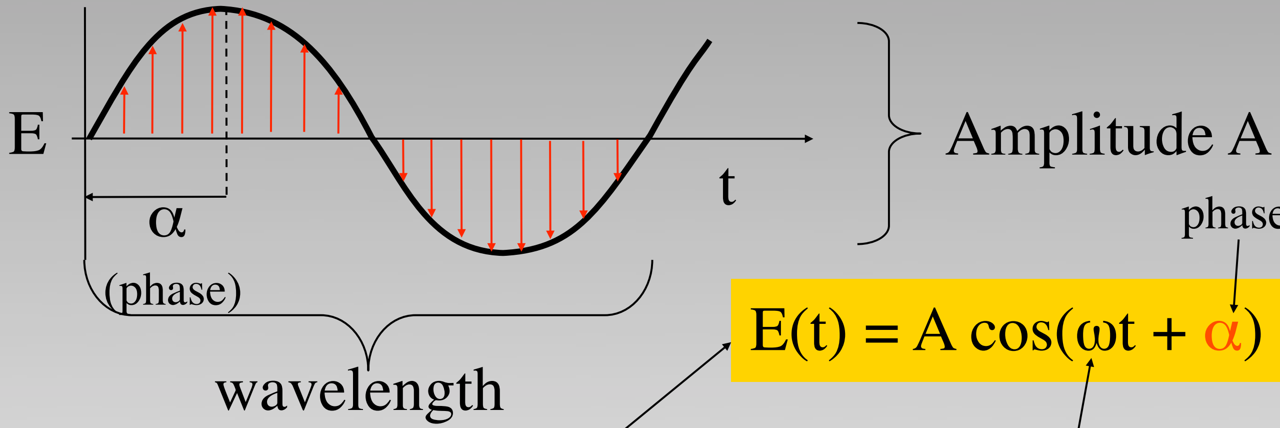
Protein Structure Determination

Lecture 2:

Wave addition

The general equation for wave

Remember:
Photons are
oscillating electric
fields*.



phase

$$E(t) = A\cos(\omega t + \alpha)$$

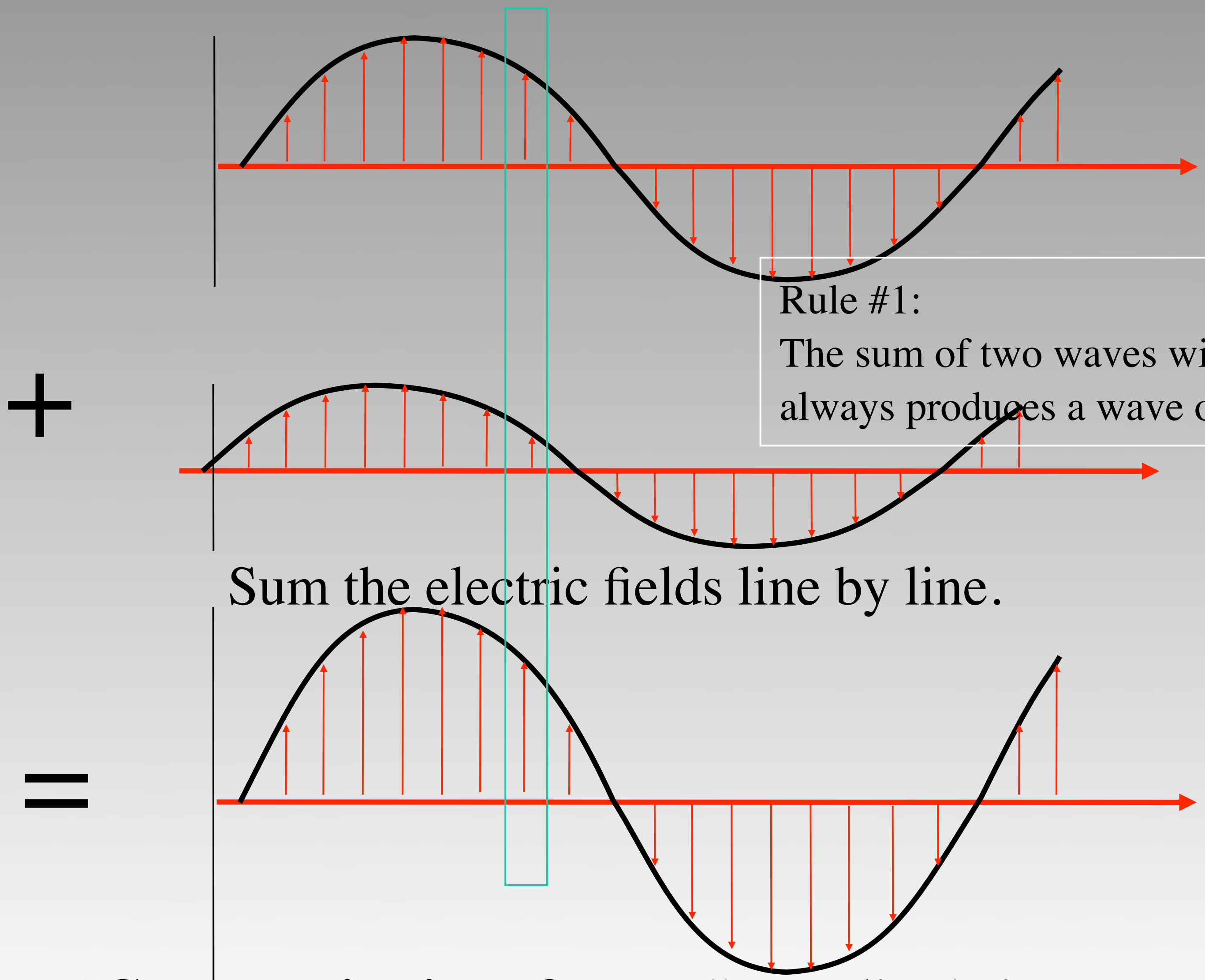
The instantaneous electric field at time **t**

$$\omega = 2\pi \underline{c/\lambda}$$

oscillation rate in cycles/second

*also an oscillating magnetic field of the same frequency, 90 degrees out of phase.

Wave addition

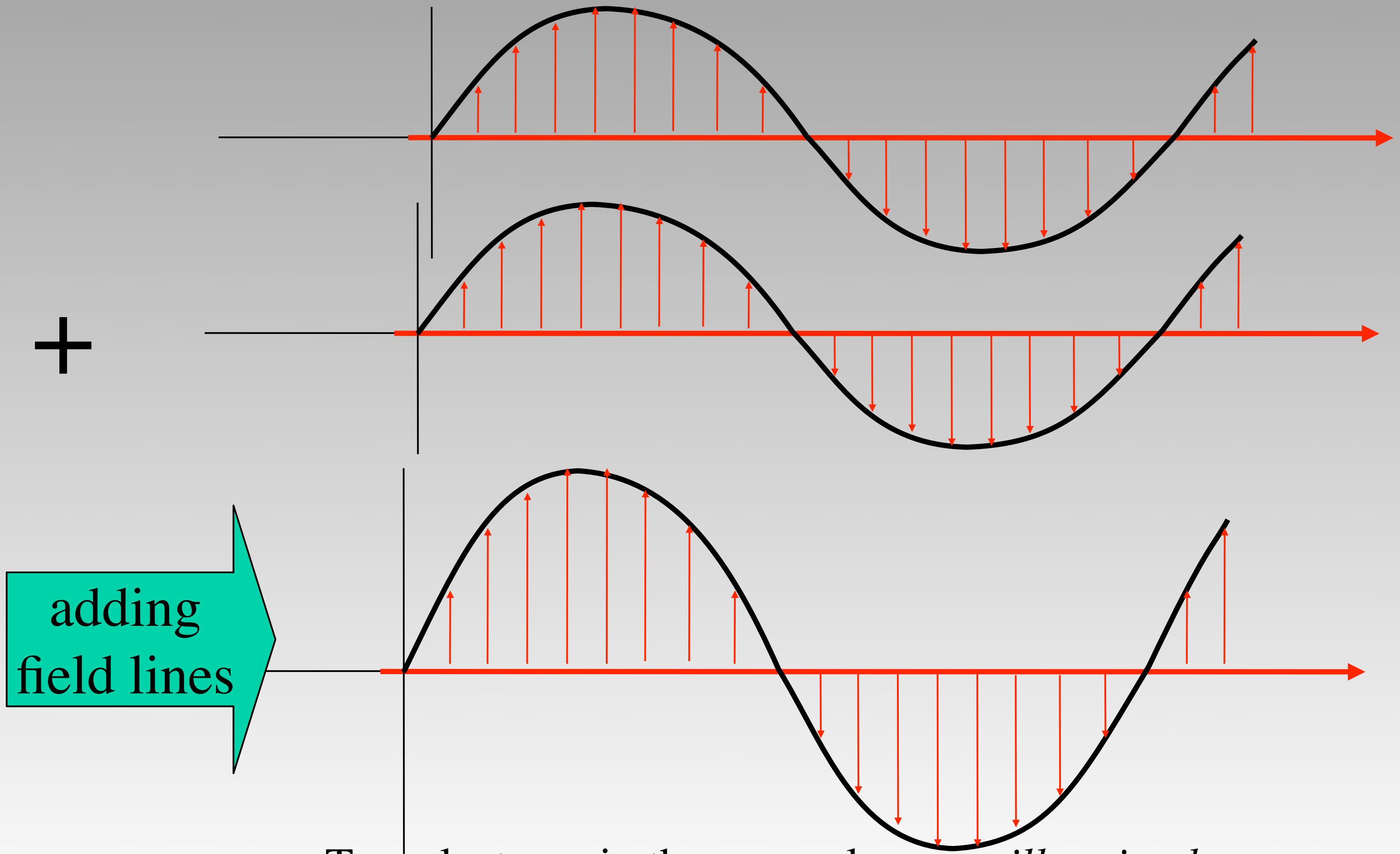


Rule #1:
The sum of two waves with wavelength λ always produces a wave of wavelength λ.

Sum the electric fields line by line.

“**Constructive interference**”: amplitude increases.

Constructive interference

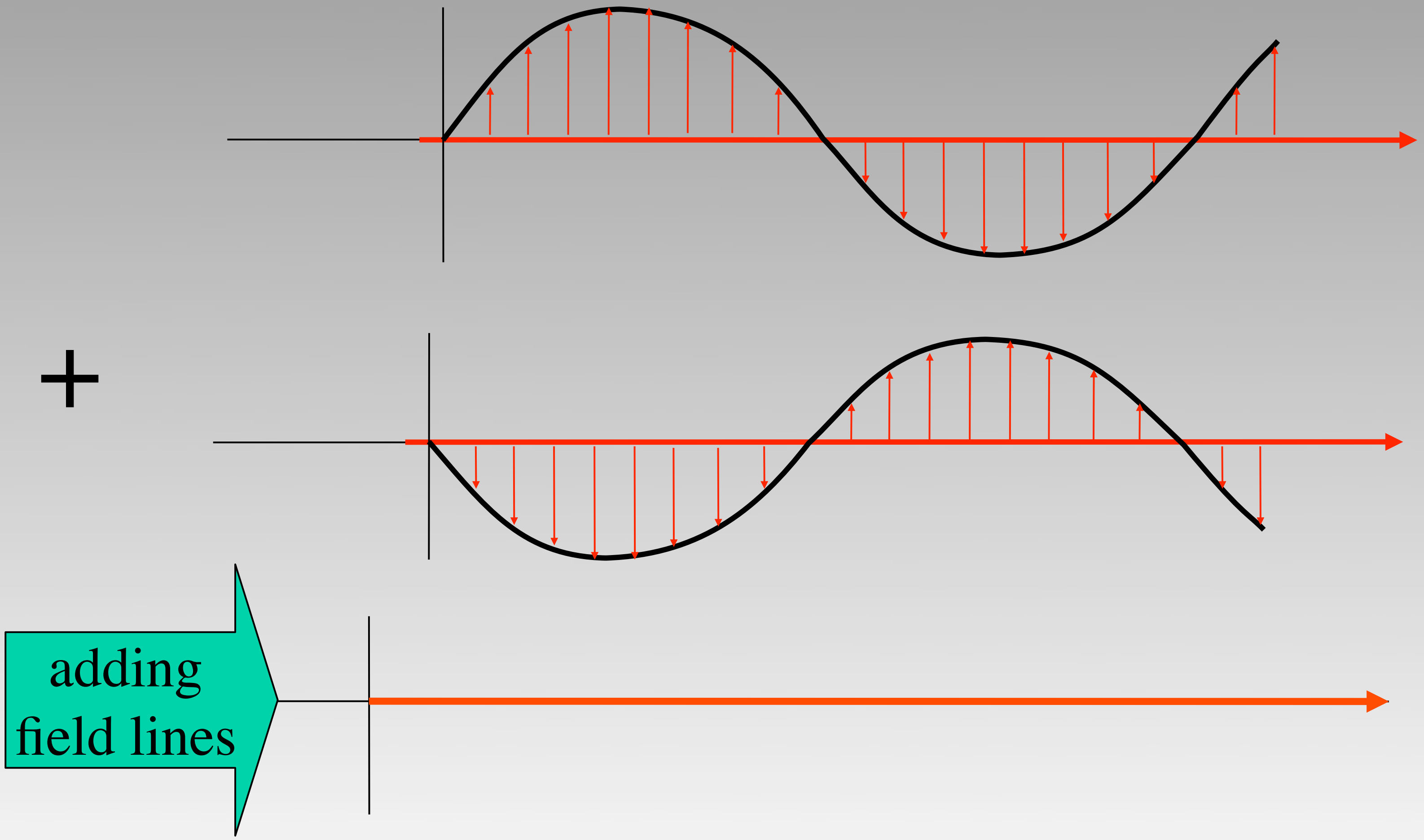


+

adding
field lines

Two electrons in the same place *oscillate in phase*.

Destructive interference



adding field lines

2 electrons separated by $\lambda/2$ *oscillate out of phase* .

Decomposing a wave into two parts

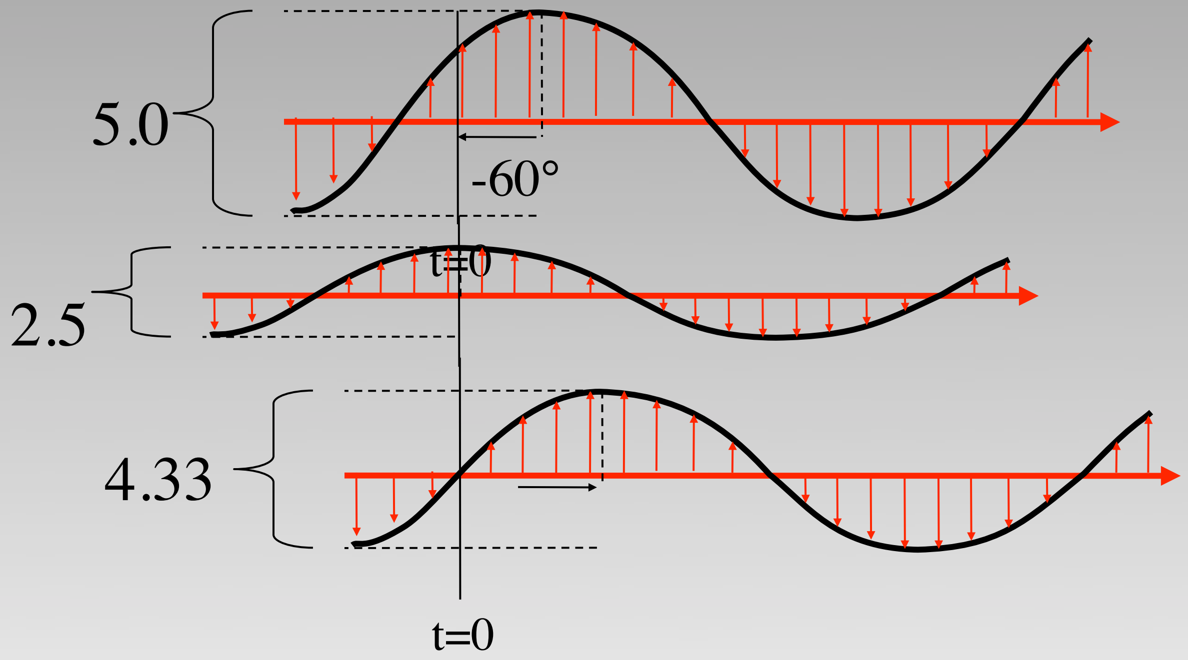
a wave

=

cosine part

+

sine part



Decomposing a wave into two parts

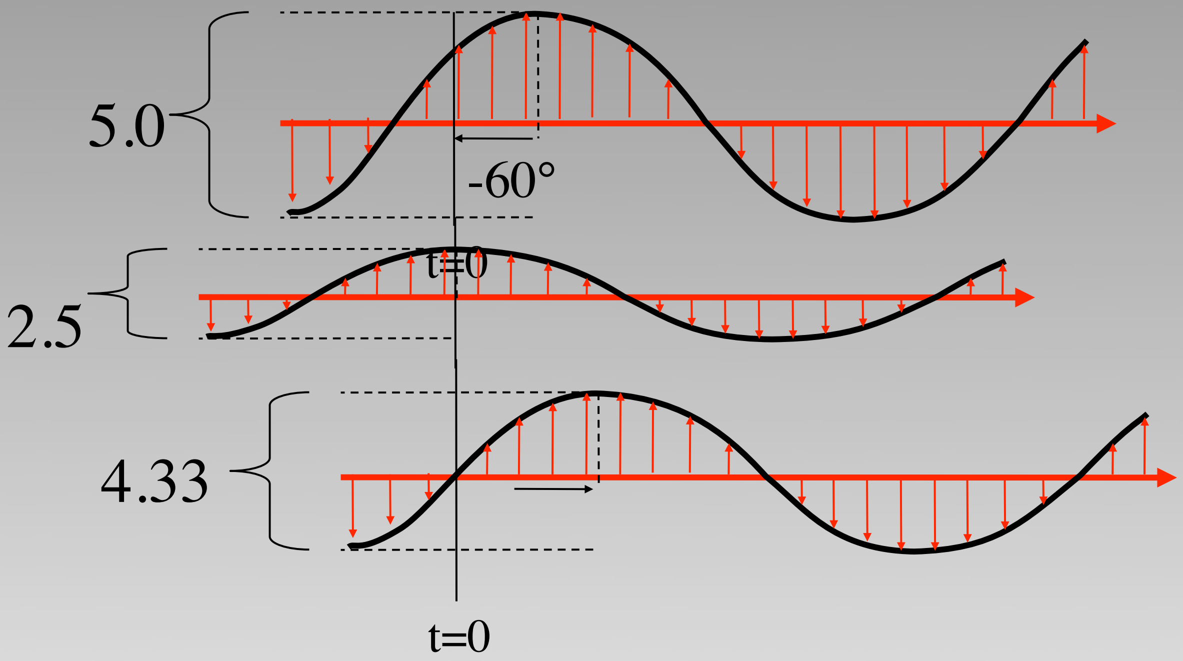
5.0 cos(ωt - 1/3π)

=

2.5 cos ωt

+

4.33 sin ωt



5.0 cos(ωt - 1/3π) =

5.0 cos(–1/3π) cos ωt - 5.0 sin(–1/3π) sin ωt =

2.5 cos ωt + 4.33 sin ωt

The sum of angles rule

$$\cos(\alpha + \beta) = \cos\alpha \cos\beta - \sin\alpha \sin\beta$$

Using the sum of angles rule on the wave equation decomposes a wave into sine and cosine parts

The general wave equation,

$$E(t) = A\cos(\omega t + \alpha)$$

Using the sum of angles rule, becomes

$$A\cos(\omega t + \alpha) = \underline{A\cos\alpha}\,\cos\omega t - \underline{A\sin\alpha}\,\sin\omega t$$

amplitude of cosine wave part

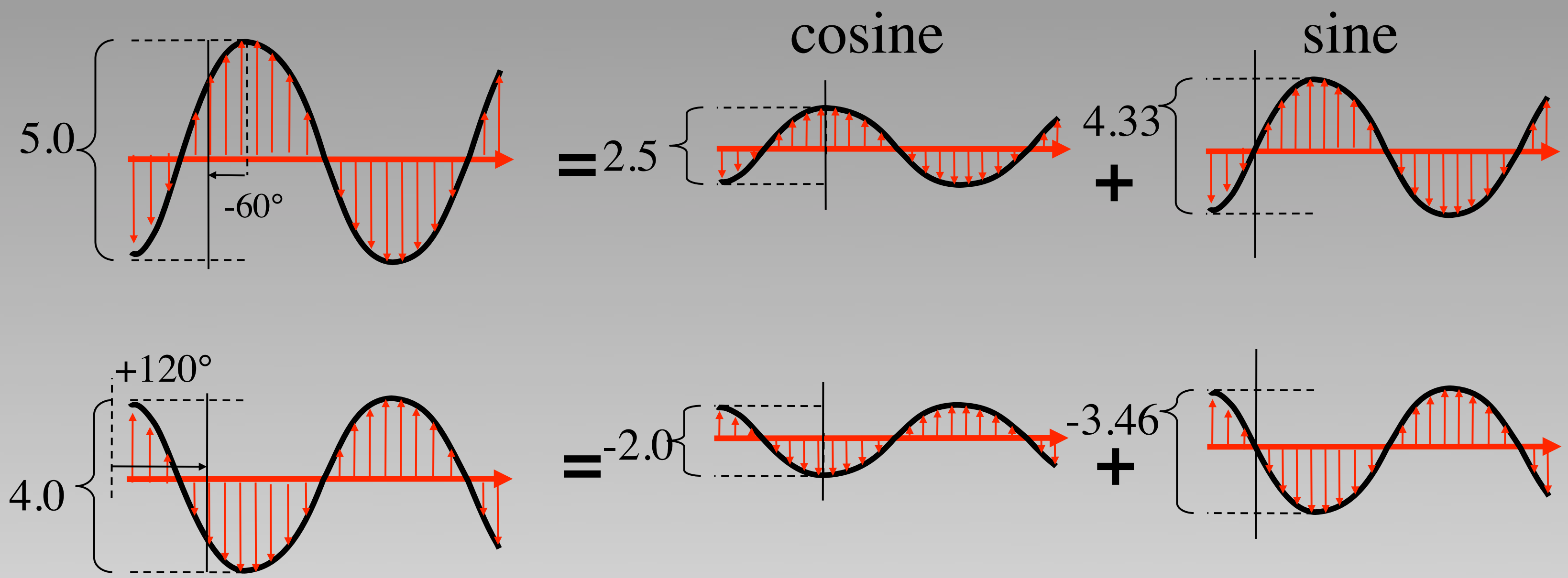
amplitude of sine wave part

A unit cosine wave.
We can call this our x-axis

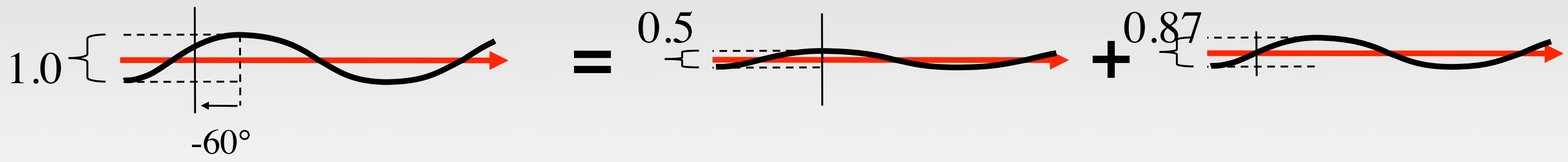
A unit sine wave.
We can call this our y-axis

Which corresponds to a point in a 2-D orthogonal coordinate system.

Adding waves by parts



Add amplitudes of cosine and sine parts, then recombine them.



Adding waves by parts

Split waves into cosine and sine parts, add them:

$$5\cos(\omega t - 60°) + 4\cos(\omega t + 120°)$$

$$= 5\{\cos(-60°)\cos(\omega t) - \sin(-60°)\sin(\omega t)\} +$$
$$4\{\cos(120°)\cos(\omega t) - \sin(120°)\sin(\omega t)\}$$

$$= [5(0.5) + 4(-0.5)]\cos(\omega t) - [5(-0.866)+4(0.866)]\sin(\omega t)$$

$$= 0.5\,\underline{\cos(\omega t)} - (-0.866)\,\underline{\sin(\omega t)}$$

reference sine wave

reference cosine wave

Cosine parts and Sine parts of waves can be summed independently, *like orthogonal coordinates*.

Adding waves by parts, part 2

Any point in orthogonal coordinates can be expressed in polar coordinates: $(x,y) = (B\cos\beta, B\sin\beta)$

So,...

$0.5\cos(\omega t) - (-0.866)\sin(\omega t) = B\cos\beta\cos(\omega t) - B\sin\beta\sin(\omega t)$

Solving for β and B...

phase= $\beta = \arctan(B\sin\beta / B\cos\beta)$

$= \arctan(-0.866/0.5)$

$= -60°$

amplitude= $B = 0.5/\cos\beta$

$= 0.5/0.5$

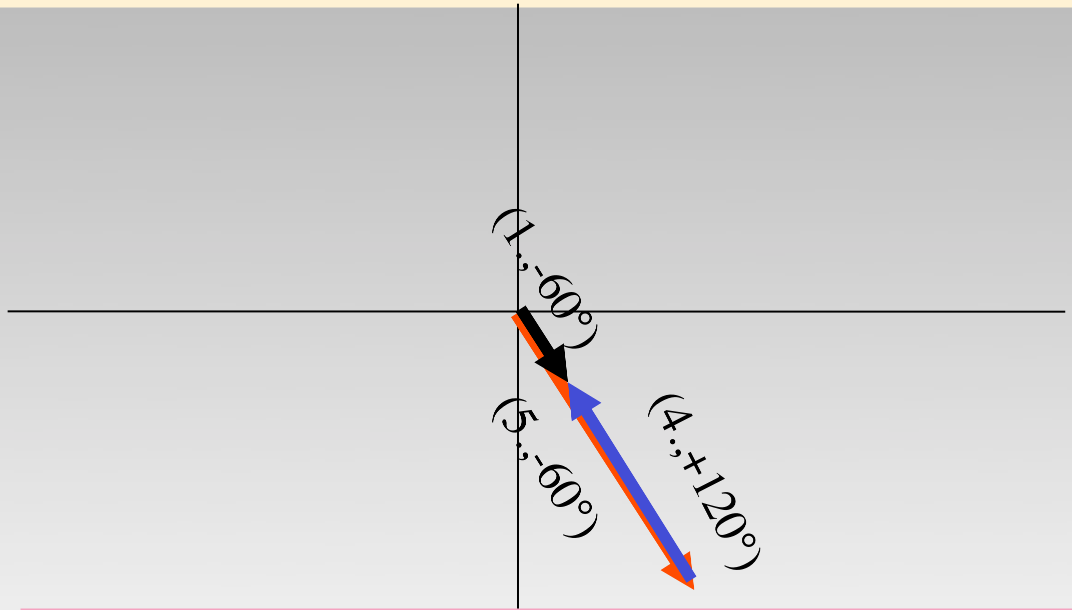
$= 1.0$

Cosine parts and Sine parts of waves can be summed independently, *like orthogonal coordinates*.

Total amplitude is Pythagorean, *like orthogonal coordinates*.

$\therefore$

Waves can be expressed in orthogonal coordinates!!



Wave addition is vector addition

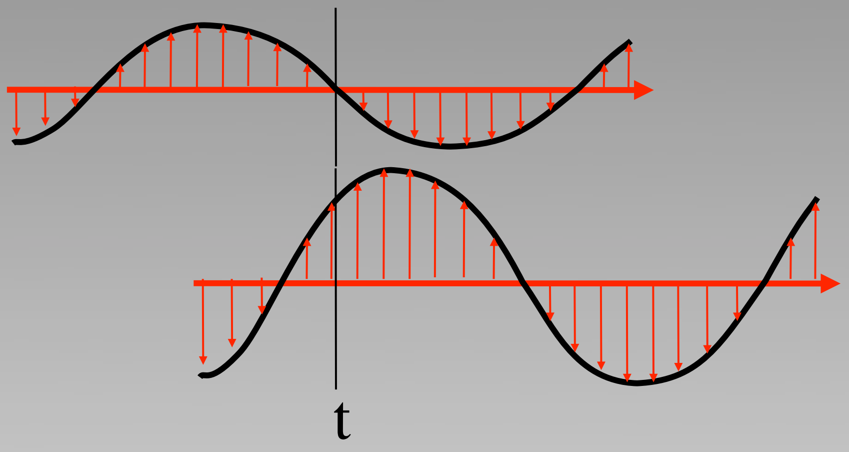
note on *arctan* function

Most calculators return a number between -90 and +90 for $\tan^{-1}(x/y)$ regardless of the sign of y.

(example: $\tan^{-1}(0/-1) = 180°$, not 0°)

For $y < 0$, add 180° to the calculator's answer.

Take home exercise: add two waves



A_1=2.0 α_1= +90°

A_2=4.0 α_2= -60°

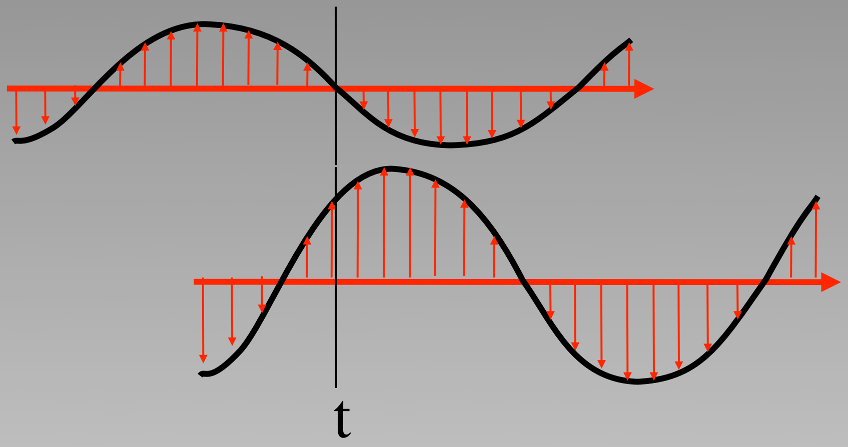
Solve this equation using the sum of angles rule:

$B\cos(\omega t+\beta) = 2.0\cos(\omega t + 90°) + 4.0\cos(\omega t - 60°)$

phase=β=______________________________

amplitude=B=______________________________

answer



$A_1=2.0$ $\alpha_1= +90°$

$A_2=4.0$ $\alpha_2= -60°$

(1)Separate each wave into sine and cosine reference waves

$$A \cos(\omega t + \alpha) = A \cos\alpha \cos\omega t - A \sin\alpha \sin\omega t$$

$$B \cos(\omega t + \beta) = B \cos\beta \cos\omega t - B \sin\beta \sin\omega t$$

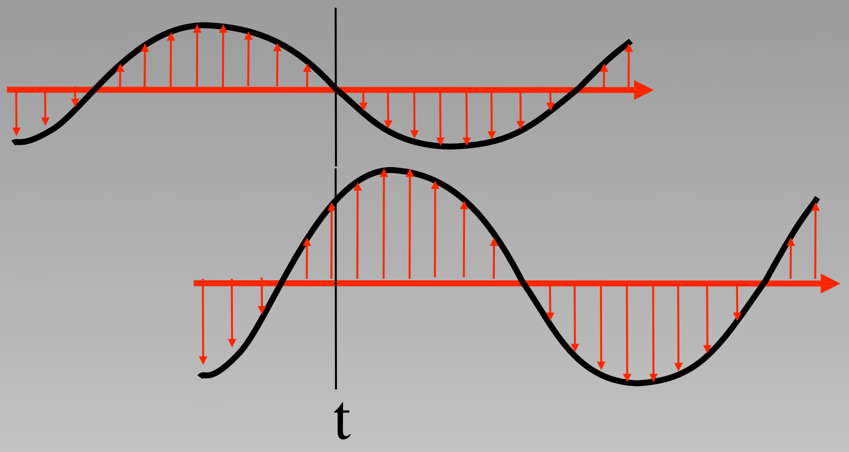
(2) Regroup

$$[A_1\cos\alpha_1 + A_2\cos\alpha_2]\cos(\omega t) - [A_1\sin\alpha_1 + A_2\sin\alpha_2]\sin(\omega t)$$

(3) New phase= $\beta=\tan^{-1}\left(\frac{[A_1\sin\alpha_1 + A_2\sin\alpha_2]}{[A_1\cos\alpha_1 + A_2\cos\alpha_2]}\right) = -36.1°$

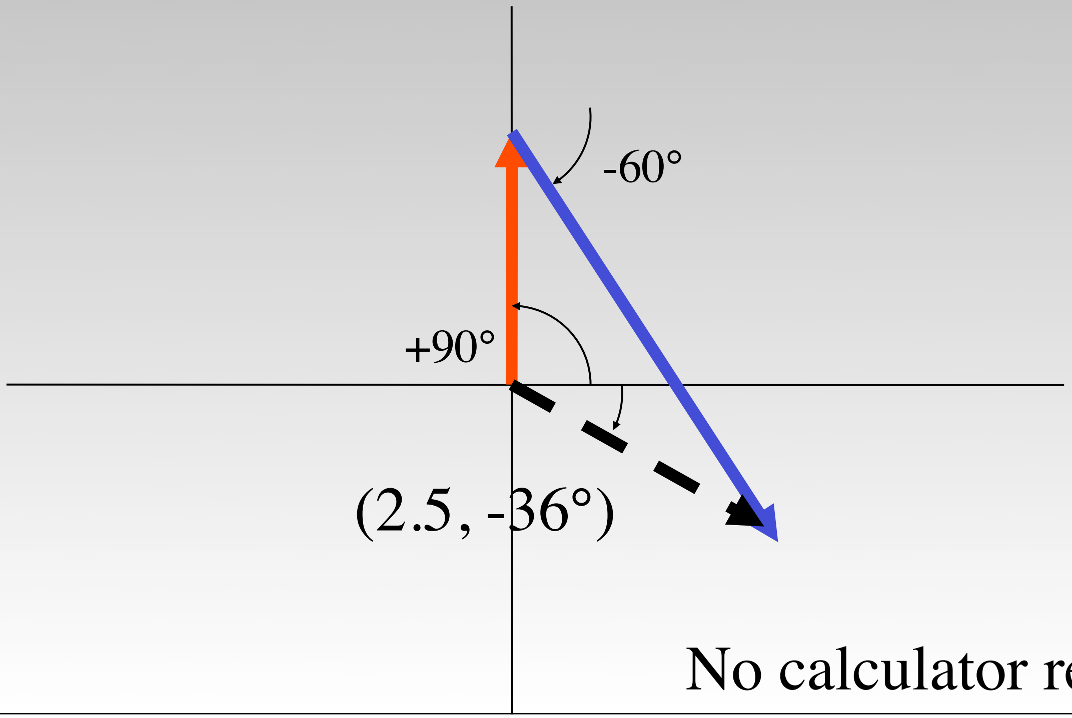
(4) New amplitude= $B= [A_1\cos\alpha_1 + A_2\cos\alpha_2]/\cos\beta = 2.47$

Same problem using paper and pencil



$A_1=2.0$ $\alpha_1= +90°$

$A_2=4.0$ $\alpha_2= -60°$



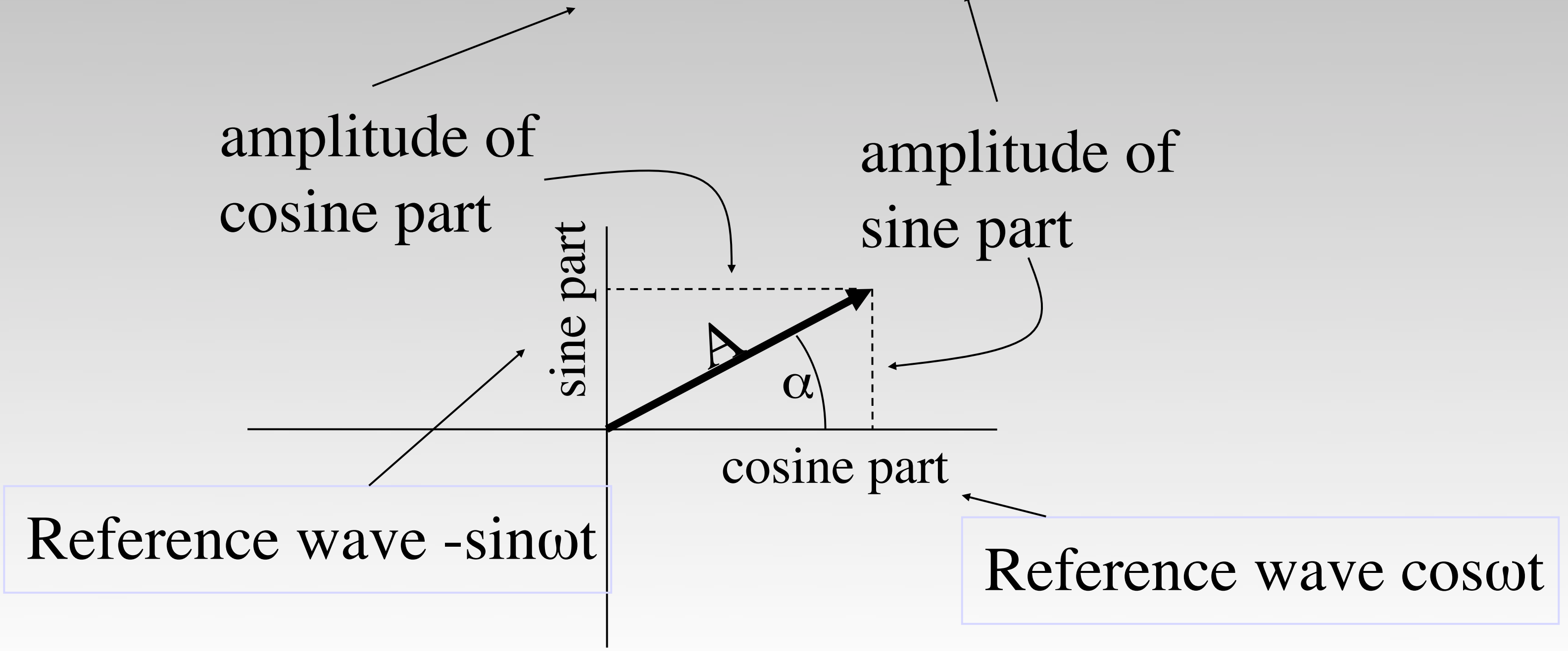
No calculator required!!

Expressing a wave in the space of sine and cosine reference waves

$E(t) = A \cos(\omega t + \alpha)$

Using the sum of angles rule:

$$A \cos(\omega t + \alpha) = \underline{A \cos\alpha} \cos\omega t - \underline{A \sin\alpha} \sin\omega t$$



amplitude of cosine part

amplitude of sine part

Reference wave -sinωt

Reference wave cosωt

For mathematical convenience, a wave can be represented as one complex number, instead of an ordered pair.

Euler's Theorem: $$e^{i\alpha} = \cos\alpha + i\sin\alpha$$

Proof: write the expansions and sum them

$$e^{\alpha} = 1 + \alpha + \alpha^2/2! + \alpha^3/3! + \alpha^4/4! + \alpha^5/5! - \cdots$$

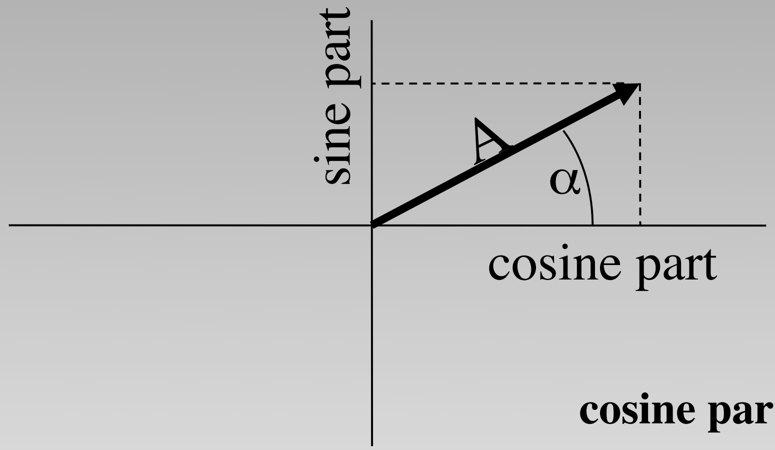
$$e^{i\alpha} = 1 + i\alpha - \alpha^2/2! - i\alpha^3/3! + \alpha^4/4! + i\alpha^5/5! - \cdots$$

$$\cos\alpha = 1 - \alpha^2/2! + \alpha^4/4! - \alpha^6/6! - \cdots$$

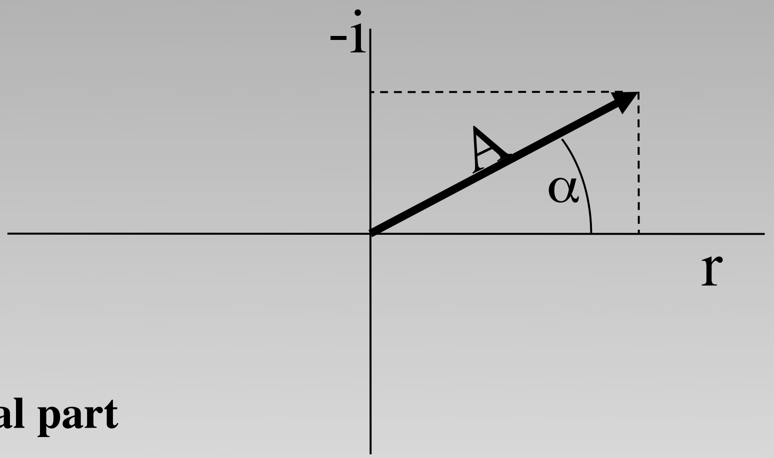
$$i\sin\alpha = i\alpha - i\alpha^3/3! + i\alpha^5/5! - i\alpha^7/7! + \cdots$$

cosine, sine space = Argand space

$(A\cos\alpha,\ A\sin\alpha)$



$Ae^{i\alpha}$



“Argand diagram”

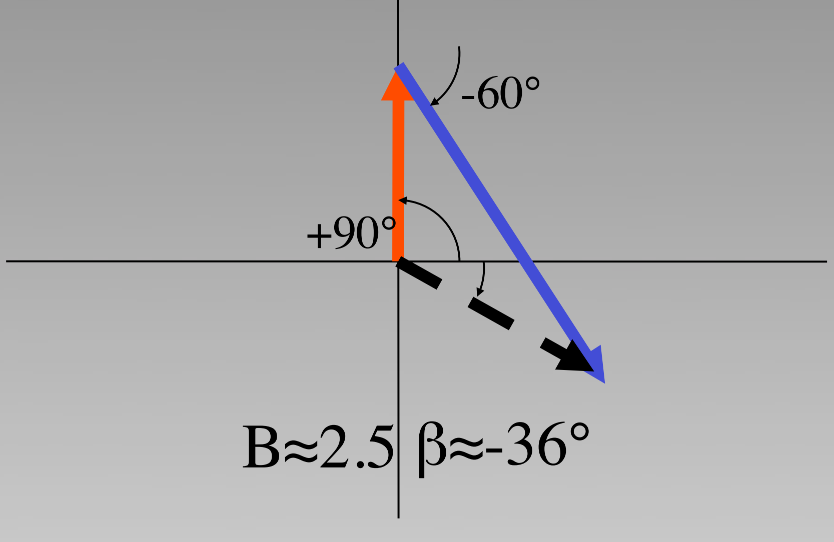
cosine part = real part

sine part = imaginary part

We may conveniently use Argand diagrams for summing waves:

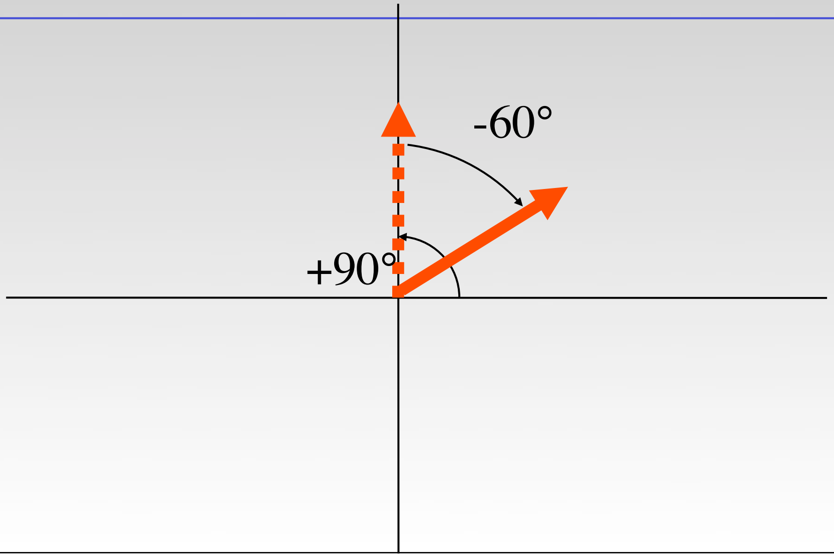
Wave addition is vector addition in Argand space

$A_1e^{i\alpha1} + A_2e^{i\alpha2}$



Multiplying complex exponentials = *phase shift*

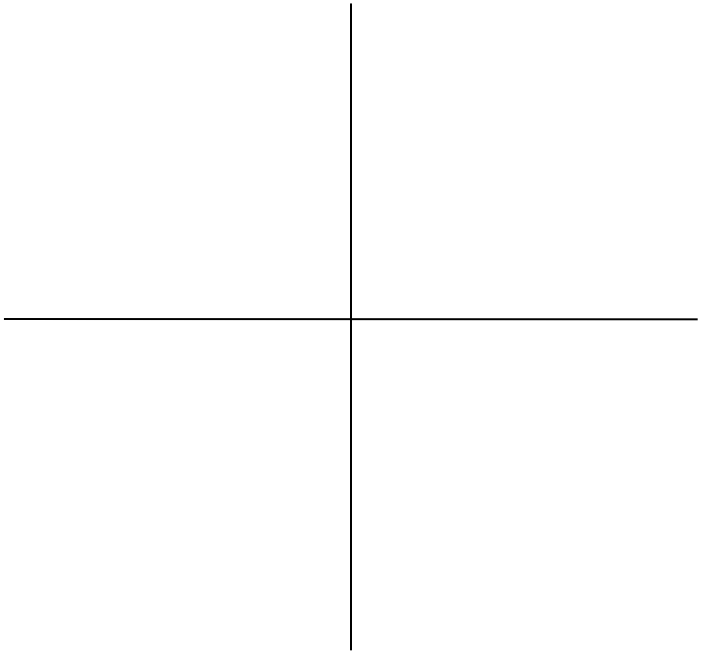
$A_1e^{i\alpha1}\, e^{i\alpha2} = A_1e^{i(\alpha1+\alpha2)}$

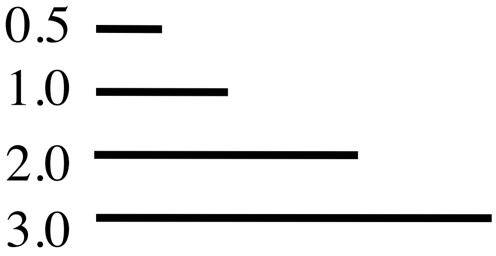


Try it: Add these waves using a protractor and ruler

Start at the origin. Add head to tail.

- 3.0, -30°
- 2.0, 180°
- 0.5, +90°
- 2.0, +45°
- 1.0, +135°
- 2.0, +120°
- 0.5, -120°

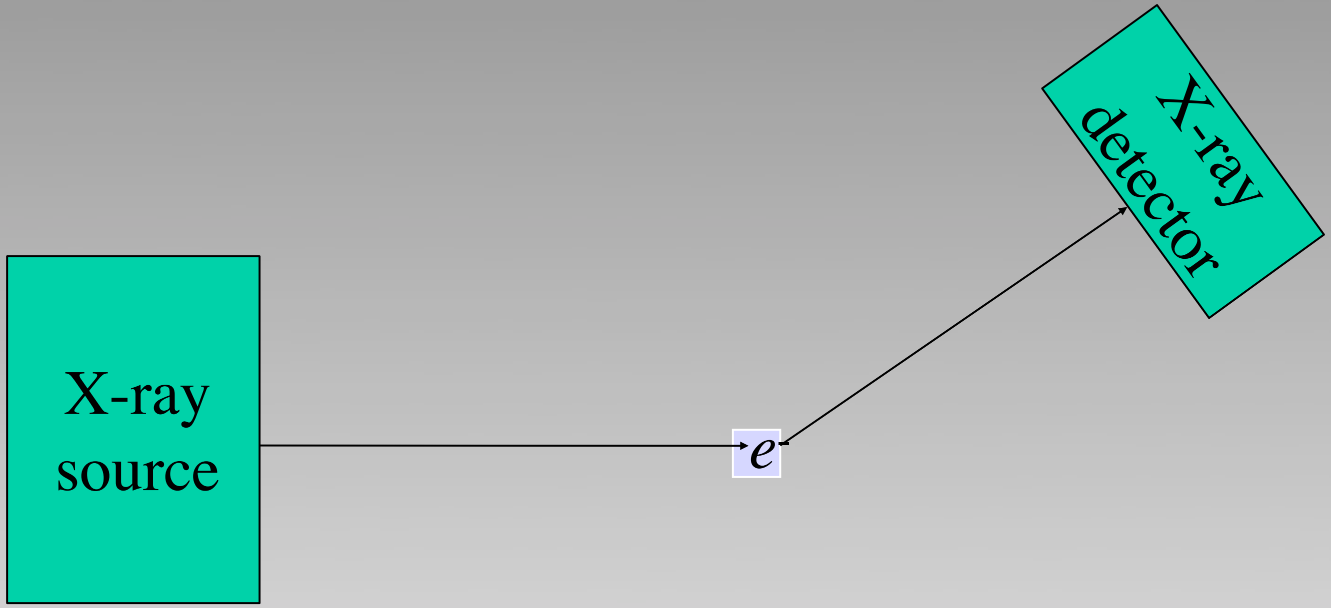




Use these bars to calibrate a makeshift ruler, if necessary.

Every electron has a phase, and the phase depends on where it is relative to the origin.

Light turns a corner at the crystal

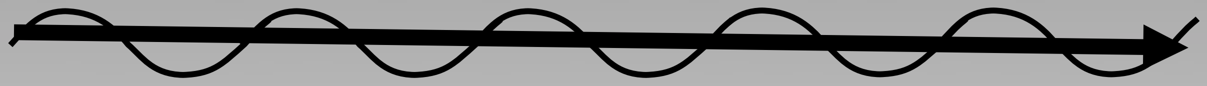


length/λ = the number of oscillations completed when hitting the detector

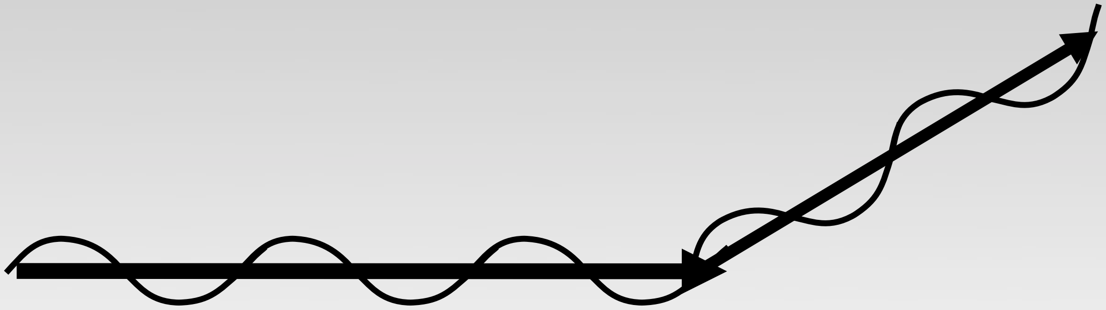
The phase is the non-integer part

Exactly *where* the light turns the corner determines the phase.

Phase depends on the distance traveled



Phase = D/ λ – nearest integer(D/λ)

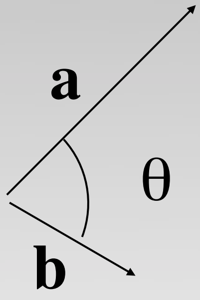


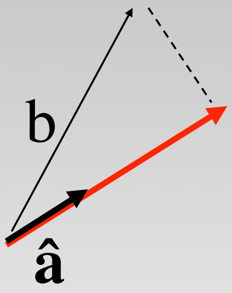
Same for scattered path

Dot product

$$\mathbf{a}\bullet\mathbf{b} = |\mathbf{a}||\mathbf{b}|\cos(\theta)$$

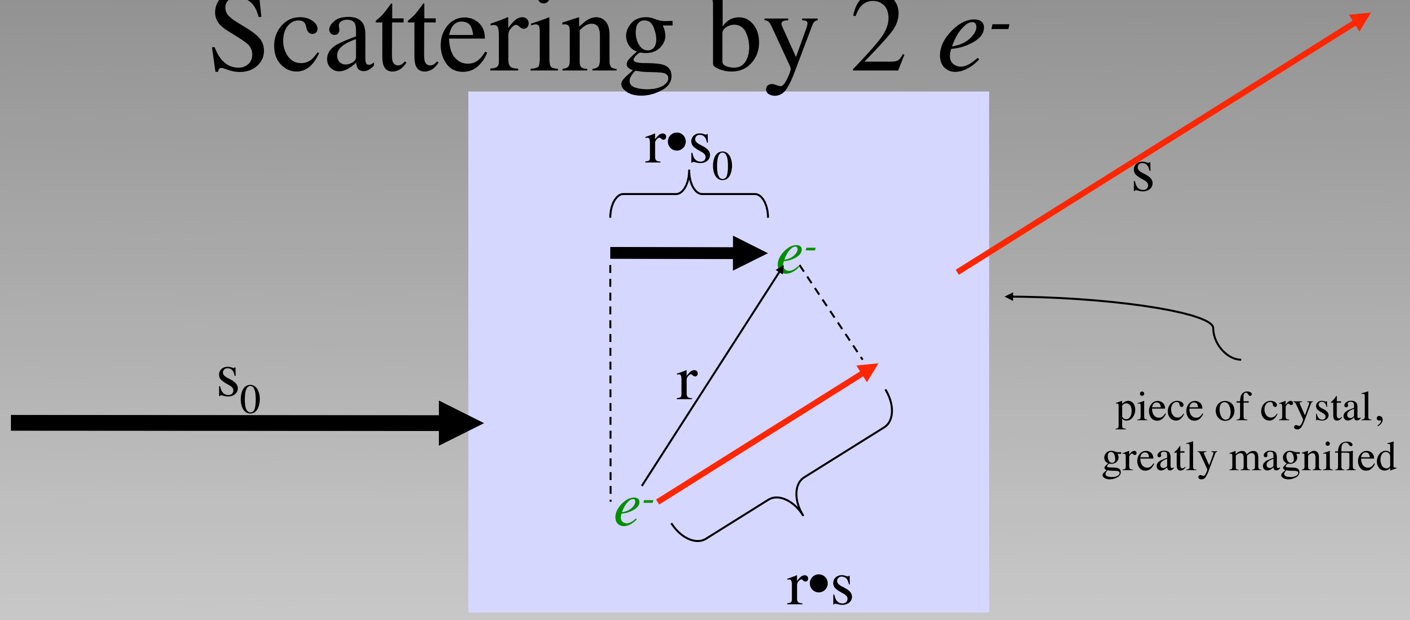
$$\mathbf{a}\bullet\mathbf{b} = a_x b_x + a_y b_y + a_z b_z$$





If **â** is a unit vector, then **â•b** is the projection of **b** on **â**.

Scattering by 2 e^-

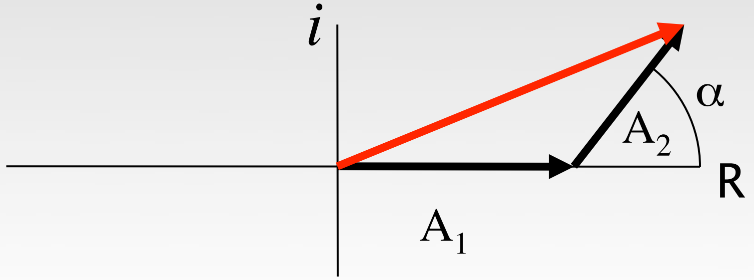


Difference in pathlength = $r \bullet s - r \bullet s_0$

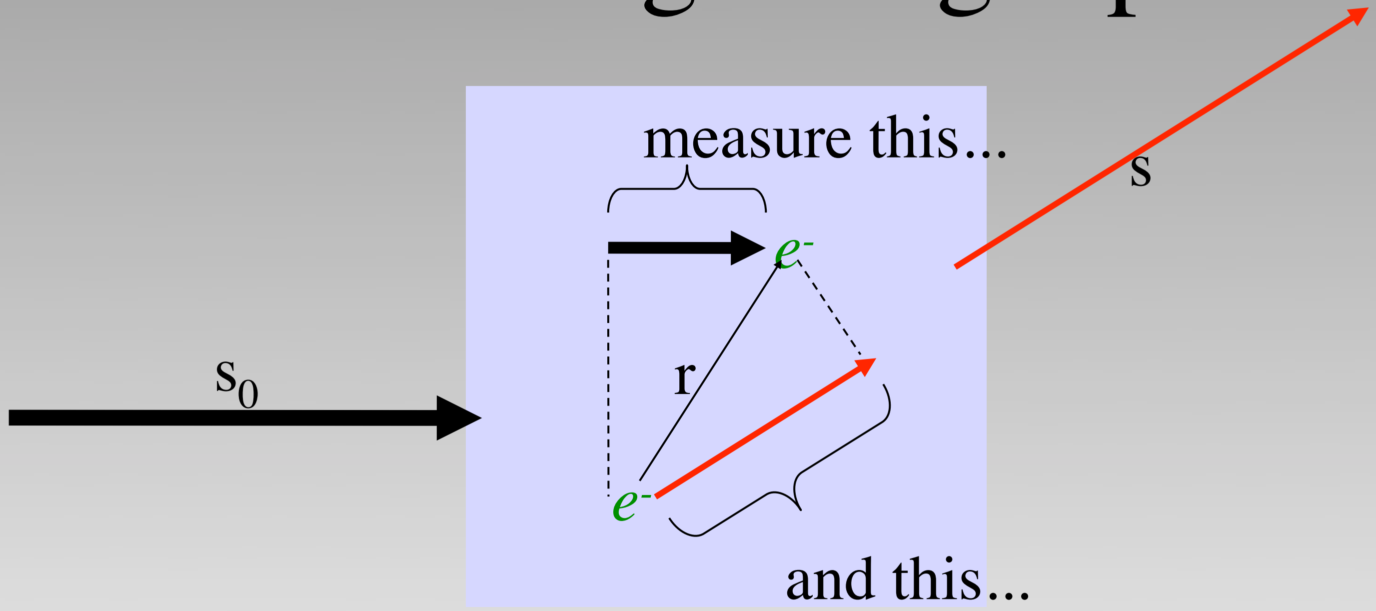
Relative phase: $\alpha = 2\pi(r \bullet s - r \bullet s_0)/\lambda$

If $e^-(1)$ scatters with amplitude A_1, and $e^-(2)$ scatters with amplitude A_2, then the sum of their scattered waves is

$$A_1 + A_2 e^{i\alpha}$$



Divide path difference by wavelength to get phase



measure this…

and this…

Get the difference, divide by the wavelength.
Multiply by 2π radians.
That's the phase difference.
Add the two waves using vectors.

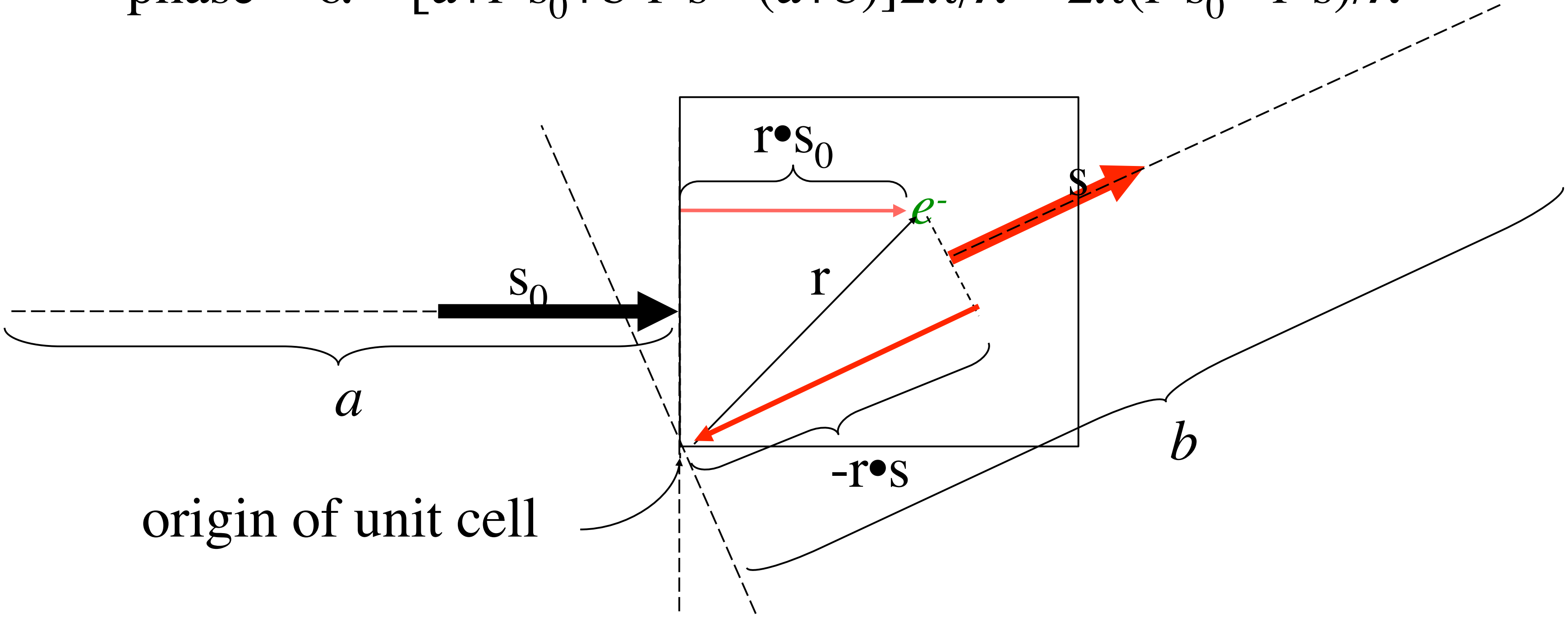
Phase equals additional distance traveled...

...divided by the wavelength

Distance from source to e^- $= a + \mathbf{r \bullet s}_0$

Distance from e^- to detector $= b - \mathbf{r \bullet s}$

$$\text{phase} = \alpha = [a + r \bullet s_0 + b - r \bullet s - (a+b)]2\pi/\lambda = 2\pi(r \bullet s_0 - r \bullet s)/\lambda$$



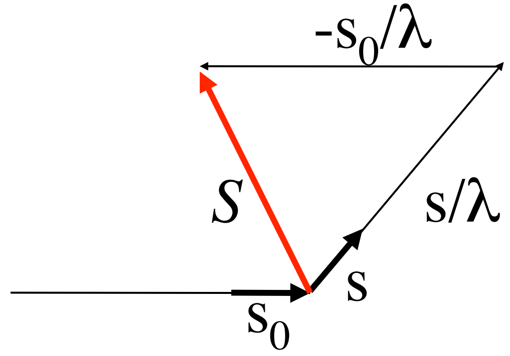
Definition of scattering vector *S*

phase of a point in space *r*:

$r = 2\pi(\mathrm{r} \bullet \mathrm{s} - \mathrm{r} \bullet \mathrm{s}_0)/\lambda$

simplifying...

$(\mathrm{r}_1 \bullet \mathrm{s} - \mathrm{r}_1 \bullet \mathrm{s}_0)/\lambda = \mathrm{r}_1 \bullet (\mathrm{s} - \mathrm{s}_0)/\lambda$



So we define the "scattering vector" *S*

$$S \equiv (\mathrm{s} - \mathrm{s}_0)/\lambda$$

Note the reciprocal Å units.
S is in *reciprocal space*!

Substituting *S* into expressions for phase:

$$\alpha_1 = 2\pi(\mathrm{r}_1 \bullet \mathrm{s} - \mathrm{r}_1 \bullet \mathrm{s}_0)/\lambda \quad = 2\pi\, S \bullet \mathrm{r}_1$$

$$\alpha_2 = 2\pi(\mathrm{r}_2 \bullet \mathrm{s} - \mathrm{r}_2 \bullet \mathrm{s}_0)/\lambda \quad = 2\pi\, S \bullet \mathrm{r}_2$$

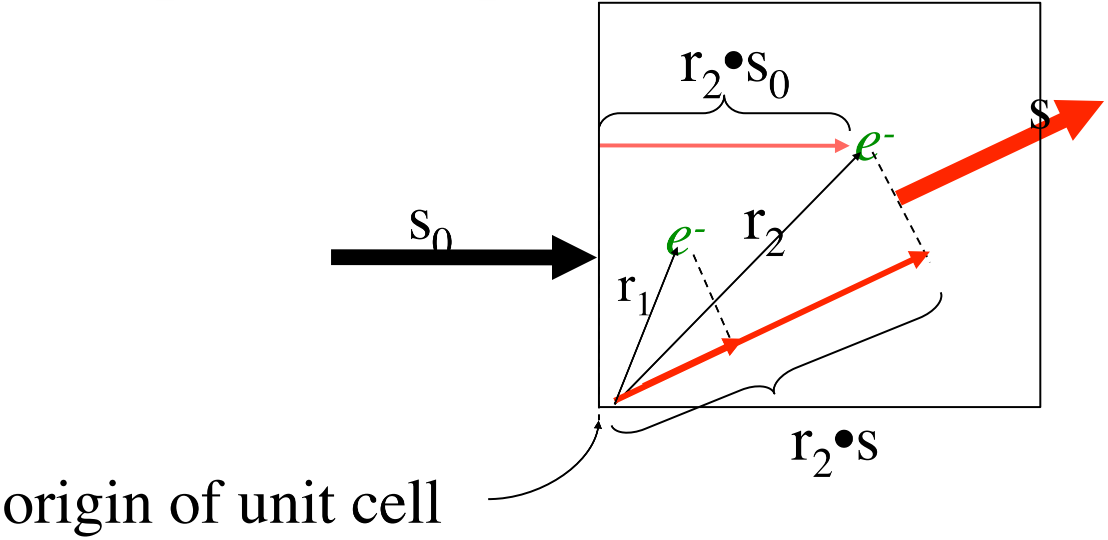
Amplitude of scatter from a point is its electron density.

$$F(S) = \sum_{k} A_k e^{i2\pi S \bullet r_k}$$

$$A_k = \rho\left(r_k\right)$$ electron density

Scattering factor for two or more regions of e^- density.

Pick any two locations in space, $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, and a direction of scatter $\boldsymbol{s}$ (a unit vector). **What is the amplitude and phase of the scattered X-rays?**



The exponent must be unit-less. Let's check:
r is in Å.
S is in 1/Å.
So units cancel!

$$\alpha_1 = 2\pi\, S \bullet r_1$$

$$\alpha_2 = 2\pi\, S \bullet r_2$$

$$F(s,s_0)=A_1e^{i\alpha_1}+A_2e^{i\alpha_2} = \sum_k A_k e^{i\alpha_k}$$

where A_k is the electron density at r_k. If we sum over all points k,

$$F(S)=\sum_k A_k e^{i2\pi S \bullet r_k}$$

Fourier transform is the sum waves from *all* points in the crystal

The amplitude of scatter from each volume unit **d*r*** *is* proportional to the electron density at the point, ρ***(r)***, times the volume unit **d*r***, and the phase is 2πS•r. This is summed over all ***dr***, so the total wave summation can be written as

$$\lim_{dr\to 0} \left[\rho(r_1) e^{i 2\pi S \bullet r_1} dr + \rho(r_2) e^{i2\pi S \bullet r_2} dr + \ldots \right.$$

$$= \int \rho(r) e^{i2\pi S \bullet r} dr$$

Please note: this is really a triple integral: dr = dx dy dz