

# Introduction to X-Ray Diffraction Physics

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These notes present, for structural biology and chemistry students who are beginning their study of crystallography, some basic principles of the physics that underlies X-ray diffraction.

Classical electromagnetic wave theory of X-ray scattering by electrons and atoms is described as background for studying X-ray diffraction analysis of the three-dimensional atomic architecture of molecules and crystals. Almost all mathematical steps are written out in explicit detail, and the topics treated include:

- Wave Properties
- Wave Superposition
- Wave Representation by Complex Exponentials
- Wave Energy
- Electromagnetic Waves
- X-Ray Scattering by a Free Electron
- X-Ray Scattering by a Bound Atomic Electron
- Dispersion Effects in X-ray Scattering
- Polarization Effects in X-ray Scattering
- Atomic Scattering Factors
- Dispersion Corrections to Atomic Scattering Factors
- Scattering Factor/Scattering Density Fourier Transform Relationships

## Wave Properties

By analogy with the surface ripples from a pebble tossed into a pond imagine, as illustrated below, a sinusoidal wave propagating from a source of harmonically oscillating disturbance in an isotropic, homogeneous medium. Near the source the wave is a spherical wave, but far from the source the curvature of the wave fronts, i.e., the surfaces of equal phase perpendicular to the direction of propagation, is negligible and the wave is a plane wave.

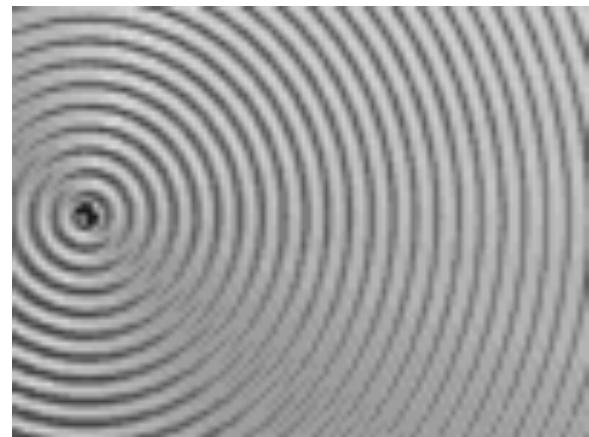
A wave is characterized by several properties:

<i>speed</i>	$c$	$(l \cdot t^{-1})$ ,	the speed of propagation;
<i>wavelength</i>	$\lambda$	$(l)$ ,	the distance crest-to-crest or trough-to-trough;
<i>wave number</i>	$\sigma = 1/\lambda$	$(l^{-1})$ ,	the number of wave cycles per unit distance;
<i>frequency</i>	$v = c/\lambda$	$(t^{-1})$ ,	the number of wave cycles per unit time;
<i>period</i>	$\tau = 1/v$	$(t)$ ,	the time per wave cycle;
<i>angular wave number</i>			
	$k = 2\pi/\lambda$	$[(rad) l^{-1}]$ ,	the number of phase angle cycles per unit distance;
<i>angular frequency</i>		$\omega = 2\pi v$	$[(rad) t^{-1}]$ , the number of phase angle cycles per unit time; and
<i>amplitude</i>	$\psi_0 = \psi_{\max}$ ,		the maximum wave displacement.

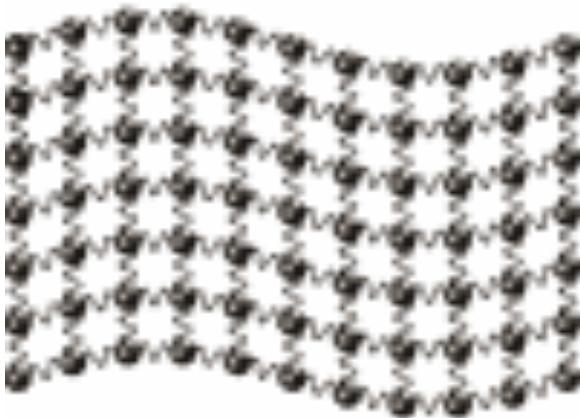
## Sinusoidal traveling wave illustrations



Water surface wave



Circular surface wave  
or cross-section of a spherical wave



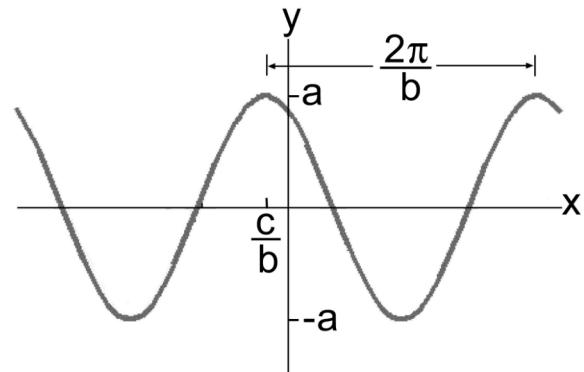
Transverse wave



Longitudinal wave

$$y = a \cos(bx - c) = a \cos\left[b\left(x - \frac{c}{b}\right)\right]$$

Amplitude	$a$
Frequency	$b$
Phase shift	$c$
Phase	$bx - c$
Wavelength	$2\pi/b$



Sinusoid function

Illustrations copied from Siltec (2004), *Computer animations of physical processes*. <http://physics.nad.ru/start.htm>

At an arbitrary point  $P$  along the path of a traveling sinusoidal plane wave, let a time zero be chosen when the wave displacement  $\psi$  at  $P$  equals the wave amplitude  $\psi_0$ . At a later time  $t$  the displacement at  $P$  will be  $\psi = \psi_0 \cos(\omega t)$ , while at a distance  $r$  further along the wave

path from  $P$  the displacement at time  $t$  will be  $\psi = \psi_0 \cos\left[\omega\left(t - \frac{r}{c}\right)\right]$ , because the wave

propagates at the finite speed  $c$  and therefore requires a time  $r/c$  to travel the distance  $r$ . In other words, the wave displacement at time  $t$  at a distance  $r$  along the wave path from a reference point  $P$  is equal to what the displacement was back at  $P$  at the *earlier* or retarded time  $t' = t - \frac{r}{c}$ .

The sinusoidally oscillating variation of the wave displacement with time and distance has various equivalent expressions in terms of the characteristic properties of the wave, viz.,

$$\begin{aligned}\psi &= \psi_0 \cos\left[\omega\left(t - \frac{r}{c}\right)\right] \\ &= \psi_0 \cos\left[2\pi v\left(t - \frac{r}{c}\right)\right] = \psi_0 \cos\left[2\pi\left(vt - \frac{r}{\lambda}\right)\right] = \psi_0 \cos\left[\frac{2\pi}{\lambda}(ct - r)\right] \\ &= \psi_0 \cos[2\pi(vt - \sigma r)] = \psi_0 \cos(\omega t - kr) = \psi_0 \cos(\omega t + \delta) = \psi_0 \cos\varphi.\end{aligned}$$

The cosine argument in these equations, expressed in any of its various equivalent forms,

$$\varphi = \omega t - \delta = \omega t - kr = 2\pi(vt - \sigma r) = \frac{2\pi}{\lambda}(ct - r) = 2\pi\left(vt - \frac{r}{\lambda}\right) = 2\pi v\left(t - \frac{r}{c}\right) = \omega\left(t - \frac{r}{c}\right),$$

(all of which are *dimensionless, as all arguments of the functions sin x, cos x, tan x, or exp x must be*) is called the *phase angle* or simply the *phase* of the wave at time  $t$  and distance  $r$ , and the distance or *path length* component of the phase,

$$\delta = kr = 2\pi\sigma r = 2\pi r/\lambda = 2\pi vr/c = \omega r/c,$$

is called the *phase shift..*

With respect to the phase  $\varphi = \omega t - kr$  at time  $t$  and distance  $r$  along the wave path, the phase

$$\varphi + \Delta\varphi = \omega t - k(r + \Delta r)$$

at time  $t$  at distance  $r + \Delta r$ , further along the wave path, is behind the phase at  $r$  by

$$\Delta\varphi = -k\Delta r = -2\pi\sigma\Delta r = -2\pi\Delta r/\lambda,$$

and the phase

$$\varphi + \Delta\varphi = \omega(t + \Delta t) - kr$$

at distance  $r$  at time  $t + \Delta t$ , after a time delay, is ahead of the phase at  $t$  by

$$\Delta\varphi = +\omega\Delta t = +2\pi v\Delta t = +2\pi c\Delta t/\lambda.$$

In general,

$$\Delta\varphi = \omega\Delta t - k\Delta r = 2\pi(v\Delta t - \sigma\Delta r) = 2\pi\left(v\Delta t - \frac{\Delta r}{\lambda}\right) = \frac{2\pi}{\lambda}(c\Delta t - \Delta r),$$

and a *time delay*  $\Delta t > 0$  produces a *phase advance*, while a *path length increase*  $\Delta r > 0$  produces a *phase lag*.

As can easily be seen by differentiation and substitution, a cosine wave,

$$\psi = \psi_0 \cos\left[\omega\left(t - \frac{x}{c}\right)\right],$$

is a solution of the one-dimensional *wave equation*,

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2},$$

which, in its generalized three-dimension form,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2},$$

governs all kinds of wave motion: transverse traveling waves, such as water surface waves and (as discussed below) light waves, with wave displacement oscillations perpendicular to the direction of wave propagation; longitudinal traveling waves, such as sound waves, with compression-rarefaction or contraction-expansion wave displacement oscillations parallel to the direction of wave propagation; and standing waves, which result from reflection and constructive interference of traveling waves, i.e., superposition of oppositely traveling waves, such as occurs with the transverse vibrations of a stretched string fixed at its end points or a stretched membrane fixed around its perimeter, or the longitudinal vibrations of a column of air in a tube.

## Wave Superposition

As shown in the following illustrations, wave superposition amounts to point-by-point addition of the displacements due to two or more component waves. Imagine two plane waves with the same frequency propagating with the same speed in the same direction but from different wave origins. Superposition of two such waves with the same frequency but different amplitudes and phase shifts gives a combined wave,

$$\psi_1 \cos(\omega t - \delta_1) + \psi_2 \cos(\omega t - \delta_2) = \psi_0 \cos(\omega t - \delta),$$

with the same frequency but a new amplitude and new phase shift. The phase difference between the two component waves,

$$\Delta\varphi = \varphi_2 - \varphi_1 = (\omega t - \delta_2) - (\omega t - \delta_1) = -(\delta_2 - \delta_1) = -2\pi\left(\frac{r_2 - r_1}{\lambda}\right) = -2\pi\frac{\Delta r}{\lambda},$$

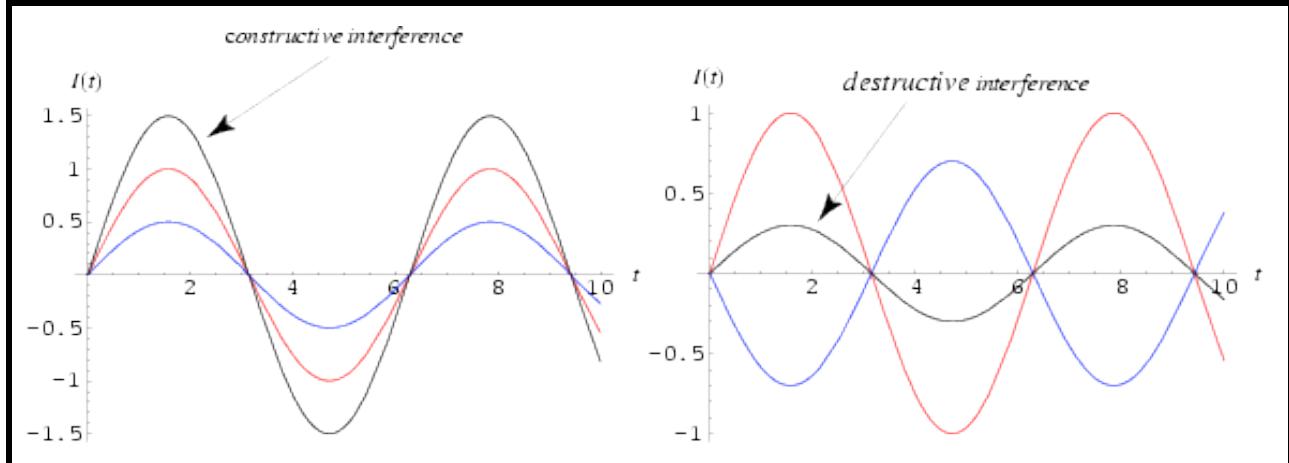
is due to the wave path length difference due to the separation between the two wave origins.

If the path lengths differ by  $|\Delta r| = n\lambda = 0, \lambda, 2\lambda, \dots$ , the phases differ by  $|\Delta\varphi| = 2n\pi = 0, 2\pi, 4\pi, \dots$ , and the waves are *in phase*: The waves superimpose crest on crest and trough on trough; and by *constructive interference* the waves strengthen one another to a larger amplitude  $\psi_0 = \psi_1 + \psi_2$ .

If, on the other hand,  $|\Delta r| = (n + \frac{1}{2})\lambda = \frac{1}{2}\lambda, \frac{3}{2}\lambda, \frac{5}{2}\lambda, \dots$ , so that  $|\Delta\varphi| = (2n + 1)\pi = \pi, 3\pi, 5\pi, \dots$ , then the waves are *out of phase*: The waves superimpose crest on trough; and by *destructive interference* the waves weaken one another to a smaller amplitude  $\psi_0 = |\psi_1 - \psi_2|$ . If in the latter case the two waves are of equal amplitude they annihilate one another.

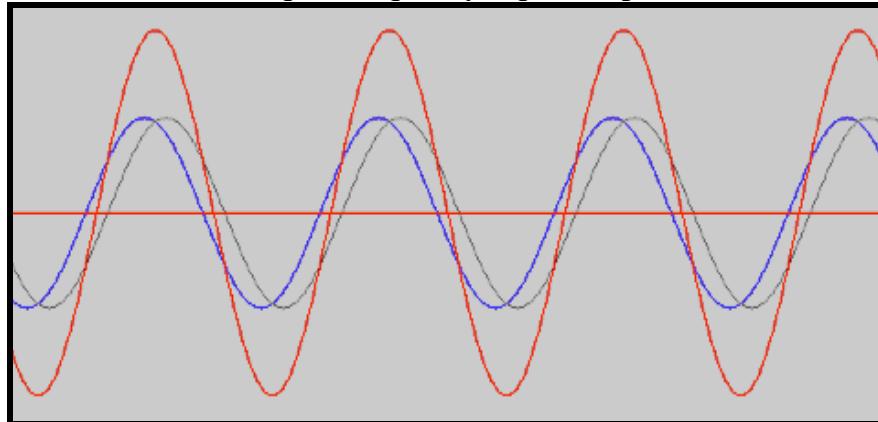
If the path length difference is neither an integral nor half-integral number of wavelengths, then: if  $|\Delta\varphi| = 2\pi|\Delta r|/\lambda < \pi/2$ , i.e.,  $|\Delta r| < \lambda/4$ , the wave interference will be constructive and produce a strengthened resultant wave with  $\psi_0 > \max(\psi_1, \psi_2)$ ; and if  $\pi/2 < |\Delta\varphi| < \pi$ , i.e.,  $\lambda/4 < |\Delta r| < \lambda/2$  the wave interference will be destructive and produce a weakened resultant wave with  $\psi_0 < \min(\psi_1, \psi_2)$ .

### Wave Superposition and Constructive and Destructive Interference

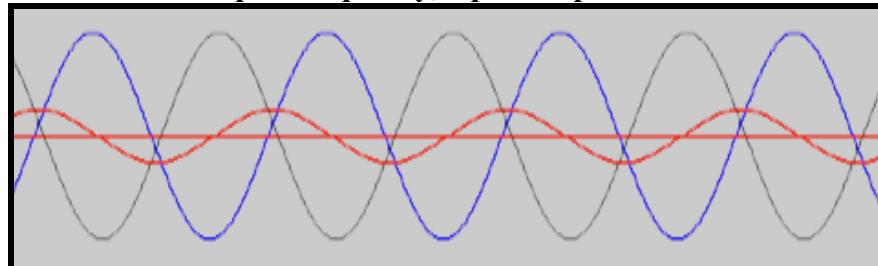


Figures copied from Weisstein (2006). <http://scienceworld.wolfram.com/physics/topics/InterferencePhenomena.html>

### Constructive interference of equal frequency, equal amplitude waves almost in phase



### Destructive interference of equal frequency, equal amplitude waves almost $\pi$ out of phase



Figures copied from Huang (2006). <http://www.phy.ntnu.edu.tw/ntnужava/viewtopic.php?t=35>

For the general case of a superposition of two waves of the same frequency but different phases,

$$\psi_1 \cos(\omega t - \delta_1) + \psi_2 \cos(\omega t - \delta_2) = \psi_0 \cos(\omega t - \delta),$$

the trigonometric identity,

$$\cos(x \pm y) = \cos x \cos y \mp \sin x \sin y,$$

can be used to rewrite the wave superposition as

$$\begin{aligned} \psi_1 \cos(\omega t - \delta_1) + \psi_2 \cos(\omega t - \delta_2) \\ = \psi_1 \cos(\omega t) \cos \delta_1 + \psi_1 \sin(\omega t) \sin \delta_1 + \psi_2 \cos(\omega t) \cos \delta_2 + \psi_2 \sin(\omega t) \sin \delta_2 \\ = (\psi_1 \cos \delta_1 + \psi_2 \cos \delta_2) \cos(\omega t) + (\psi_1 \sin \delta_1 + \psi_2 \sin \delta_2) \sin(\omega t). \end{aligned}$$

Similarly, for the resultant combined wave,

$$\begin{aligned} \psi_1 \cos(\omega t - \delta_1) + \psi_2 \cos(\omega t - \delta_2) \\ = \psi_0 \cos(\omega t - \delta) \\ = \psi_0 \cos(\omega t) \cos \delta + \psi_0 \sin(\omega t) \sin \delta. \end{aligned}$$

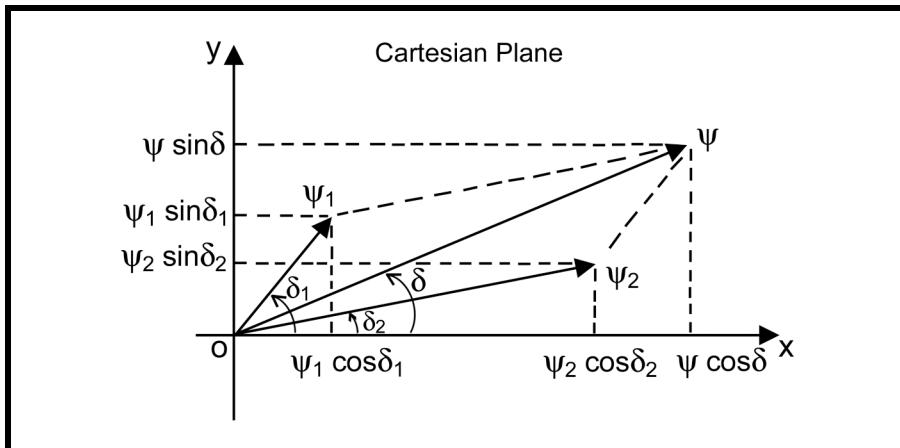
Then, equating the corresponding coefficients of  $\cos(\omega t)$  and  $\sin(\omega t)$  gives

$$\begin{cases} \psi_1 \cos \delta_1 + \psi_2 \cos \delta_2 = \psi_0 \cos \delta \\ \psi_1 \sin \delta_1 + \psi_2 \sin \delta_2 = \psi_0 \sin \delta. \end{cases}$$

This result shows that the wave superposition corresponds formally to a vector addition  $\vec{\psi}_1 + \vec{\psi}_2 = \vec{\psi}_0$ , where  $\psi_1 \cos \delta_1$  and  $\psi_1 \sin \delta_1$  correspond to, respectively, the  $x$ - and  $y$ -components of  $\vec{\psi}_1$ , and similarly for the components of  $\vec{\psi}_2$  and  $\vec{\psi}_0$ , as illustrated below.

Then, corresponding to the length  $|\vec{\psi}_0|$  and direction  $\delta$  of the resultant vector, the amplitude and phase shift of the combined wave resulting from the wave superposition are given by

$$\begin{cases} \psi_0 = \left[ (\psi_0 \cos \delta)^2 + (\psi_0 \sin \delta)^2 \right]^{1/2} = \left[ (\psi_1 \cos \delta_1 + \psi_2 \cos \delta_2)^2 + (\psi_1 \sin \delta_1 + \psi_2 \sin \delta_2)^2 \right]^{1/2} \\ \delta = \tan^{-1} \left( \frac{\psi_0 \sin \delta}{\psi_0 \cos \delta} \right) = \tan^{-1} \left( \frac{\psi_1 \sin \delta_1 + \psi_2 \sin \delta_2}{\psi_1 \cos \delta_1 + \psi_2 \cos \delta_2} \right). \end{cases}$$



In the obvious way, the results for two waves are readily generalized for  $n$  waves: The superposition of  $n$ -waves of the same frequency but different amplitudes and phases gives a combined wave with

$$\psi_0 \cos(\omega t - \delta) = \sum_{j=1}^n \psi_j \cos(\omega t - \delta_j),$$

where

$$\psi_0 = \left[ \left( \sum_{j=1}^n \psi_j \cos \delta_j \right)^2 + \left( \sum_{j=1}^n \psi_j \sin \delta_j \right)^2 \right]^{1/2} \quad \text{and} \quad \delta = \tan^{-1} \left( \frac{\sum_{j=1}^n \psi_j \sin \delta_j}{\sum_{j=1}^n \psi_j \cos \delta_j} \right).$$

## Wave Representation by Complex Exponential Functions

The Euler relationship,

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

which links the trigonometric functions and complex exponential functions via the formulae,

$$e^{ix} = \cos x + i \sin x \quad \cos x = (e^{ix} + e^{-ix})/2$$

$$e^{-ix} = \cos x - i \sin x \quad \sin x = (e^{ix} - e^{-ix})/2i,$$

provides a simpler way to carry out wave superposition via the alternative mathematical form for wave representation in terms of complex numbers, the properties of which are summarized in the following table and figure.

By the Euler relationship, the cosine superposition

$$\psi_0 \cos(\omega t - \delta) = \sum_{j=1}^n \psi_j \cos(\omega t - \delta_j)$$

is the real part of a complex exponential superposition

$$\psi_0 \exp[i(\omega t - \delta)] = \sum_{j=1}^n \psi_j \exp[i(\omega t - \delta_j)],$$

which, since  $a^{x+y} = a^x a^y$ , reduces to

$$\psi_0 e^{i\omega t} e^{-i\delta} = \sum_{j=1}^n \psi_j e^{i\omega t} e^{-i\delta_j}$$

$$\psi_0 e^{-i\delta} = \sum_{j=1}^n \psi_j e^{-i\delta_j}.$$

Then, by equating real (cosine) and imaginary (sine) parts, the complex exponential superposition straightforwardly gives the key result

$$\begin{cases} \psi_0 \cos \delta = \sum_{j=1}^n \psi_j \cos \delta_j \\ \psi_0 \sin \delta = \sum_{j=1}^n \psi_j \sin \delta_j, \end{cases}$$

which in turn yields real values  $\psi_0$  and  $\delta$  from the complex exponential superposition.

## Complex Numbers

imaginary unit, $i$	$i^2 = -1, \quad i^{-1} = -i, \quad i(-i) = -i^2 = 1$
complex numbers	
Cartesian form	$\begin{cases} z = x + iy \\ =  z  e^{i\varphi} \\ =  z (\cos \varphi + i \sin \varphi) \end{cases}$
polar form	
trigonometric form	
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  $z \rightarrow z^* \Leftrightarrow i \rightarrow -i$

complex conjugate

Cartesian form	$\begin{cases} z^* = x - iy \\ =  z  e^{-i\varphi} \\ =  z (\cos \varphi - i \sin \varphi) \end{cases}$
polar form	
trigonometric form	

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 
$$\begin{aligned} z_1 z_2 &= (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + x_2 y_1) \\ &= |z_1| |z_2| \exp[i(\varphi_1 + \varphi_2)] \end{aligned}$$

division 
$$\begin{aligned} \frac{z_1}{z_2} &= \frac{x_1 + iy_1}{x_2 + iy_2} = \frac{z_1 z_2^*}{z_2 z_2^*} = \frac{(x_1 + iy_1)(x_2 - iy_2)}{x_2^2 + y_2^2} \\ &= \frac{|z_1|}{|z_2|} \exp[i(\varphi_1 - \varphi_2)] \end{aligned}$$

**The Euler Relationship, "Euler's Jewel"**

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

**The Euler Identity, "The most beautiful equation in the world"**

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

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

### Complex numbers on the Argand or complex plane

$$z = x + iy = |z| e^{i\varphi} = |z|(\cos \varphi + i \sin \varphi), \quad |z| = \sqrt{x^2 + y^2}, \quad \varphi = \tan^{-1}(y/x)$$

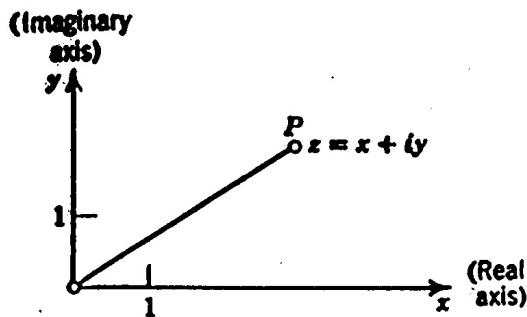


Fig. 15. The complex plane.

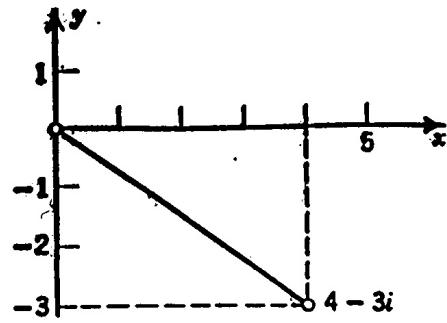


Fig. 16. The number  $4 - 3i$  in the complex plane.

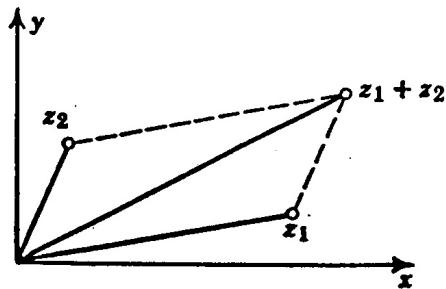


Fig. 17. Addition of complex numbers.

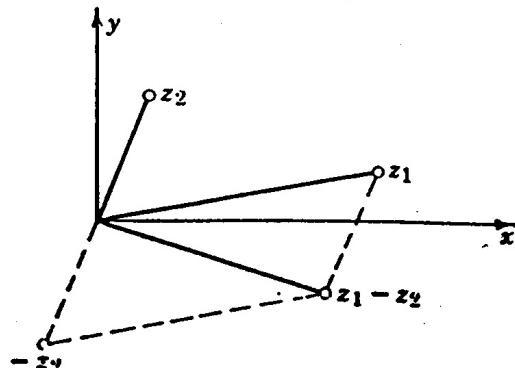


Fig. 18. Subtraction of complex numbers.

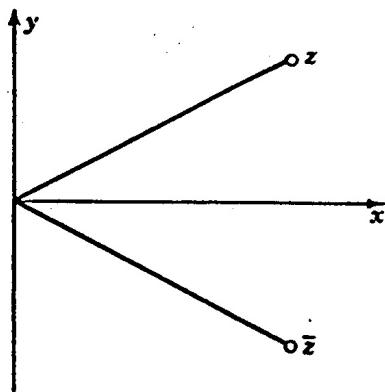


Fig. 19. Conjugate complex numbers.

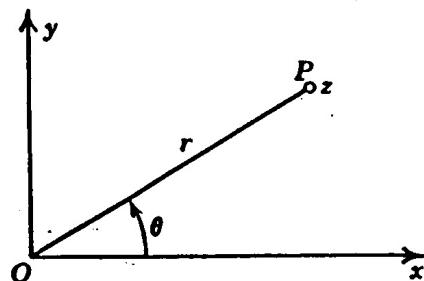


Fig. 20. Trigonometric form of complex numbers.

In much of physics, especially in all the physics of oscillatory phenomena, mathematical analysis in terms of complex variables is often the most convenient theoretical formalism. Recall that a complex variable,

$$z = x + iy = |z| e^{i\varphi} = |z|(\cos \varphi + i \sin \varphi),$$

has real and imaginary parts

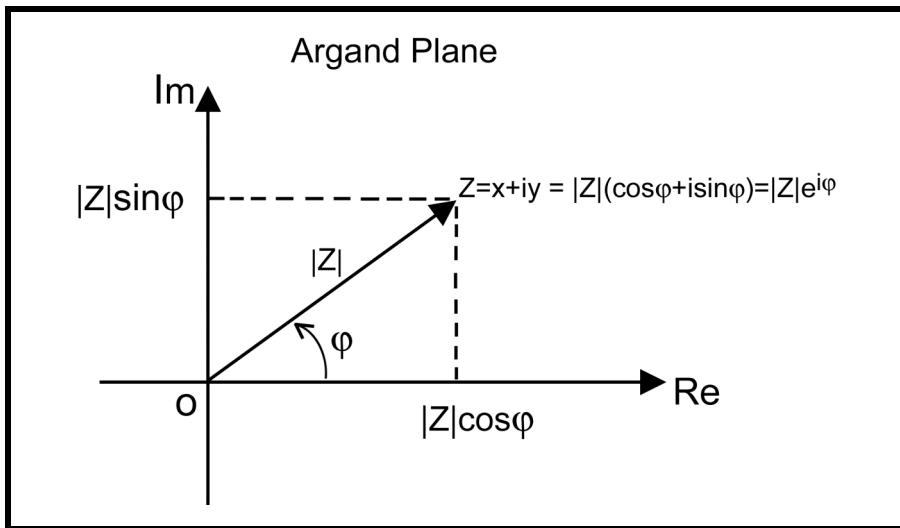
$$\operatorname{Re}(z) = x = |z| \cos \varphi \quad \text{and} \quad \operatorname{Im}(z) = y = |z| \sin \varphi ,$$

and it has magnitude or modulus,

$$|z| = \sqrt{|z|^2} = \sqrt{zz^*} = \left[ (x+iy)(x-iy) \right]^{1/2} = \sqrt{x^2+y^2} ,$$

and phase,

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



For wave phase differences as discussed above, a phase change  $\Delta\varphi$  multiplies the complex exponential representation of a wave by the quantity  $e^{i\Delta\varphi}$ , and rotates the vector representation in the Argand or complex plane by the angle  $\Delta\varphi$ . That is, given

$$z = |z| e^{i\varphi} = |z|(\cos \varphi + i \sin \varphi),$$

a phase change  $\Delta\varphi$  gives

$$z' = z e^{i\Delta\varphi} = |z| e^{i\varphi} e^{i\Delta\varphi} = |z| e^{i(\varphi + \Delta\varphi)} = |z| [\cos(\varphi + \Delta\varphi) + i \sin(\varphi + \Delta\varphi)].$$

Note that an experimentally observable, physically measurable quantity cannot be complex-valued. Any observable, measurable quantity must be real-valued; however, it might be represented mathematically by the real part, or the magnitude or squared magnitude, or the phase of a complex variable.

## Wave Energy

A wave transmits the energy expended in creating or sustaining the disturbance that is the source of the wave. For example, the ripples from a pebble tossed into a pond carry away the kinetic energy lost by the pebble upon impact with the water surface.

If a wave propagates in an elastic material medium in which each volume element of mass  $m$  executes simple harmonic motion, the equation of motion is

$$ma = F = -kx$$

$$ma + kx = 0$$

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0,$$

where  $a$  is the acceleration imparted by the elastic restoring force,  $k$  is the elastic force constant, and  $x$  is the oscillating displacement. [Above, the symbol  $k$  denoted wave number ( $k = 2\pi/\lambda$ ), but here it denotes the force constant ( $k = -F/x$ ).]

The differential equation of simple harmonic motion has a solution for the oscillating displacement,

$$x = x_0 e^{i(\omega t - \delta)} \quad \left( x = x_0 [\cos(\omega t - \delta) + i \sin(\omega t - \delta)] \right),$$

and differentiation gives the oscillating velocity and acceleration,

$$v = \frac{dx}{dt} = i\omega x_0 e^{i(\omega t - \delta)} = i\omega x \quad \left( v = i\omega x_0 [\cos(\omega t - \delta) + i \sin(\omega t - \delta)] \right. \\ \left. = -\omega x_0 [\sin(\omega t - \delta) - i \cos(\omega t - \delta)] \right),$$

$$a = \frac{dv}{dx} = \frac{d^2x}{dt^2} = -\omega^2 x_0 e^{i(\omega t - \delta)} = -\omega^2 x \quad \left( a = -\omega^2 x_0 [\cos(\omega t - \delta) + i \sin(\omega t - \delta)] \right).$$

[In parentheses to the right of the complex exponential equations, the equivalent complex trigonometric equations are given. Physical values for the oscillating displacement, velocity, and acceleration are given by the real parts of the complex expressions, viz.,  $\text{Re}(x) = x_0 \cos(\omega t - \delta)$ ,  $\text{Re}(v) = -\omega x_0 \sin(\omega t - \delta)$ , and  $\text{Re}(a) = -\omega^2 x_0 \cos(\omega t - \delta)$ , respectively.]

Substitution of  $a = -\omega^2 x$  into the equation of motion gives the relationship between the elastic force constant and the natural oscillation frequency,

$$-\omega^2 x + \frac{k}{m}x = 0 \\ k = m\omega^2.$$

By the chain rule,  $\frac{dy}{dx} = \frac{dy}{du} \frac{du}{dx}$ , the acceleration can also be written as

$$a = \frac{dv}{dt} = \frac{dv}{dx} \frac{dx}{dt} = v \frac{dv}{dx}.$$

Then the equation of motion can be rewritten as

$$mv \frac{dv}{dx} + kx = 0,$$

and integration gives

$$\int mv dv + \int kx dx = C$$

$$\frac{1}{2}mv^2 + \frac{1}{2}kx^2 = C.$$

The latter result expresses the conservation of the constant total energy equal to the sum of the kinetic energy  $T = \frac{1}{2}mv^2$  and potential energy  $V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$  of the oscillating mass  $m$ .

In terms of the constants of the oscillatory motion, the constant total energy is given by

$$U = T + V$$

$$= \frac{1}{2}mv^2 + \frac{1}{2}m\omega^2x^2$$

$$= \frac{1}{2}m[-\omega x_0 \sin(\omega t - \delta)]^2 + \frac{1}{2}m\omega^2[x_0 \cos(\omega t - \delta)]^2$$

$$= \frac{1}{2}m\omega^2x_0^2[\sin^2(\omega t - \delta) + \cos^2(\omega t - \delta)]$$

$$U = \frac{1}{2}m\omega^2x_0^2.$$

(Note that, here, the real parts of the complex trigonometric expressions for  $v$  and  $x$  were substituted because  $U$ ,  $T$ , and  $V$  must be real-valued.)

Thus, the total energy in the wave is proportional to the squared amplitude of the oscillating displacement, and in each wave cycle the total energy oscillates between potential energy and kinetic energy: The potential energy is maximum and the kinetic energy is zero at the extremes of the oscillating displacement, and the kinetic energy is maximum and the potential energy is zero at the points of zero displacement.

As in the simple harmonic oscillator example, it is true *in general* that the energy in a wave is proportional to the square of the wave amplitude,

$$U \propto \psi_0^2.$$

The energy transmitted per unit time per unit area  $S$  of wave front, i.e., the power  $P$  per unit area, is called the *intensity*,

$$I = (U/t)/S = P/S.$$

The intensity is therefore, like the energy, proportional to the square of the wave amplitude,

$$I \propto \psi_0^2.$$

Since the area of a spherical wave front is  $S = 4\pi r^2$ , the intensity of a spherical wave is, by the principle of energy conservation, proportional to the inverse square of the wave path length,

$$I \propto 1/r^2.$$

It follows that the amplitude of a spherical wave is proportional to the inverse path length,

$$\psi_0 \propto 1/r.$$

## Electromagnetic Waves

By the mid 19<sup>th</sup> century, optical studies of reflection, refraction, interference, and diffraction phenomena had shown that light manifests wave behavior, and that the various colors of visible light differ by wavelength. In the late 19<sup>th</sup> century, the theory of electrodynamics based on the electric and magnetic field equations discovered by James Clerk Maxwell (1831-1879) provided not only a unified explanation of the phenomena of electricity and magnetism but also the insight that light is an electromagnetic wave phenomenon.

Electrodynamical theory shows that while a static charge creates an electric field, and a moving charge creates also a magnetic field, an accelerated charge radiates electromagnetic energy. Acceleration of a charge produces a ripple in its electric and magnetic fields that propagates in all directions. The rippling change in the electric field produces a rippling change in the magnetic field and *vice versa*, and the propagating ripple radiates the energy expended to produce the force that produced the charge acceleration. Electromagnetic radiation from accelerated charges was found to propagate with the speed of light, and visible light with wavelengths of  $\sim 400$  nm (violet) to  $\sim 700$  nm (red) was shown to form part of the electromagnetic spectrum, which extends in a continuum from  $\gamma$ -rays with wavelengths of 1 pm or less, produced by nuclear disintegrations, to radio waves with wavelengths of 1 km or more, produced by oscillating electric circuits. Across the whole electromagnetic spectrum, the only light sources in the universe are accelerated electrical charges.

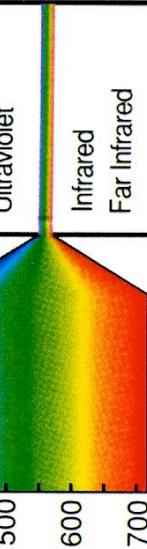
The formulation of classical electrodynamics based on the Maxwell electromagnetic field equations was the greatest theoretical synthesis in physics since the formulation of mechanics based on the laws of motion discovered by Isaac Newton (1642-1727). In the same way that Newton's equations unified the laws of celestial and terrestrial motions, Maxwell's equations unified all the empirical Coulomb, Gauss, Ampere, and Faraday laws of electricity and magnetism and – by revealing that light is a wave propagation of electric and magnetic field oscillations – all the empirical reflection, refraction, interference, diffraction, and polarization laws of visible light optics. The electromagnetic theory showed that, in SI mks units, the electric permittivity  $\epsilon_0$  and magnetic permeability  $\mu_0$  of free space, which had been derived from electrical measurements, and the speed of light  $c$  in free space, which had been derived from astronomical and optical measurements, were related by  $\epsilon_0 \mu_0 c^2 = 1$ . The remarkable result

$c = 1/\sqrt{\epsilon_0 \mu_0}$  prompted Maxwell's statement: "This velocity is so nearly that of light that it seems we have strong reason to conclude that light itself... is an electromagnetic disturbance in the form of waves propagating through the electromagnetic field according to electromagnetic laws."

Even in its limitations, the classical theory of electrodynamics is historic: In the early 20<sup>th</sup> century, the inability of the classical theory to account for the frame-of-reference invariance of the speed of light, the blackbody radiation spectrum, the photoelectric effect, and atomic line spectra stimulated development of the modern theories of relativity and quantum mechanics, which revealed the equivalence of matter and energy, the particle nature of electromagnetic energy, and the wave nature of matter.

# THE ELECTROMAGNETIC SPECTRUM

Frequency $\nu$ (Hz)	Wavelength $\lambda = c/\nu$ (m)	Type of Radiation	Typical Process	Energy (eV)	Wavenumber $\bar{\nu} = 1/\lambda$ (cm <sup>-1</sup> )
$10^{21}$	$10^{-13}$ (1 X-unit)		$\gamma$ -Rays	$(1 \text{ MeV})10^6$	$10^{11}$
$10^{18}$ (1 EHz)	$10^{-10}$ (1 Å) $10^{-9}$ (1 nm)	$\lambda$ (nm)	X-Rays	$(1 \text{ keV})10^3$	$10^8$
$10^{15}$ (1 PHz)	$10^{-6}$ (1 μm)	400	Vacuum Ultraviolet	$10^5$	
$10^{12}$ (1 THz)	$10^{-3}$ (1 mm) $10^{-2}$ (1 cm)	500	Ultraviolet	$10^4$	
$10^9$ (1 GHz)	$10^{-2}$ (1 km)	600	Infrared	$10^2$	
$10^6$ (1 MHz)	1	700	Far Infrared		
$10^3$ (1 kHz)			Microwaves		
			Radiowaves		
			Nuclear Spin Transition (NMR)	$(1 \mu\text{eV})10^{-6}$	$10^{-3}$
				$(1 \text{ neV})10^{-9}$	$10^{-6}$
				$(1 \text{ peV})10^{-12}$	$10^{-9}$



$1 \text{ eV} = 1.602177 \times 10^{-19} \text{ J}$ ;  $\hbar = 6.626075 \times 10^{-34} \text{ J}\cdot\text{s}$  (Planck Constant);  $c = 2.997925 \times 10^8 \text{ m}\cdot\text{s}^{-1}$  (light velocity)  
 $1 \text{ Å} = 10^{-10} \text{ m} = 10^{-8} \text{ cm} = 2.997925 \times 10^{18} \text{ s}^{-1}$  (light frequency)  $\sim 1.239852 \times 10^4 \text{ eV}$  (energy of light quantum)

**The Maxwell equations.** The Maxwell equations are a set of four vector differential equations that interrelate electric and magnetic fields in space and time. In SI mks units, the Maxwell equations in free space, (and the laws of electricity and magnetism that they subsume) are:

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon_0}, \quad (\text{Gauss's law for electric fields})$$

$$\vec{\nabla} \cdot \vec{B} = 0, \quad (\text{Gauss's law for magnetic fields})$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad (\text{Faraday's law of induction})$$

$$\vec{\nabla} \times \vec{B} = \mu_0 \vec{J} + \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}, \quad (\text{Ampere's law for constant current plus Maxwell's extension for varying current})$$

where  $\vec{E} = \vec{E}(x, y, z, t)$  and  $\vec{B} = \vec{B}(x, y, z, t)$  are, respectively, the electric and magnetic fields;

$\vec{\nabla} = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}$  is the vector differential operator called “del”;  $\rho$  is charge density

(charge per unit volume) and  $\vec{J}$  is current density (current per unit area of surface, or charge per unit time per unit area); and  $\epsilon_0 = 8.85 \times 10^{-12} \text{ C}^2 \cdot \text{N}^{-1} \cdot \text{m}^{-2}$  and  $\mu_0 = 4\pi \times 10^{-7} \text{ C}^{-2} \cdot \text{N} \cdot \text{s}^2$  are, respectively, the electric permittivity and magnetic permeability of free space.

The del operator has the properties:

$$\vec{\nabla} \varphi = \text{grad } \varphi = \hat{i} \frac{\partial \varphi}{\partial x} + \hat{j} \frac{\partial \varphi}{\partial y} + \hat{k} \frac{\partial \varphi}{\partial z},$$

$$\vec{\nabla} \cdot \vec{A} = \text{div } \vec{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z},$$

$$\vec{\nabla} \times \vec{A} = \text{curl } \vec{A} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} = \hat{i} \left( \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) + \hat{j} \left( \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) + \hat{k} \left( \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right),$$

where  $\varphi$  is any scalar quantity and  $\vec{A} = \hat{i}A_x + \hat{j}A_y + \hat{k}A_z$  is any vector quantity. The vector operators  $\vec{\nabla}$ ,  $\vec{\nabla} \cdot$ , and  $\vec{\nabla} \times$  are called, respectively, the gradient, divergence, and curl operators. The scalar “del square” operator,

$$\nabla^2 = \vec{\nabla} \cdot \vec{\nabla} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2},$$

is called the Laplacian operator.

The four Maxwell equations state that:

- Electric charges produce electric fields.
- Magnetic monopoles do not exist.
- Time varying magnetic fields produce electric fields.
- Time varying electric fields and electric currents produce magnetic fields.

**Electromagnetic Waves.** In a region of free space far from any charges or currents, where  $\rho = 0$  and  $\vec{J} = 0$ , Maxwell's equations reduce to

$$\begin{aligned}\vec{\nabla} \cdot \vec{E} &= 0, \\ \vec{\nabla} \cdot \vec{B} &= 0, \\ \vec{\nabla} \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t}, \\ \vec{\nabla} \times \vec{B} &= \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}.\end{aligned}$$

By application of the  $ABC = BAC - CAB$  identity for a vector triple product,

$$\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B}),$$

the curl operation on the third Maxwell equation gives

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = \vec{\nabla}(\vec{\nabla} \cdot \vec{E}) - (\vec{\nabla} \cdot \vec{\nabla})\vec{E} = \vec{\nabla}(\vec{\nabla} \cdot \vec{E}) - \nabla^2 \vec{E} = -\frac{\partial}{\partial t}(\vec{\nabla} \times \vec{B}),$$

which, with substitution of the first and fourth equations, gives

$$\nabla^2 \vec{E} = \epsilon_0 \mu_0 \frac{\partial^2 \vec{E}}{\partial t^2}.$$

Analogously, the curl operation on the fourth Maxwell equation leads to

$$\nabla^2 \vec{B} = \epsilon_0 \mu_0 \frac{\partial^2 \vec{B}}{\partial t^2}.$$

Thus, the Maxwell equations lead to a pair of equations with the form of wave equations,

$$\nabla^2 \psi = \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2},$$

for travelling waves of coupled electric and magnetic fields in free space, far from the charges or currents that are the source of the fields. The electromagnetic waves propagate with speed  $c = (\epsilon_0 \mu_0)^{-1/2}$ , the result that inspired Maxwell's assertion that light is an electromagnetic wave phenomenon.

In the Gaussian cgs system of units (in which  $\epsilon_0 = \mu_0 = 1$  and which, except where it is specifically stated otherwise, are used hereafter throughout these notes) the Maxwell equations in free space have an even more symmetrical appearance,

$$\begin{aligned}\vec{\nabla} \cdot \vec{E} &= 4\pi\rho, \\ \vec{\nabla} \cdot \vec{B} &= 0, \\ \vec{\nabla} \times \vec{E} &= -\frac{1}{c} \frac{\partial \vec{B}}{\partial t}, \\ \vec{\nabla} \times \vec{B} &= \frac{1}{c} \frac{\partial \vec{E}}{\partial t} + \frac{4\pi}{c} \vec{J},\end{aligned}$$

As can be easily verified by differentiation and substitution, the wave equations of the Maxwell electromagnetic field in free space with  $\rho = 0$  and  $\vec{J} = 0$  have a solution,

$$\begin{cases} E_x = a_0 \cos\left[\frac{2\pi}{\lambda}(ct - z)\right], & E_y = 0, & E_z = 0, \\ B_x = 0, & B_y = a_0 \cos\left[\frac{2\pi}{\lambda}(ct - z)\right], & B_z = 0, \end{cases}$$

which represents ( $x$  and  $y$ ) transverse, ( $z$ ) traveling, sinusoidal, plane waves of oscillating electric and magnetic fields. The field oscillations propagate with velocity  $c$ ; in Gaussian cgs units, they have equal amplitudes  $E_0 = B_0 = a_0$ ; they are in phase; and they are mutually perpendicular to one another and to the direction of wave propagation, as shown in the following illustrations.

The Maxwell equations in free space with  $\rho = 0$  and  $\vec{J} = 0$  also have a second solution,

$$\begin{cases} E_x = 0, & E_y = b_0 \cos\left[\frac{2\pi}{\lambda}(ct - z)\right], & E_z = 0, \\ B_x = b_0 \cos\left[\frac{2\pi}{\lambda}(ct - z)\right], & B_y = 0, & B_z = 0. \end{cases}$$

Both solutions represent monochromatic, linearly-polarized, electromagnetic plane waves propagating in the  $z$  direction, but the two solutions differ with respect to the direction of polarization of the electromagnetic wave, which is conventionally taken to be the direction of the electric field oscillations. Thus the first wave is  $x$ - and the second is  $y$ -polarized. A  $z$ -traveling wave with an arbitrary direction of polarization can always be resolved into perpendicular  $x$ - and  $y$ -polarization components.

It can be shown from the Maxwell equations that the instantaneous rate of energy transfer by an electromagnetic wave in free space is given by

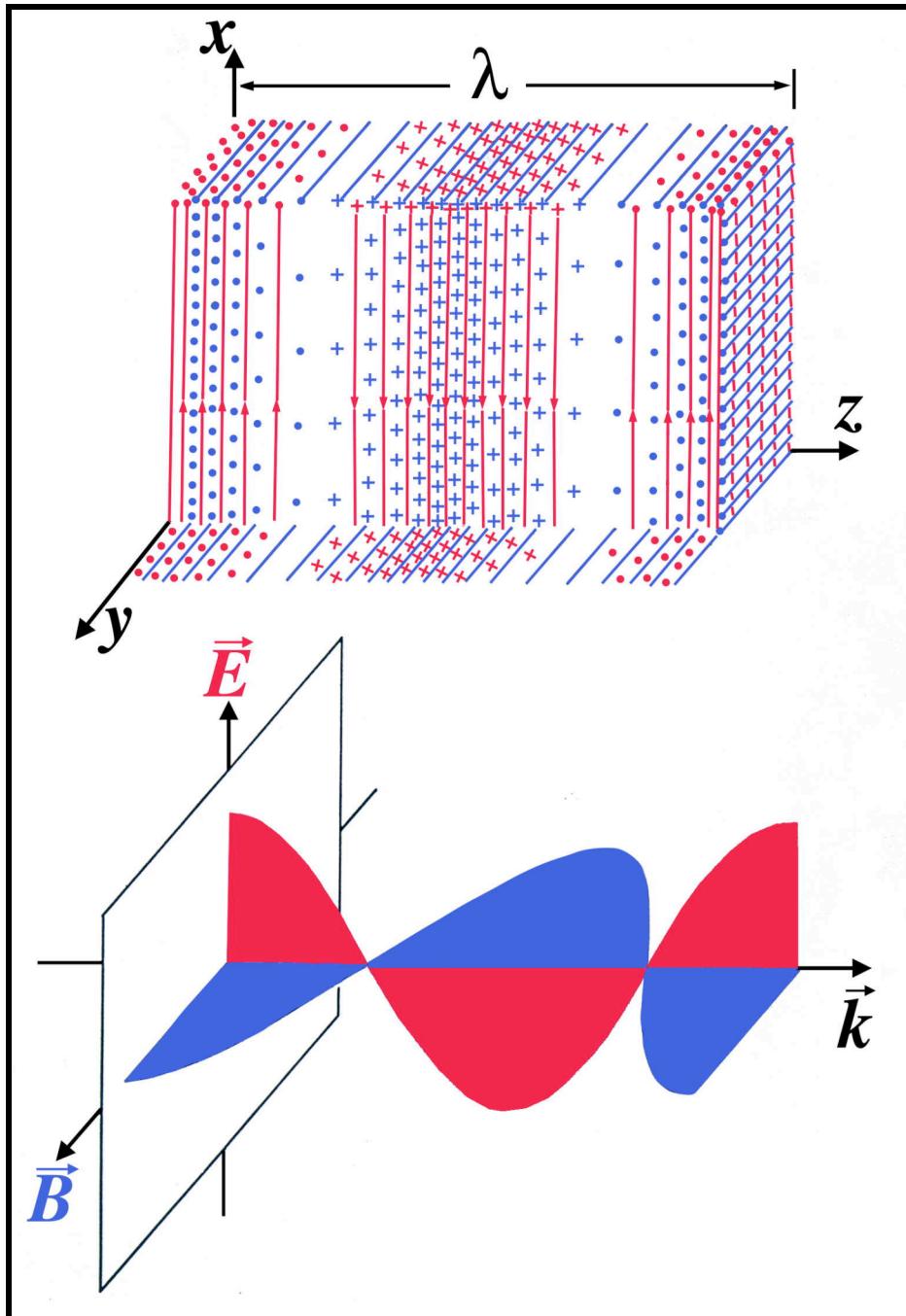
$$\vec{\Pi} = \frac{c}{4\pi} \vec{E} \times \vec{B},$$

which is called the Poynting vector, after its discoverer. The intensity of the electromagnetic radiation is then the average over a wave period of the instantaneous energy transfer rate,

$$I = \langle \Pi \rangle = \frac{c}{4\pi} \langle EB \rangle = \frac{c}{4\pi} \langle E^2 \rangle = \frac{c}{8\pi} E_0^2,$$

where the latter three equalities follow because: the oscillating fields  $\vec{E}$  and  $\vec{B}$  are perpendicular; in Gaussian cgs units, they have equal magnitudes  $E = |\vec{E}| = |\vec{B}| = B$ ; and they have average magnitude  $\langle E^2 \rangle = \frac{1}{2} E_0^2$  equal to half the squared amplitude because the field oscillations are sinusoidal and  $\langle \cos^2 x \rangle = \langle \sin^2 x \rangle = \frac{1}{2}$ .

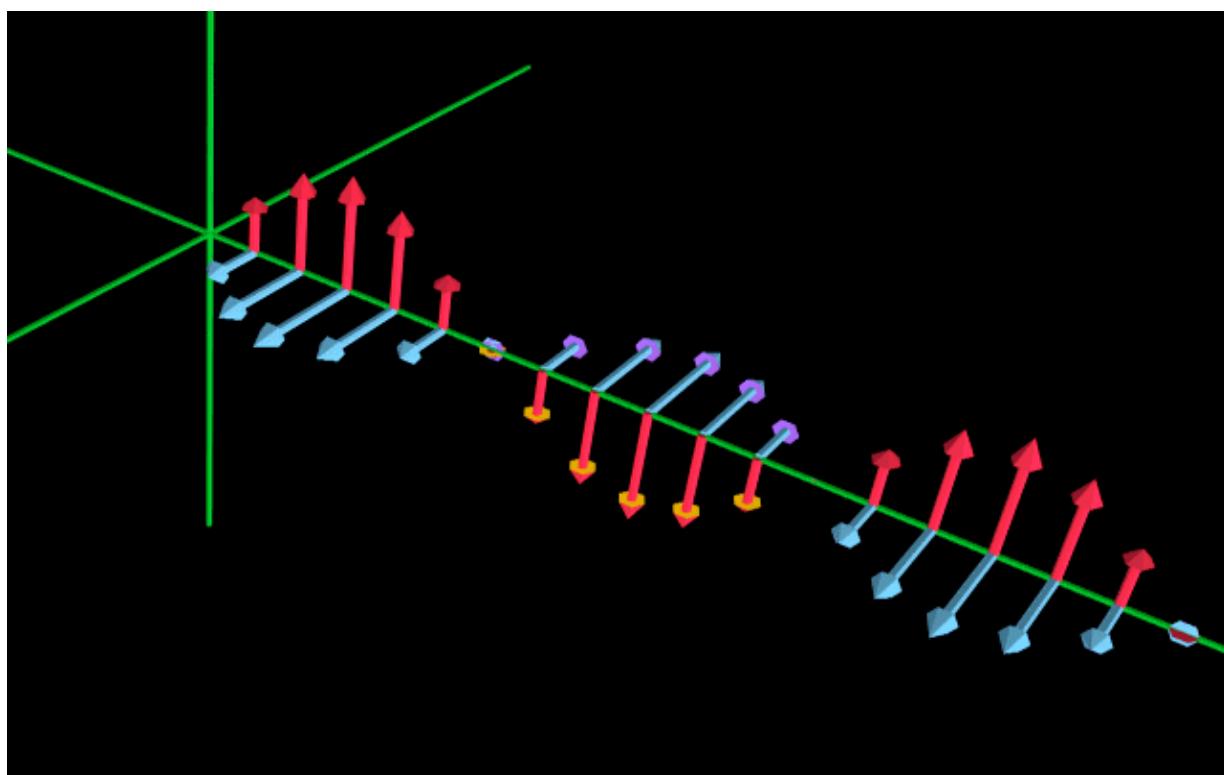
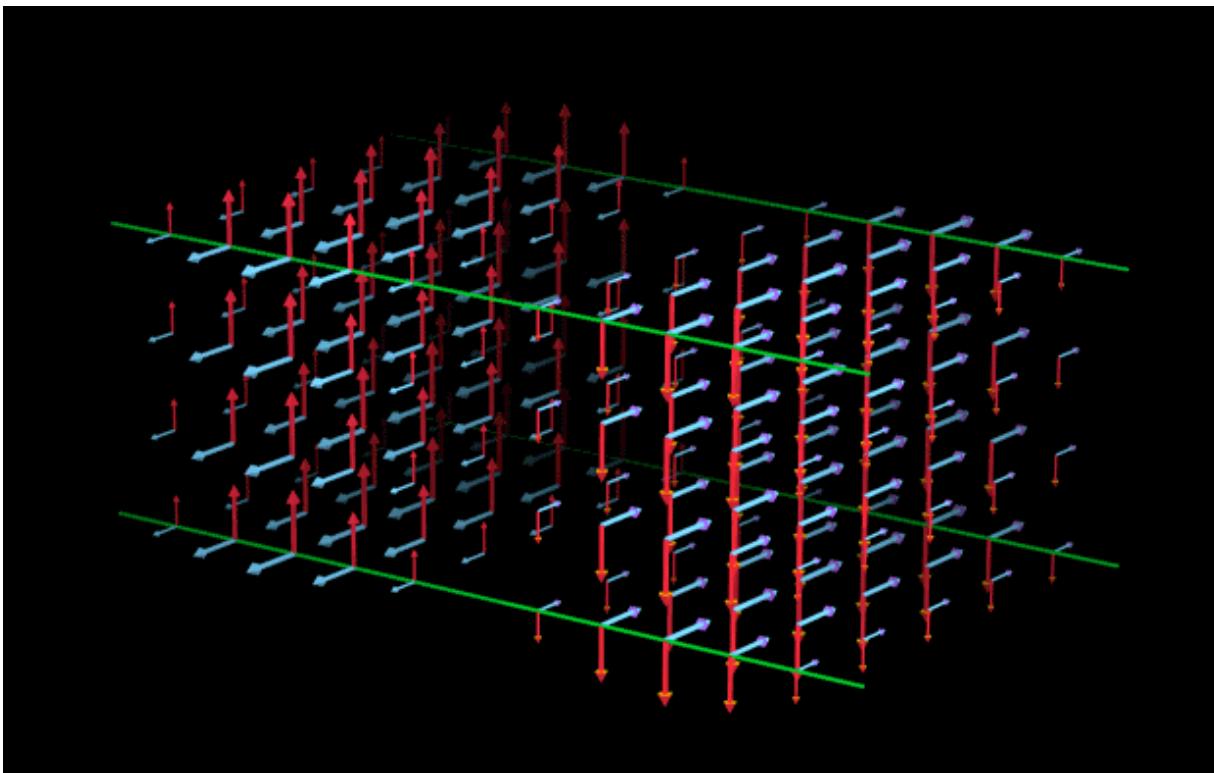
## Illustrations of an electromagnetic plane wave



$$\begin{cases} E_x = a_0 \cos\left[\frac{2\pi}{\lambda}(ct - z)\right], & E_y = 0, & E_z = 0, \\ B_x = 0, & B_y = a_0 \cos\left[\frac{2\pi}{\lambda}(ct - z)\right], & B_z = 0. \end{cases}$$

Figure adapted from Sears (1958).

## Electromagnetic plane wave illustrations



Images copied from <http://www.cs.brown.edu/stc/outrea/greenhouse/nursery/physics/home.html>

Both solutions represent monochromatic, linearly-polarized, electromagnetic plane waves propagating in the  $z$  direction, but the two solutions differ with respect to the direction of polarization of the electromagnetic wave, which is conventionally taken to be the direction of the electric field oscillations. Thus the first wave is  $x$ - and the second is  $y$ -polarized. A  $z$ -traveling wave with an arbitrary direction of polarization can always be resolved into perpendicular  $x$ - and  $y$ -polarization components.

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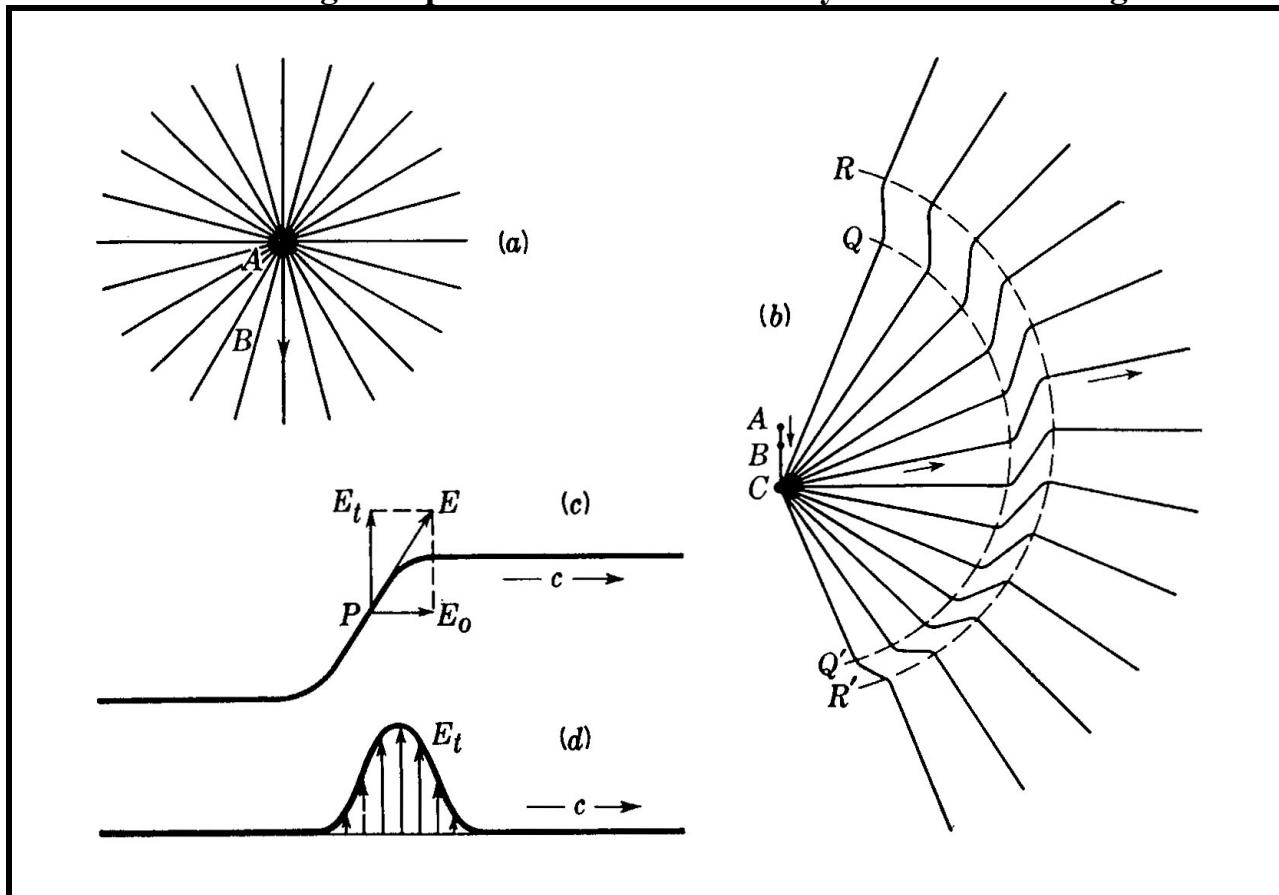
- the oscillating fields  $\vec{E}$  and  $\vec{B}$  are perpendicular;
- in Gaussian cgs units, they have equal magnitudes  $E = |\vec{E}| = |\vec{B}| = B$ ; and
- they have mean-square magnitude  $\langle E^2 \rangle = \frac{1}{2} E_0^2$  equal to half the squared amplitude because the field oscillations are sinusoidal and  $\langle \cos^2 x \rangle = \langle \sin^2 x \rangle = \frac{1}{2}$ .

**Electromagnetic radiation.** Universally, the phenomenon of electromagnetic radiation is due to charge acceleration (a velocity increase, decrease, or change of direction) and can be described in terms of classical laws of electricity and magnetism as follows.

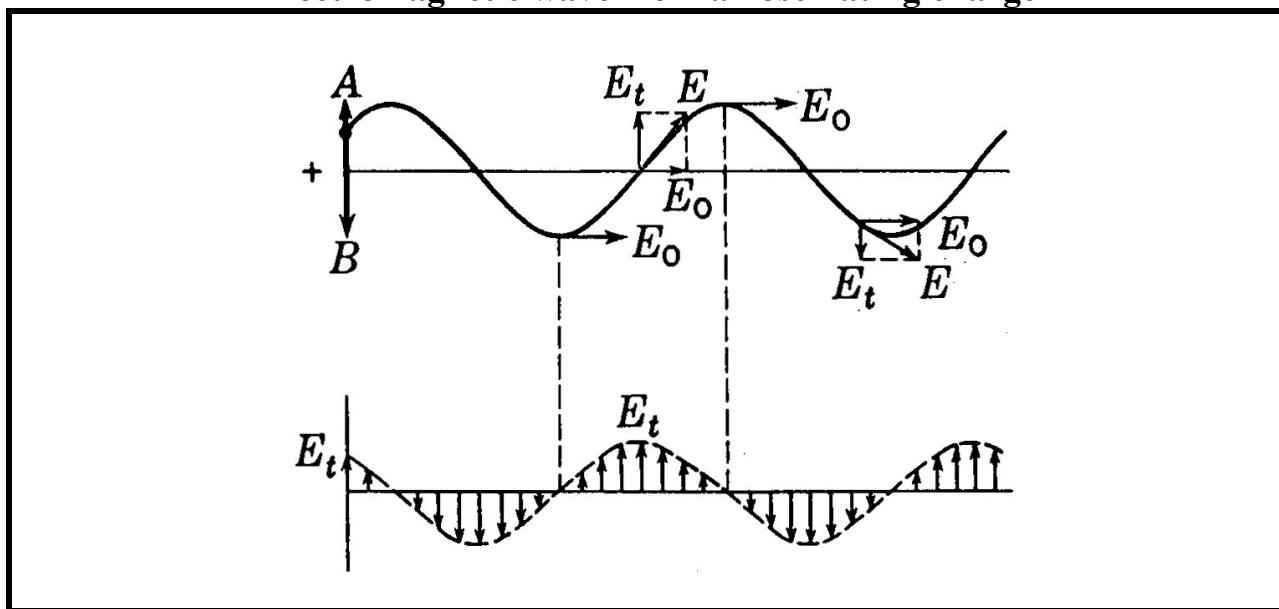
- Around a static charge there is a radial electric field, which stores energy. For example, by the principle of conservation of energy, the field between the plates of a charged capacitor stores the energy that was expended to charge the plates. At a point at  $\vec{r}$  from a static charge  $q$  in free space, the electric field strength is  $\vec{E} = \frac{q}{r^2} \left( \frac{\vec{r}}{r} \right)$  and the energy density at any point in the field can be shown to be  $u = \frac{E^2}{8\pi}$ . If a probe charge  $q'$  were introduced at a point  $\vec{r}$  from a static charge  $q$ , the energy stored in the electric field due to  $q$  would produce on  $q'$  the Coulomb force  $\vec{F} = q' \vec{E} = \frac{q' q}{r^2} \left( \frac{\vec{r}}{r} \right)$ . Indeed, the force per unit probe charge,  $\vec{F}/q' = \vec{E}$ , defines the electric field strength.

- Around a charge in uniform motion with constant velocity  $v \ll c$  there is also a magnetic field transverse to the radial electric field, and both fields store energy. From the Biot-Ampere law for the magnetic field due to a uniform current in an element of straight conductor, the magnetic field at a point at  $\vec{r}$  from a charge  $q$  that is moving with a constant nonrelativistic velocity  $\vec{v}$  in free space is  $\vec{B} = \frac{1}{c} \frac{q}{r^2} \vec{v} \times \left( \frac{\vec{r}}{r} \right) = \frac{1}{c} \vec{v} \times \vec{E}$ , and the energy density in the electromagnetic field at  $\vec{r}$  can be shown to be  $u = \frac{1}{8\pi} (E^2 + B^2)$ . At a point in an electromagnetic field in free space where the field strengths are  $\vec{E}$  and  $\vec{B}$ , the energy stored in the field would produce on a charge  $q'$  moving with a constant velocity  $\vec{v}$  the Lorentz force  $\vec{F} = q' \left[ \vec{E} + \left( \frac{\vec{v}}{c} \times \vec{B} \right) \right]$ . Note that the Lorentz force is that due to external fields acting on a moving charge, not the fields of the charge itself.
- Around an accelerated charge, the energy expended to produce the force that produced the acceleration is not stored in the electric and magnetic fields surrounding the moving charge; rather, it is radiated as a ripple or kink that propagates with radial velocity  $c$  in the electromagnetic field around the accelerated charge. In effect, while the electric and magnetic fields can adjust to follow the uniform motion of a charge moving with constant velocity, the fields cannot adjust to follow a changing motion of an accelerated charge. As illustrated in the following figures, an acceleration that changes either the speed or direction of motion, or both, produces transverse field components  $\vec{E}_\perp = \vec{E}_t$  and  $\vec{B}_\perp = \vec{B}_t$  that are perpendicular to one another and to the radial field components  $\vec{E}_\parallel = \vec{E}_0$  and  $\vec{B}_\parallel = \vec{B}_0 = \frac{\vec{v}}{c} \times \vec{E}_0$ . The transverse field components propagate radially with velocity  $c$  and constitute the electromagnetic radiation. The energy density in the electromagnetic radiation is  $u = \frac{1}{8\pi} (E_t^2 + B_t^2) = \frac{E_t^2}{4\pi}$ , and if the energy density, which has dimensions energy per unit volume, is multiplied by the propagation velocity, which has dimensions distance per unit time, the product has dimensions energy per unit time per unit area, i.e., intensity. The result  $I = c \langle u \rangle = \frac{c}{4\pi} \langle E_t^2 \rangle$ , where the average is over the duration of an acceleration pulse or the period of an oscillating acceleration, is the same as was given above in terms of the Poynting vector.

### Electromagnetic pulse from a momentarily accelerated charge



### Electromagnetic wave from an oscillating charge



Figures copied from Jenkins and White (1957).

## Figure legends (Jenkins and White, 1957)

### Electromagnetic pulse from a momentarily accelerated charge:

- (a) Radial lines of force in the electric field  $\vec{E}$  around a static positive charge  $q_A$  at A. A point probe charge  $q_B$  at B would experience a force  $\vec{F} = q_B \vec{E} = (q_A q_B / r_{AB}^2) (\vec{r}_{AB} / r_{AB})$ .
- (b) Electric field after the charge initially at rest at A at  $t_0$  is uniformly accelerated to B at  $t_1$  during the time interval  $t_{AB} = t_1 - t_0$  and then continues in uniform motion from B at  $t_1$  to C at  $t_2$  during the time interval  $t_{BC} = t_2 - t_1$ .  
 Since the speed of propagation of electromagnetic field effects  $c$  is finite:
- The field beyond the outer arc RR', which has radius  $r_A = c(t_{AB} + t_{BC}) = c(t_2 - t_0)$  and is centered on A, where the acceleration began, is that from the static charge at A. At time  $t_2$  the arc RR' traces the minimum distance at which the beginning of the acceleration could be detected at time  $t_2$ .
  - The field within the inner arc QQ', which has radius  $r_B = ct_{BC} = c(t_2 - t_1)$  and is centered on B, where the acceleration ended and the uniform motion began, is that from the uniformly moving charge at C. At time  $t_2$  the arc QQ' traces minimum distance at which the end of the accelerated motion and beginning of the uniform motion could be detected.
  - Between the two arcs is a “kink” or “ripple” in the field due to the acceleration pulse.
- (c) The field  $\vec{E}$  at any point is tangent to the line of force through the point, and can be resolved into a radial component  $\vec{E}_\parallel = \vec{E}_0$  and a transverse component  $\vec{E}_\perp = \vec{E}_t$ , which:
- Is zero along straight, radial lines of force;
  - Has its largest value midway along the kink in a line of force that is perpendicular to the charge acceleration direction;
  - Is directed opposite the acceleration direction, since the lines of force are continuous across the kinks; and
  - Falls to zero along lines of force that are parallel to the acceleration direction.
- (d) The transverse components produced by a uniform acceleration for a discrete time interval form an electromagnetic pulse that propagates with speed  $c$ .

### Electromagnetic wave from an oscillating charge:

- Sinusoidal oscillation of a point positive charge between A and B produces sinusoidal oscillations of the transverse component  $\vec{E}_\perp = \vec{E}_t$  of the electric field  $\vec{E}$ . The radial component  $\vec{E}_\parallel = \vec{E}_0$  remains constant.
- The charge oscillations and the field oscillations have the same frequency, but they differ in phase by  $\pi/2$ .

**Feynman's electromagnetic field equations.** The phenomenon of electromagnetic radiation can also be described in terms of equations for the electric and magnetic fields of a moving charge, which Richard Feynman (1918-1988) derived from the Maxwell equations and presented in some lectures on synchrotron radiation (Feynman, *ca.* 1950, as cited by Feynman *et al.*, 1962; see also Janah *et al.*, 1988 and Dushek and Kuzmin, 2004).

In Gaussian cgs units, Feynman's equations for the electric field  $\vec{E}$  and magnetic field  $\vec{B}$  at time  $t$  at a fixed point  $P(x, y, z)$  due to an arbitrarily moving point charge  $q$  are

$$\begin{cases} \vec{E}(x, y, z, t) = q \left[ \frac{\hat{r}}{r^2} + \frac{r}{c} \frac{d}{dt} \left( \frac{\hat{r}}{r^2} \right) + \frac{1}{c^2} \frac{d^2 \hat{r}}{dt^2} \right], \\ \vec{B}(x, y, z, t) = \hat{r} \times \vec{E}, \end{cases}$$

where, since electromagnetic field effects are transmitted at the finite speed  $c$ , the fields at time  $t$  at point  $P$  depend on the position vector  $\vec{r} = \vec{r}(t')$  from  $q$  to  $P$ , and its unit direction

$$\text{vector } \hat{r} = \frac{\vec{r}}{|\vec{r}|} = \frac{\vec{r}}{r} = \hat{r}(t'), \text{ at the earlier, retarded time } t' = \left( t - \frac{r}{c} \right).$$

In Feynman's electric field equation, the first term  $(q\hat{r}/r^2)$  can be recognized as the Coulomb field of a static charge; the second term can be seen to be the time rate of change of the Coulomb field of a moving charge  $\frac{d}{dt}(q\hat{r}/r^2)$  multiplied by the time  $(r/c)$  needed to transmit a change in the field through a distance  $r$  at speed  $c$ ; but the third term, the product of an acceleration  $\frac{d^2 \hat{r}}{dt^2}$  and the quantity  $(q/c^2)$ , is non-Coulombic and represents the electric field component of the electromagnetic radiation.

At a far distant fixed point  $P$ , at  $\vec{r}$  from  $q$ , a small displacement of  $q$  changes the direction of  $\vec{r}$  but leaves its length  $r$  essentially unchanged, so that for large  $r$ ,

$$\frac{d}{dt} \left( \frac{\hat{r}}{r^2} \right) \approx \frac{1}{r^2} \frac{d\hat{r}}{dt},$$

and Feynman's equation for the electric field at large  $r$  may be rewritten as

$$\vec{E} \approx q \left( \frac{\hat{r}}{r^2} + \frac{1}{rc} \frac{d\hat{r}}{dt} + \frac{1}{c^2} \frac{d^2 \hat{r}}{dt^2} \right).$$

In addition, for large and therefore essentially constant  $r$ ,

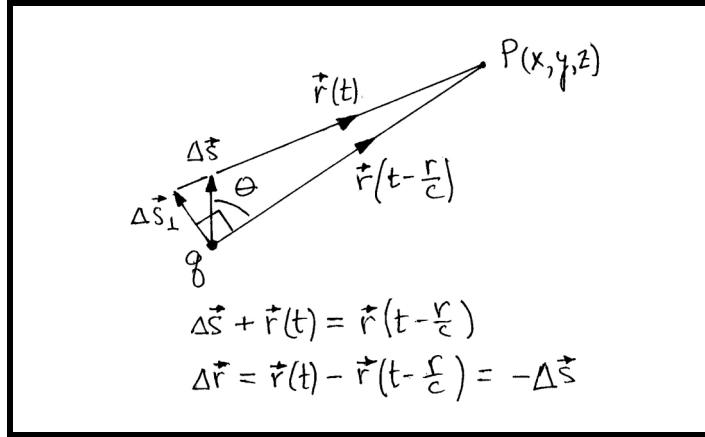
$$\frac{d\hat{r}}{dt} = \frac{d}{dt} \left( \frac{\vec{r}}{r} \right) \approx \frac{1}{r} \frac{d\vec{r}}{dt} \quad \text{and} \quad \frac{d^2 \hat{r}}{dt^2} \approx \frac{1}{r} \frac{d^2 \vec{r}}{dt^2},$$

so that at large  $r$ ,

$$\vec{E} \approx q \left( \frac{\hat{r}}{r^2} + \frac{1}{r^2 c} \frac{d\vec{r}}{dt} + \frac{1}{rc^2} \frac{d^2 \vec{r}}{dt^2} \right).$$

Furthermore, in the view from  $P$  back to  $q$ , the time derivatives of  $\vec{r}$  for a displacement  $\Delta\vec{s}$  of  $q$  depend on only the component of  $\Delta\vec{r} = \vec{r}(t) - \vec{r}\left(t - \frac{r}{c}\right) = -\Delta\vec{s}$  that is perpendicular to  $\vec{r}\left(t - \frac{r}{c}\right)$ . The perpendicular component is  $\Delta\vec{r}_\perp = -\Delta\vec{s}_\perp$ , where  $\Delta s_\perp = \Delta s \sin\theta$  and  $\theta$  is the angle between  $\Delta\vec{s}$  and  $\vec{r}\left(t - \frac{r}{c}\right)$ ; and the negative sign occurs because  $\Delta\vec{s}$  and  $\Delta\vec{r}$  are antiparallel.

**Vector diagram showing that at  $P$  at  $\vec{r}$  from  $q$ ,  $\Delta\vec{r}_\perp = -\Delta\vec{s}_\perp$ , where  $\Delta s_\perp = \Delta s \sin\theta$ .**



It follows that the time derivatives of  $\hat{r}$  at large  $r$  may be written in terms of the perpendicular components of the time derivatives  $d\vec{s}/dt = \vec{v}$  and  $d\vec{v}/dt = d^2\vec{s}/dt^2 = \vec{a}$ . Thus,

$$\begin{aligned}\frac{d\hat{r}}{dt} &= \frac{d}{dt}\left(\frac{\vec{r}}{r}\right) \approx \frac{1}{r} \frac{d\vec{r}_\perp}{dt} = -\frac{1}{r} \frac{d\vec{s}_\perp}{dt} = -\frac{\vec{v}_\perp}{r}, \\ \frac{d^2\hat{r}}{dt^2} &\approx \frac{d}{dt}\left(-\frac{\vec{v}_\perp}{r}\right) = -\frac{1}{r} \frac{d\vec{v}_\perp}{dt} = -\frac{\vec{a}_\perp}{r},\end{aligned}$$

where the negative signs occur because  $\Delta\vec{r} = -\Delta\vec{s}$ , and the components of displacement, velocity, and acceleration perpendicular to a unit vector  $\hat{r}$  are given by

$$\begin{aligned}\vec{s}_\perp &= (\hat{r} \times \vec{s}) \times \hat{r}, & s_\perp &= s \sin\theta, \\ \vec{v}_\perp &= (\hat{r} \times \vec{v}) \times \hat{r}, & v_\perp &= v \sin\theta, \\ \vec{a}_\perp &= (\hat{r} \times \vec{a}) \times \hat{r}, & a_\perp &= a \sin\theta,\end{aligned}$$

respectively, where  $\theta$  is the angle that  $\vec{s}$ ,  $\vec{v}$ , and  $\vec{a}$  make with  $\hat{r}$ .

Substituting the perpendicular velocity and acceleration expressions for the time derivatives of  $\hat{r}$ , Feynman's equations for the electric and magnetic fields far from a moving charge become

$$\begin{cases} \vec{E} \approx q \left( \frac{\hat{r}}{r^2} - \frac{\vec{v}_\perp}{r^2 c} - \frac{\vec{a}_\perp}{rc^2} \right), \\ \vec{B} = \hat{r} \times \vec{E}. \end{cases}$$

The Feynman electromagnetic field equations state that:

- For a static charge  $q$ , the electric field at  $\vec{r}$  from  $q$  is the radial Coulomb field  $\vec{E} = \frac{q}{r^2} \left( \frac{\vec{r}}{r} \right)$ , and the magnetic field is  $\vec{B} = \left( \frac{\vec{r}}{r} \right) \times \vec{E} = 0$  because  $\vec{r} \times \vec{r} = 0$ .
- For a charge  $q$  moving uniformly with a constant, nonrelativistic velocity  $v \ll c$ , the electric field at  $\vec{r}$  from  $q$  is the radial field  $\vec{E} = \frac{q}{r^2} \left( \frac{\vec{r}}{r} - \frac{\vec{v}_\perp}{c} \right) \approx \frac{q}{r^2} \left( \frac{\vec{r}}{r} \right)$ , where  $\vec{v}_\perp$  is the component of  $\vec{v}$  that is perpendicular to  $\vec{r}$ ; and the magnetic field is  $\vec{B} = \left( \frac{\vec{r}}{r} \right) \times \vec{E} = -\frac{q}{cr^2} \left( \frac{\vec{r}}{r} \right) \times \vec{v}_\perp$ , which is transverse to  $\vec{E}$  has magnitude  $B = -\frac{qv \sin \theta}{cr^2}$ , where  $\theta$  is the angle between  $\vec{v}$  and  $\vec{r}$ .
- For an accelerated charge  $q$ , the electric and magnetic fields at large  $r$ , far from  $q$ , reduce to the transverse fields due to the third term in Feynman's electric field equation, viz.,  $\vec{E} = -\frac{q\vec{a}_\perp}{c^2 r}$  and  $\vec{B} = \left( \frac{\vec{r}}{r} \right) \times \vec{E} = -\frac{q}{c^2 r} \left( \frac{\vec{r}}{r} \right) \times \vec{a}_\perp$ , where  $\vec{a}_\perp$  is the component of  $\vec{a}$  that is perpendicular to  $\vec{r}$ , because the first two, radial terms in Feynman's equation, which fall off as  $r^{-2}$  and are therefore short-range, become negligible compared to the third, transverse term, which falls off as only  $r^{-1}$  and is therefore long-range.

The transverse, long-range,  $r^{-1}$  electric and magnetic fields due to acceleration of a charge constitute electromagnetic radiation. At a position  $\vec{r}$ , far from a charge  $q$ , that experiences a momentary acceleration  $\vec{a}$ , the instantaneous electric and magnetic fields are

$$\begin{cases} \vec{E} = -\frac{q\vec{a}_\perp}{c^2 r} = -\frac{q}{c^2 r} (\hat{r} \times \vec{a}) \times \hat{r} = -\frac{q}{c^2 r} \left( \frac{\vec{r}}{r} \times \vec{a} \right) \times \frac{\vec{r}}{r}, & E = -\frac{q a \sin \theta}{c^2 r}, \\ \vec{B} = \frac{\vec{r}}{r} \times \vec{E}, \end{cases}$$

where:  $\theta$  is the angle between  $\vec{a}$  and  $\vec{r}$ ; the negative sign means that  $\vec{E}$  is directed opposite the component of  $\vec{a}$  that is perpendicular to  $\vec{r}$ ; and, since the radiation propagates at the finite speed  $c$ , the electromagnetic radiation fields at time  $t$ , depend on the position  $\vec{r} = \vec{r}(t')$  and acceleration  $\vec{a} = \vec{a}(t')$  at the earlier, retarded time,  $t' = t - \frac{r}{c}$ . The  $r^{-1}$  dependence of  $E$  is a characteristic of the spherical propagation of the radiation.

**Directions of the electric and magnetic fields  $\vec{E}$  and  $\vec{B}$  at  $P$   
due to acceleration of a point charge  $q$  at  $O$**

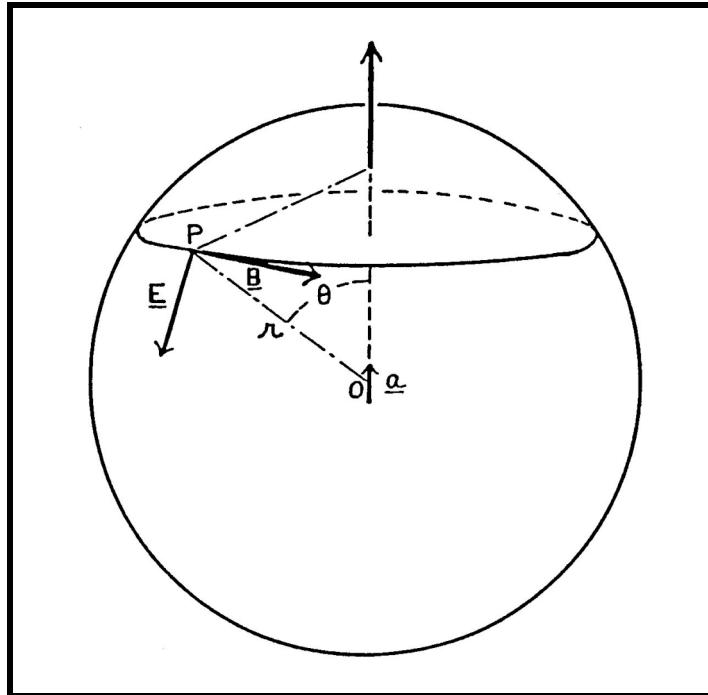


Figure copied from Compton and Allison (1935)

The result from classical electrodynamical theory for the electric field component of the electromagnetic radiation field far from an accelerated charge

$$E = -\frac{q a \sin \theta}{c^2 r}$$

is sufficiently important for the following description of X-ray scattering by an electron that, for pedagogic purposes, the result is re-derived below via two closely similar, largely geometric demonstrations.

**Electric Field due to an Accelerated Charge.** The figures below labeled Figures 3, 4, and 5 illustrate dogleg kinks in the lines of force in the field around a point positive charge, initially at rest, then accelerated from O to O' during time  $\Delta t$ , and then allowed to continue in uniform motion with constant velocity  $a\Delta t$  in a straight line to point P at time  $t$ . Along a kink in a line of force, such as in the region labeled  $V_k$  in Figures 3 and 4, that makes an angle  $\theta$  with the direction of motion, the transverse  $E_{\perp}$  (Maxwell) component and the radial  $E_{\parallel}$  (Coulomb) component of the electric field stand in the same ratio as the lengths of the perpendicular transverse leg AB and radial leg BC of the triangle ABC in Figure 5. Thus,

$$\frac{E_{\perp}}{E_{\parallel}} = \frac{AB}{BC} = -\frac{(a\Delta t)t \sin\theta}{c\Delta t} = -\frac{ta \sin\theta}{c},$$

where the negative sign occurs because, since the line of force is continuous across the kink,  $\vec{E}_{\perp}$  is antiparallel to the perpendicular component of acceleration,  $\vec{a}_{\perp} = \vec{a}_{\theta}$  in Figure 5.

#### Kinked lines of force in the electric field around a point charge accelerated from O to O'

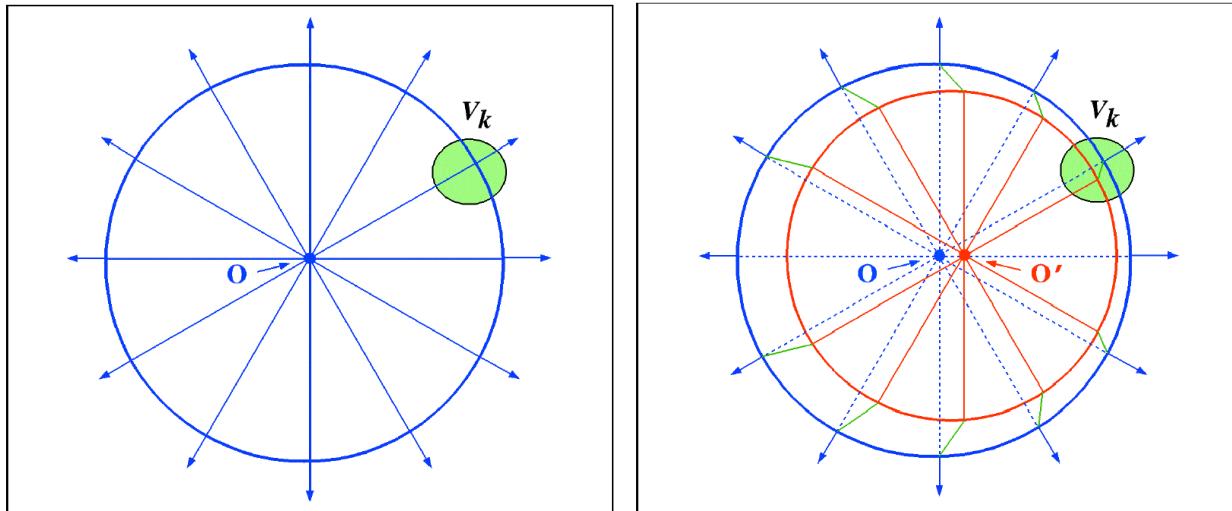


Figure 3: Electric lines of flux around a point charge

Figure 4: Field line kink due to accelerating charge

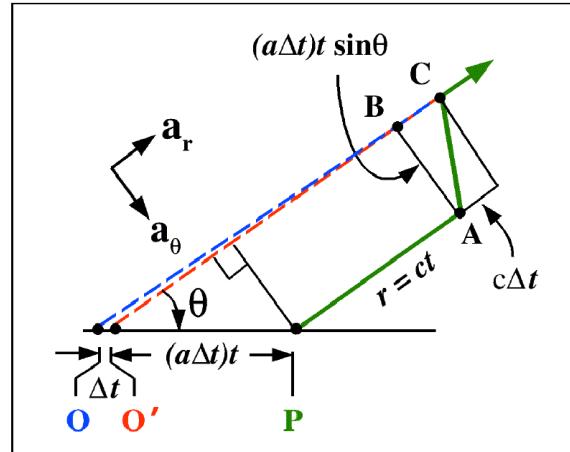


Figure 5: Kink detail

Figures 3, 4, and 5 copied from Gisin and Pantic-Tanner (2002).

<http://www.ieee.org/organizations/pubs/newsletters/emcs/winter02/how.html>

At the outer kink radius,  $r = c(t + \Delta t) \approx ct$ , so that  $t \approx \frac{r}{c}$  and

$$\frac{E_{\perp}}{E_{\parallel}} = -\frac{rasin\theta}{c^2}.$$

Then, since the radial (Coulomb) field component is

$$E_{\parallel} = \frac{q}{r^2},$$

it follows that the transverse (Maxwell) field component is

$$E_{\perp} = -\frac{qasin\theta}{c^2 r},$$

*QED.*

Since for the radial field component  $E_{\parallel} \propto r^{-2}$ , while for the transverse field component  $E_{\perp} \propto r^{-1}$ , the short-range  $r^{-2}$  radial field becomes negligible at large distances from the accelerated charge while the long-range  $r^{-1}$  transverse field, the electromagnetic radiation field, persists.

Essentially this same demonstration had been presented in 1903 by J.J. Thomson, discoverer of the electron.

#### Kink in a line of force in the electric field around an accelerated point charge

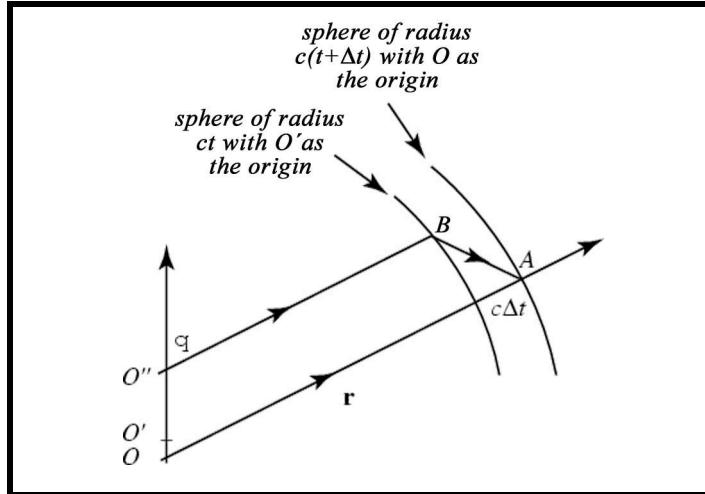


Figure copied from Weisstein (2006). <http://scienceworld.wolfram.com/physics/ElectricDipoleRadiation.html>

Referring to the above diagram, a point particle with positive charge  $q$  starting from rest at position  $O$  is accelerated during a short time interval  $\Delta t$  to point  $O'$ . The particle then continues in a straight line at constant velocity  $v = a\Delta t$ , and arrives at point  $O''$  at a time  $\Delta t + t$ . An observer at point  $A$ , a distance  $r + c\Delta t = c(t + \Delta t)$  from  $O$  and at an angle  $\theta = \angle O'OA$  from the direction of motion would see the radial electric field of the stationary

particle; an observer at point  $B$ , at a radial distance  $r = ct$  from  $O''$  and also at angle  $\theta$  from the direction of motion would see a radial electric field centered on  $O''$ .

Assume  $OA$  and  $O''B$  to be parallel. Then, by similar triangles,

$$\begin{aligned}\frac{E_{\perp}}{E_{\parallel}} &= \frac{-(OO'+O'O'')\sin\theta}{c\Delta t} = \frac{-[(a\Delta t)\Delta t + (a\Delta t)t]\sin\theta}{c\Delta t} \\ &= \frac{-a(\Delta t+t)\sin\theta}{c\Delta t} = \frac{-(a\Delta t)t\sin\theta}{c\Delta t} = -\frac{at\sin\theta}{c} = -\frac{ar\sin\theta}{c^2},\end{aligned}$$

where: it is assumed that  $\Delta t$  is small enough that  $\Delta t + t \approx t$ ; the acceleration  $a = a(t')$  and distance  $r = r(t')$  are those at the retarded time  $t' = t - \frac{r}{c}$ ; and the negative sign appears because, since the field line of force is continuous across the kink,  $\vec{E}_{\perp}$  is antiparallel to the component of  $\vec{a}$  that is perpendicular to  $\vec{r}$ .

By definition, the radial component of the field at the kink is the Coulomb field

$$E_{\parallel} = \frac{q}{(r+c\Delta t)^2} \approx \frac{q}{r^2},$$

where it is assumed that  $\Delta t$  is small enough that  $r + c\Delta t \approx r$ .

It then follows that the transverse component of the field at the kink is the Maxwell field

$$E_{\perp} = E_{\parallel} \left( -\frac{ar\sin\theta}{c^2} \right) = \left( \frac{q}{r^2} \right) \left( -\frac{ar\sin\theta}{c^2} \right),$$

and

$$E_{\perp} = -\frac{q a \sin\theta}{c^2 r},$$

*QED* (Thomson, 1903).