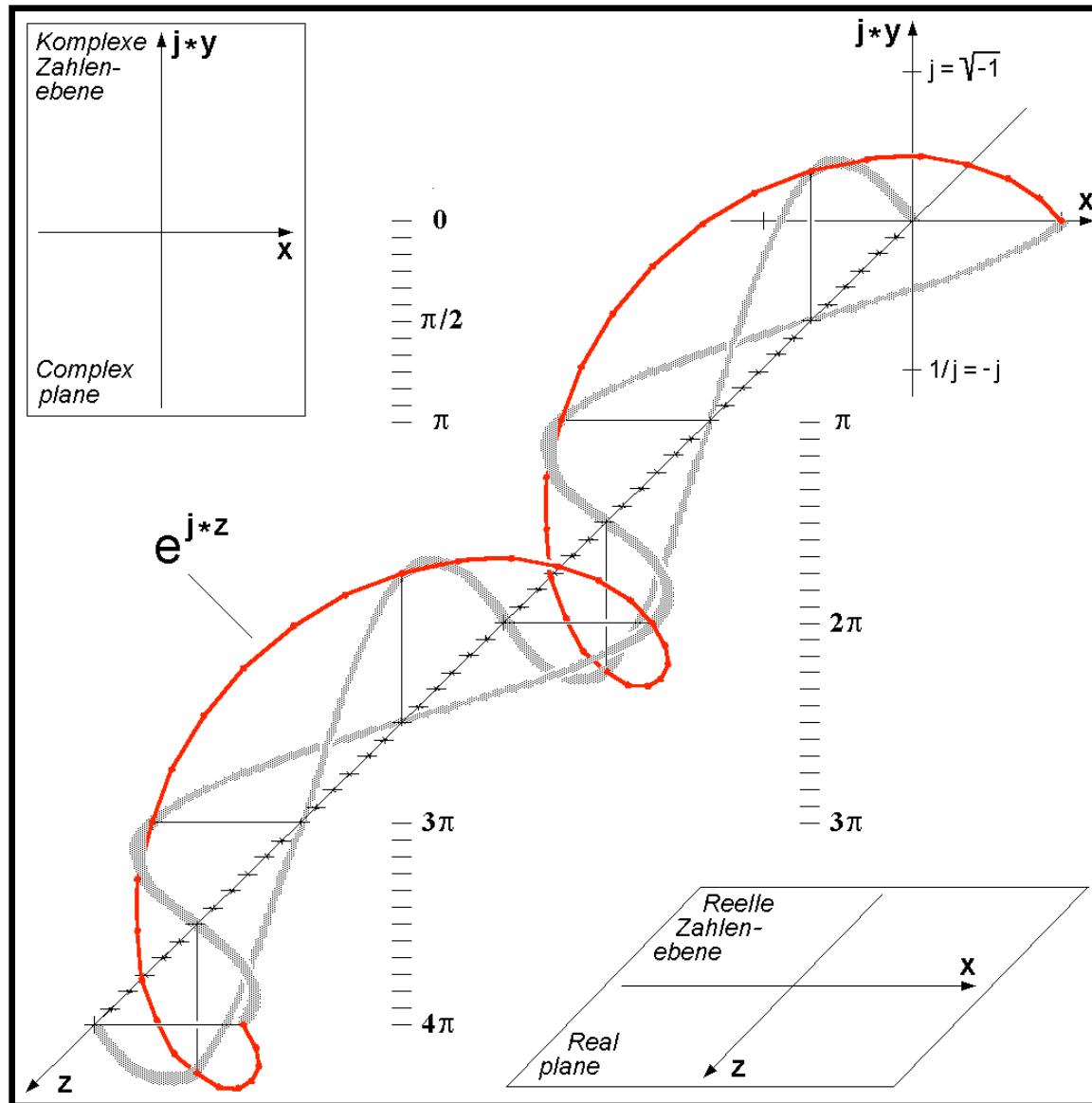
http://upload.wikimedia.org/wikipedia/commons/7/7d/Sin_drawing_process.gif

Relationships of the sine and cosine functions to the circle and helix



Unit Circle

The Euler Relationship in 3-D



Sine and Cosine Sum of Angles Formulae by Plane Geometry

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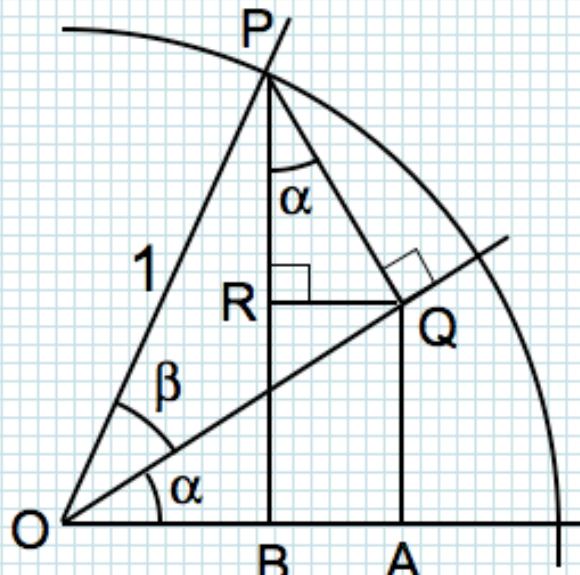
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$$\sin(\alpha + \beta) = PB = RB + PR = AQ + PR = \sin \alpha \cos \beta + \cos \alpha \sin \beta$$



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



Il ne reste plus que les coefficients 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

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

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

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

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

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

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'institut national." Nouveau Bulletin des sciences par la Société philomathique de Paris, N°. 6, Paris (Bernard), March 1808, pp. 112-116.

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

$$F_{hkl} \\ \rho(x,y,z)$$

$$F_{hkl} = |F_{hkl}| e^{i\varphi_{hkl}} \quad \begin{matrix} \xrightleftharpoons[\mathcal{F}^{-1}]{\mathcal{F}} & \rho(x,y,z) \end{matrix} \quad \left\{ \begin{array}{ll} \mathcal{F}[F_{hkl}] = \rho(x,y,z) & \text{Fourier synthesis} \\ \mathcal{F}^{-1}[\rho(x,y,z)] = F_{hkl} & \text{Fourier analysis} \end{array} \right.$$