Diffraction: The core theory

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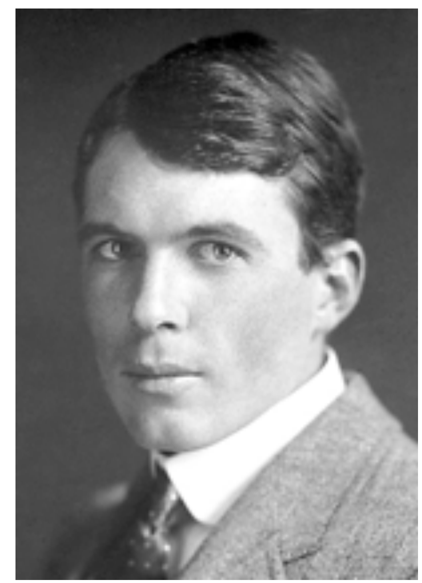
The theory of scattering of light by matter....the basis for x-ray crystallography and an application of the Fourier transform.

Christiaan Huygens
1629 - 1695

Thomas Young
1773 - 1829



William Lawrence Bragg
1890 - 1971

Still linear systems at the large variable limit….

	n = 1	n = 2 or 3	n >> 1	continuum
Linear	exponential growth and decay single step conformational change fluorescence emission pseudo first order kinetics	second order reaction kinetics linear harmonic oscillators simple feedback control sequences of conformational change	electrical circuits molecular dynamics systems of coupled harmonic oscillators equilibrium thermodynamics diffraction, Fourier transforms	Diffusion Wave propagation quantum mechanics viscoelastic systems
Nonlinear	fixed points bifurcations, multi stability irreversible hysteresis overdamped oscillators	anharmonic oscillators relaxation oscillations predator-prey models van der Pol systems Chaotic systems	systems of non-linear oscillators non-equilibrium thermodynamics protein structure/ function neural networks the cell ecosystems	Nonlinear wave propagation Reaction-diffusion in dissipative systems Turbulent/chaotic flows

adapted from S. Strogatz

The theory of diffraction

a. light as waves ... basic properties
b. An optical diffraction experiment to build our intuition.
c. Wave addition and the Argand diagram.
d. x-ray scattering ... simple to complex structures.
e. The molecular transform.
f. x-ray scattering from a crystal of molecules.
g. The crystal transform.

Why x-rays for solving atomic structures?

According to the Abbe (1840-1905) Theory of the microscope, a distance dx is resolvable by light of wavelength λ in ideal circumstances according to the rule:

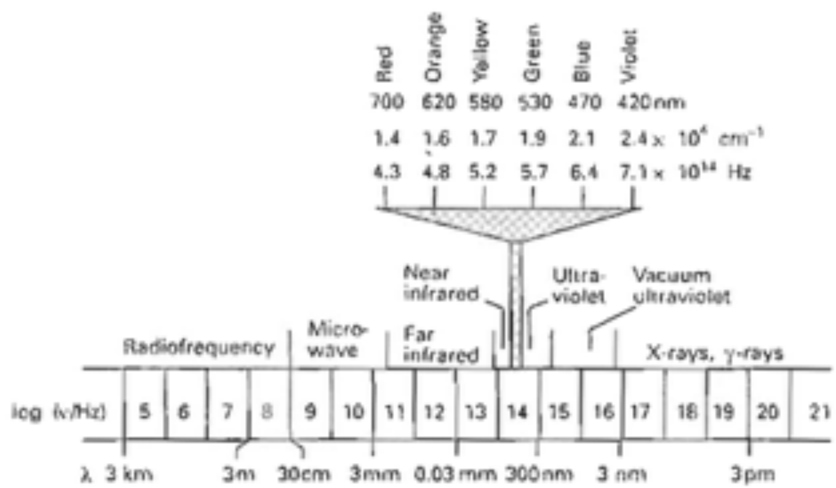
$$\boxed{dx = \frac{\lambda}{2\,(N.A)}}$$

, where N.A is numerical aperture.

The point is that with visible light [400-700 nm ... or 4,000 - 7,000 Å], we can at best resolve spacings of ~250nm.

Why x-rays for solving atomic structures?

In order to resolve things at atomic scale (1-1.5Å), we need much higher energy (smaller wavelength) electromagnetic radiation, more like 0.5→2Å. This is in the middle of the x-ray portion of the electromagnetic spectrum.



The need for a theory of diffraction...

So ... then shouldn't we just build a microscope that uses x-rays rather than visible light?

The need for a theory of diffraction...

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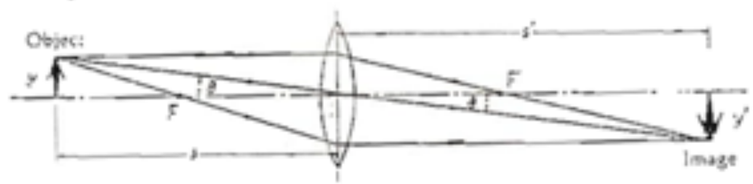
Well... there's a problem. In microscopes, images are formed by scattering of light by the object and subsequent focusing of the scattered waves by a lens.



But ... xrays are so high in energy that they penetrate everything (almost). Thus, there is no xray lens and we cannot focus the scattered radiation into an image.

A demo...

The need for a theory of diffraction...

So how do we solve this problem?

We collect the diffraction pattern upon irradiating a sample with x-rays and we use the theory of diffraction to calculate the structure from this pattern.

The key concept here is that the diffraction pattern contains all the information required to reconstruct the object! How? And what is the nature of the way in which the diffraction pattern stores the information?

Some mathematical preliminaries…complex numbers!

A complex number has the form . . .

$$z = x + iy \quad \text{where} \quad i = \sqrt{-1}$$

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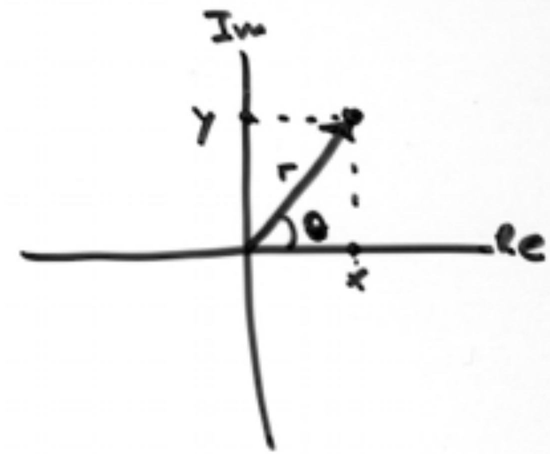

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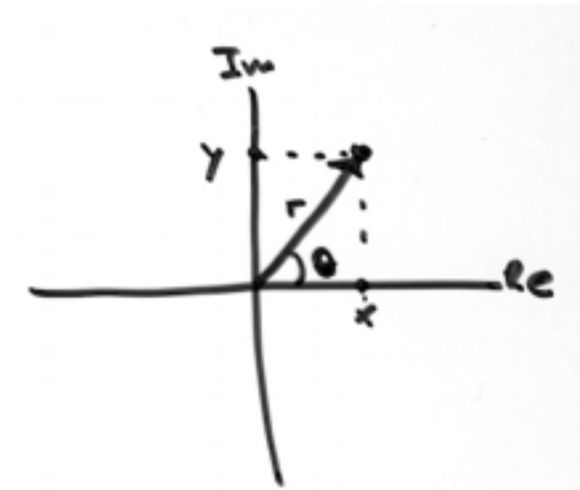

Can also write it in polar coordinates ...

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

$$\theta = \arctan\left[\frac{y}{x}\right]$$

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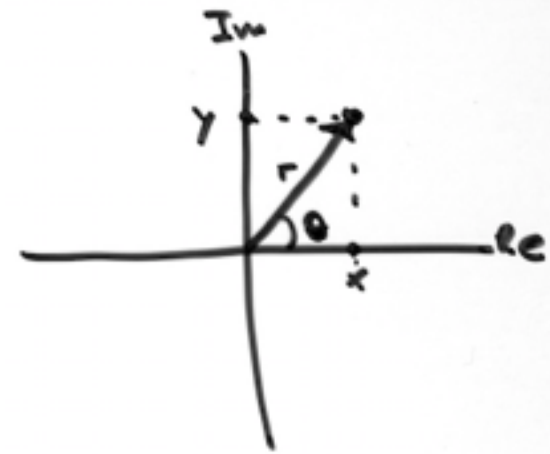

Can also write it in polar coordinates ...

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

$$\theta = \arctan\left[\frac{y}{x}\right]$$

Note that

$$x = r\cos\theta$$
$$y = r\sin\theta$$

So..

$$z = r\cos\theta + i\sin\theta$$

Some mathematical preliminaries…complex numbers!

Now for Euler's formula… relates exponential function to trigonometric functions!

power series definitions of a few key functions:

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$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

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$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1}$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n}$$

Some mathematical preliminaries…Euler's formula

So… $e^{x+iy} = e^{x}e^{iy}$

Some mathematical preliminaries…Euler's formula

So…

$$e^{x+iy} = e^x e^{iy}$$

$$= e^x\left[1 + yi + \frac{(yi)^2}{2!} + \frac{(yi)^3}{3!} + \cdots\right]$$

$$= e^x\left[1 + yi - \frac{y^2}{2!} - i\frac{y^3}{3!} + \frac{y^4}{4!} + i\frac{y^5}{5!} + \cdots\right]$$

$$= e^x\left[\left(1 - \frac{y^2}{2!} + \frac{y^4}{4!} + \cdots\right) + i\left(y - \frac{y^3}{3!} + \frac{y^5}{5!} + \cdots\right)\right]$$

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$$= e^x\left[\cos y + i \sin y\right]$$

because….

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1}$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n}$$

Some mathematical preliminaries…Euler’s formula

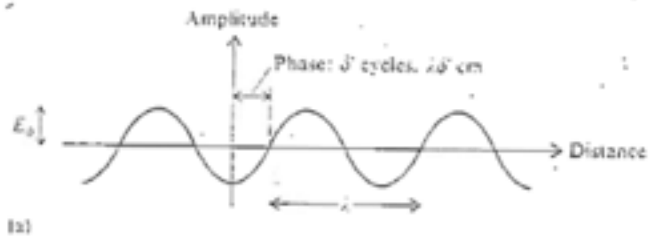
This is Euler's formula. When $z = x + iy$ is purely imaginary $(x=0)$

$$e^{iy} = \cos y + i \sin y$$

One of the great formula’s of mathematics….

The basics...

(I) X-rays are photons.



a. E_0 is amplitude

b. λ is wavelength (in Å)

c. ν is frequency $= \frac{c}{\lambda}$ (in 1/sec or Hz)

d. ω is angular frequency $= 2\pi\nu = 2\pi \frac{c}{\lambda}$

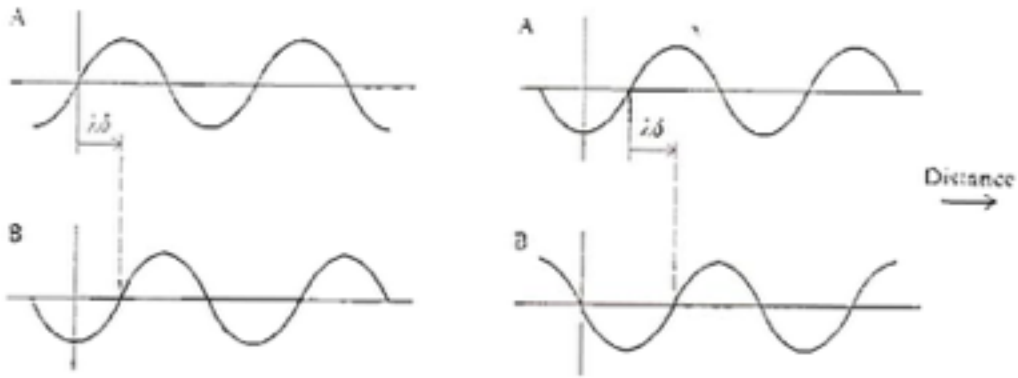
Like all electromagnetic radiation, an xray is a wave that propagates in time and space. It has characteristic amplitude (E_0 here) which gives its intensity and characteristic wavelength (λ).

The phase (α or ϕ) is how much of one wavelength the wave is displaced from a reference point.

So... given a phase α and a wavelength λ, the wave is displaced by $\alpha \cdot \lambda$ Å.

The basics...

Note that phase is a relative quantity



$t = 0$
B *leads* by δ cycles

$t = t$
B *still* leads by δ

Now, ways of representing a wave...

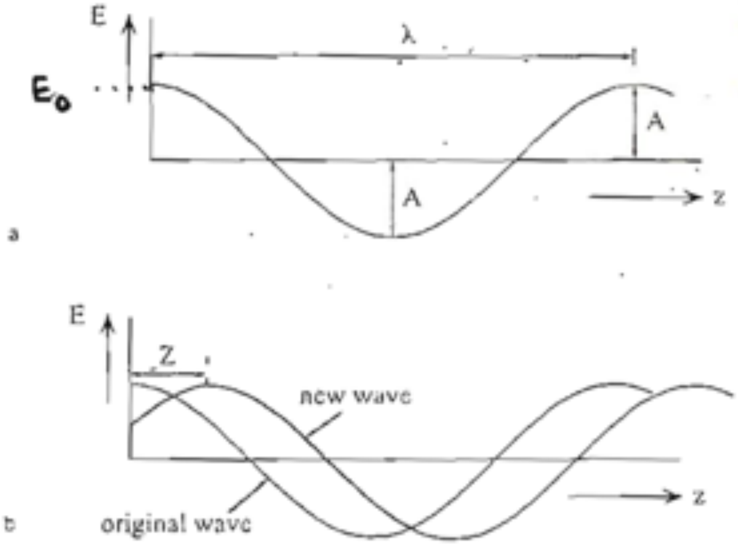


Figure 4.1. (a) The electric component of an electromagnetic wave. A is the amplitude and λ the wavelength. The accompanying magnetic component is perpendicular to the electric one, but we do not need to consider it here. (b) A new wave, displaced over a distance Z. is added.

a. E_0 = amplitude

b. λ = wavelength

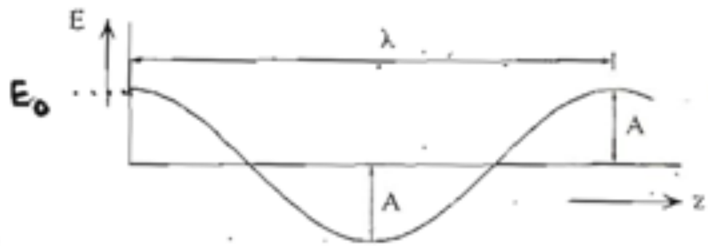
c. $\omega = 2\pi \frac{c}{\lambda}$ where...

$\frac{c}{\lambda} = \nu$, the frequency.

ω is in radians/sec.

Light as a traveling electromagnetic wave....

Now, ways of representing a wave...



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Now, one way of representing a wave is as a cosine function:

$$\boxed{E(t) = E_0 \cos(\omega t)}$$

Let's check this....

when $t=0$, $E(t) = E_0 \cos(0) = E_0$

$t = \frac{\lambda}{c}$, $E(t) = E_0 \cos(2\pi) = E_0$

$t = \frac{1}{2}\frac{\lambda}{c}$, $E(t) = E_0 \cos(\pi) = -E_0$

$t = \frac{1}{4}\frac{\lambda}{c}$, $E(t) = E_0 \cos(\frac{\pi}{2}) = 0$

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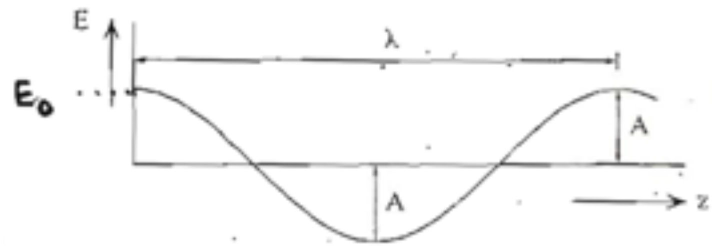

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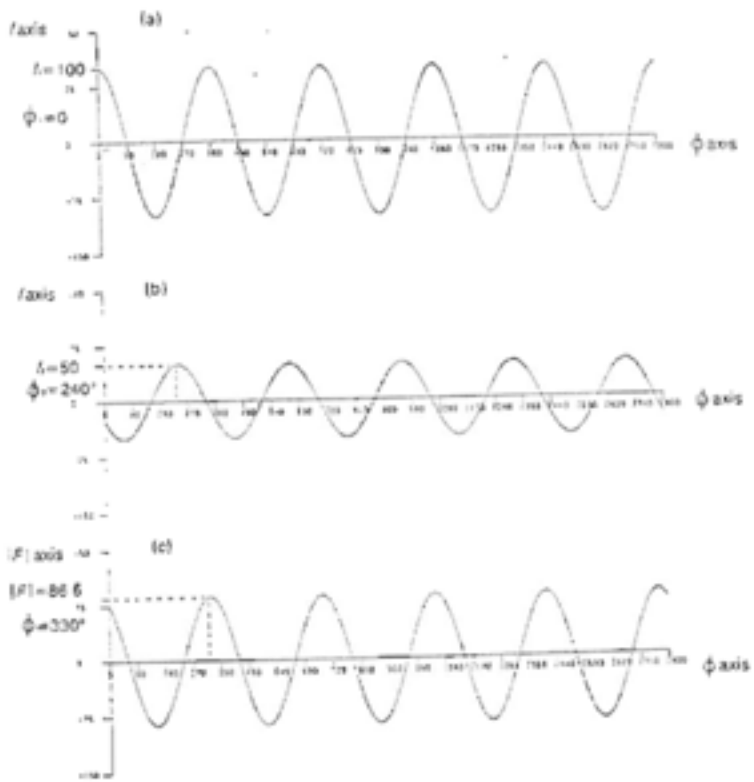
If a phase shift is added, then...

$$\boxed{E(t) = E_0 \cos(\omega t + \alpha)}$$

Two waves can be added, but the result is a little non-intuitive:



$f_1 = 100$
$\phi_1 = 0$

$f_2 = 50$
$\phi_2 = 240°$
(~ 0.6 radians)

$|F| = 86.6$
$\phi = 330°$

So, adding two waves of different amplitude and phase but same wavelength gives a new wave of the same wavelength....but different and new amplitude and phase

Let's understand this ...

wave 1: $E_1(t) = f_1 \cos(\omega t)$

wave 2: $E_2(t) = f_2 \cos(\omega t + \alpha)$

How to add these? We know that the new wave will have same angular frequency ω $\left[\omega = 2\pi \frac{c}{\lambda}\right]$, but how can we predict the amplitude and phase?

Well...

$$E_2(t) = f_2 \cos(\omega t + \alpha)$$

$$= f_2 \cos\alpha \cos\omega t - f_2 \sin\alpha \sin\omega t$$

$$= \underline{f_2 \cos\alpha} \cos\omega t + \underline{f_2 \sin\alpha} \cos(\omega t + 90^\circ)$$

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The addition rules:

$\cos(A+B) = \cos A \cos B - \sin A \sin B$

$\cos(A-B) = \cos A \cos B + \sin A \sin B$

$\sin(A+B) = \sin A \cos B + \cos A \sin B$

$\sin(A-B) = \sin A \cos B - \cos A \sin B$

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$$= \underline{f_2 \cos\alpha} \cos\omega t + \underline{f_2 \sin\alpha} \cos(\omega t + 90°)$$

Thus, any wave with an amplitude (f_2) and a phase angle α can be viewed as a sum of two waves with angular frequency ω:

1. $f_2 \cos\alpha$ [amplitude] and 0 [phase]

2. $f_2 \sin\alpha$ [amplitude] and 90° [phase]

Now let's introduce a simple graphical way of seeing this .... the Argand diagram.

$$E_2(t) = f_2 \cos(\omega t + \alpha)$$

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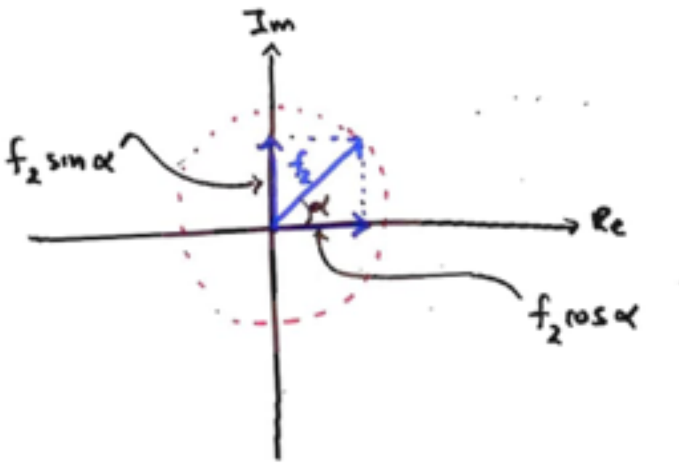
we can plot the two waves as:



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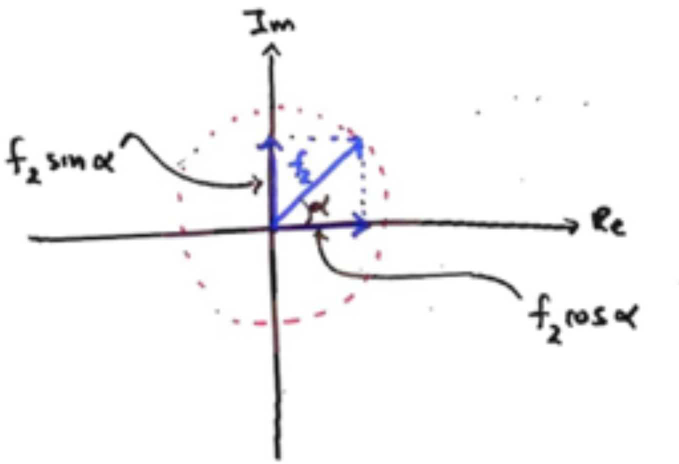
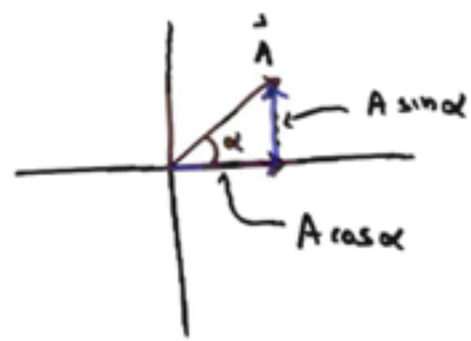
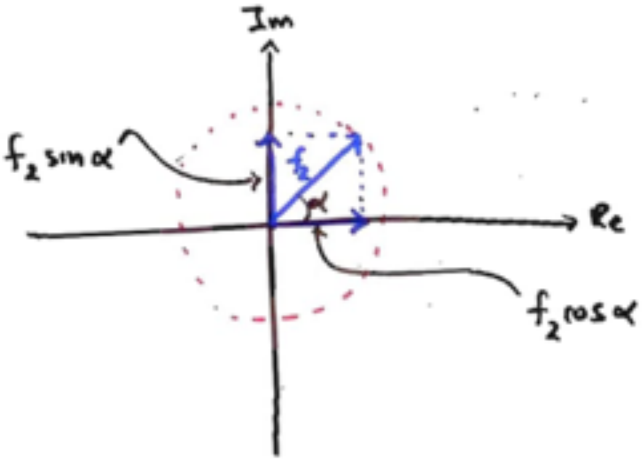


Now, remember that given a vector $\vec{A}$:



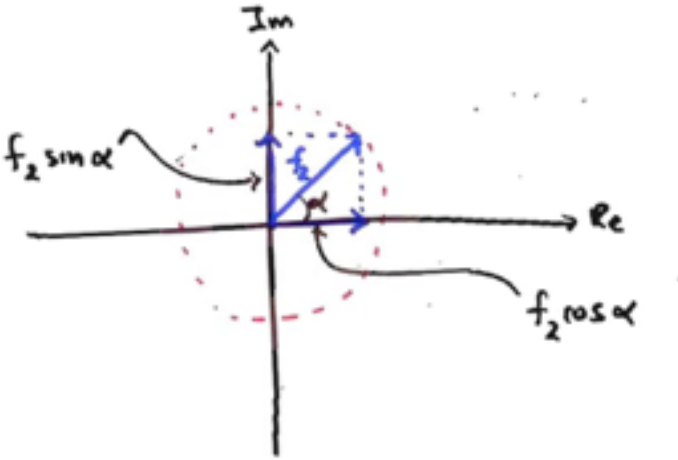
we can plot the two waves as:



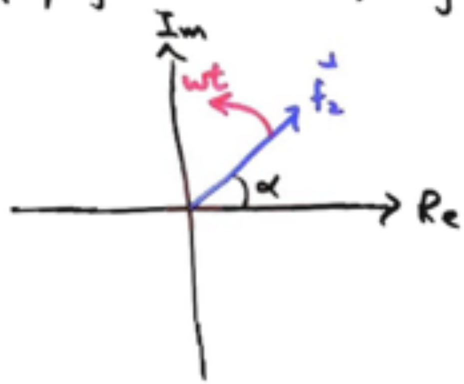
- So .... the wave $E_2(t) = f_2 \cos(\omega t + \alpha)$ is a vector $\vec{f_2}$ at time $t=0$ that makes an angle α with the real axis. This is the phase shift.

- It has projections $f_2 \cos\alpha$ with the real axis and $f_2 \sin\alpha$ with the imaginary axis.

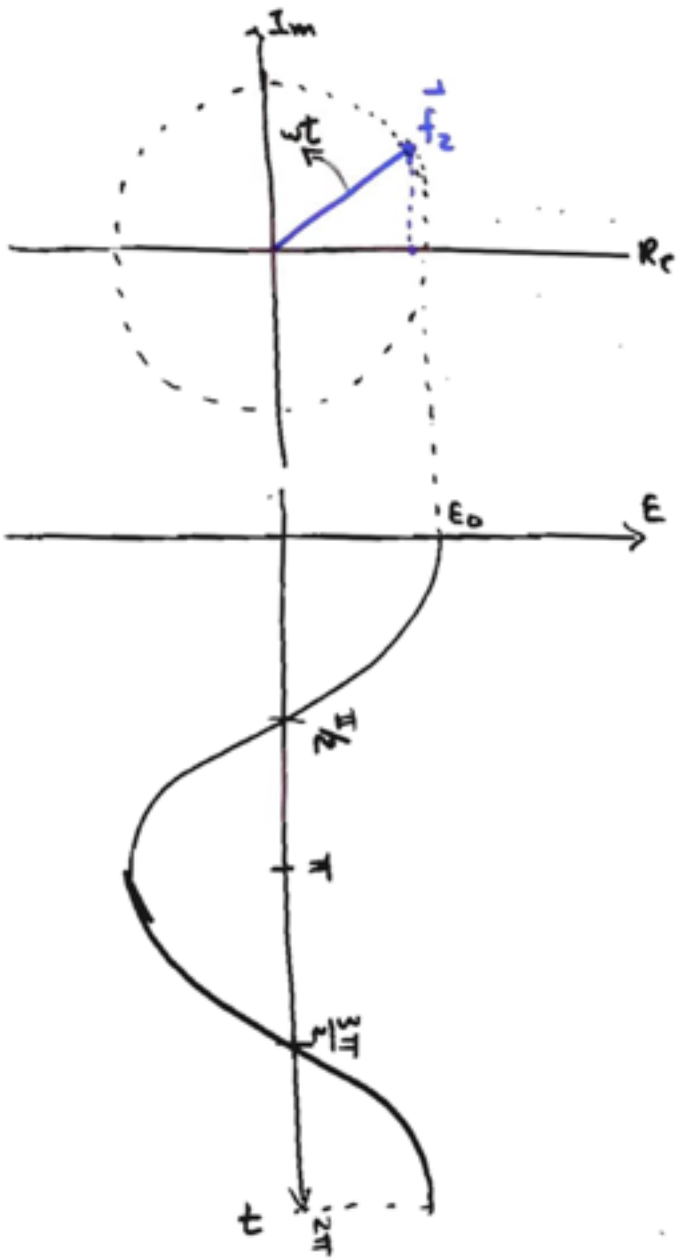
we can plot the two waves as:



- As the wave propagates in time, it goes around with angular velocity ωt.



Do you see that its projection on the real axis is the cosine wave?



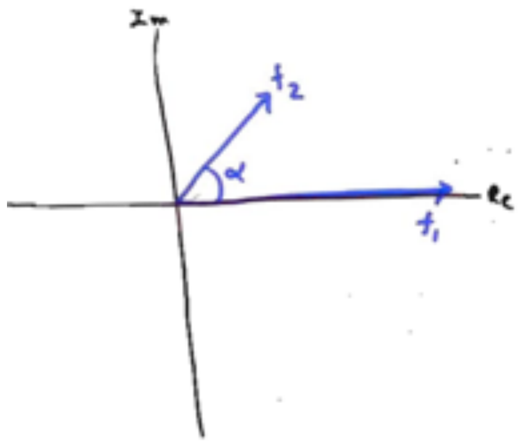
$$\omega t = 2\pi\nu t = \frac{2\pi c}{\lambda} t$$

So, the rotation of the vector in the Argand diagram describes a propagating wave in its projection on the real axis...

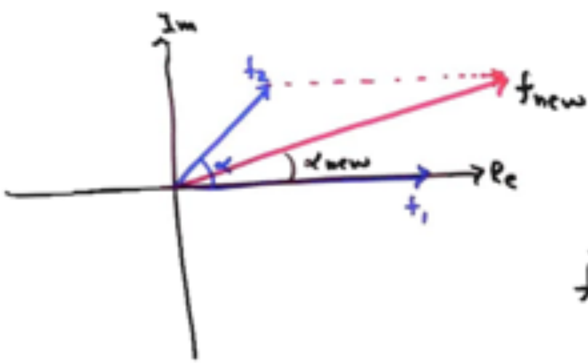
Why is this a good way to look at oscillating waves?

Remember, we started wanting to just add two wave:

$$E_1(t) = f_1 \cos \omega t$$
$$E_2(t) = f_2 \cos(\omega t + \alpha)$$



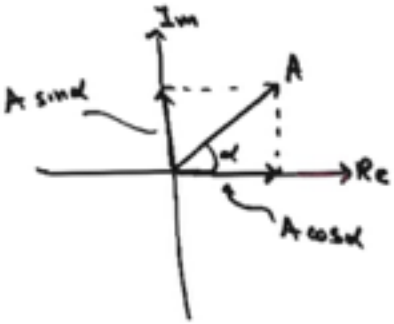
To add $\vec{f}_1$ and $\vec{f}_2$ (that is add waves $E_1(t)$ and $E_2(t)$):



$$\vec{f}_{new} = f_{new} \cos(\omega t + \alpha_{new})$$

So we can add waves by adding their vector diagrams in this representation...

Now ... back to the Argand diagram for a further simplification ...



we said vector A goes around and around at speed ωt. But all of our vectors always rotate at ωt since λ never changes in our experiment!

$$\omega = 2\pi\nu = \frac{2\pi c}{\lambda}$$

The only things that ever change in a diffraction experiment are A and α.

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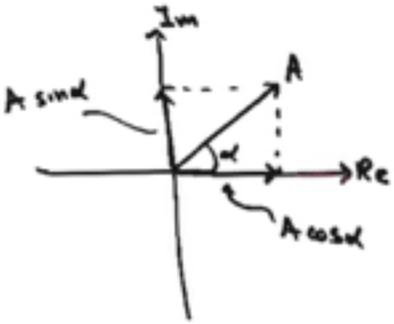

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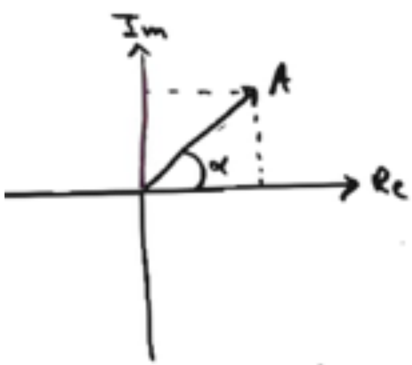
Thus, let's just simplify and write our wave as:



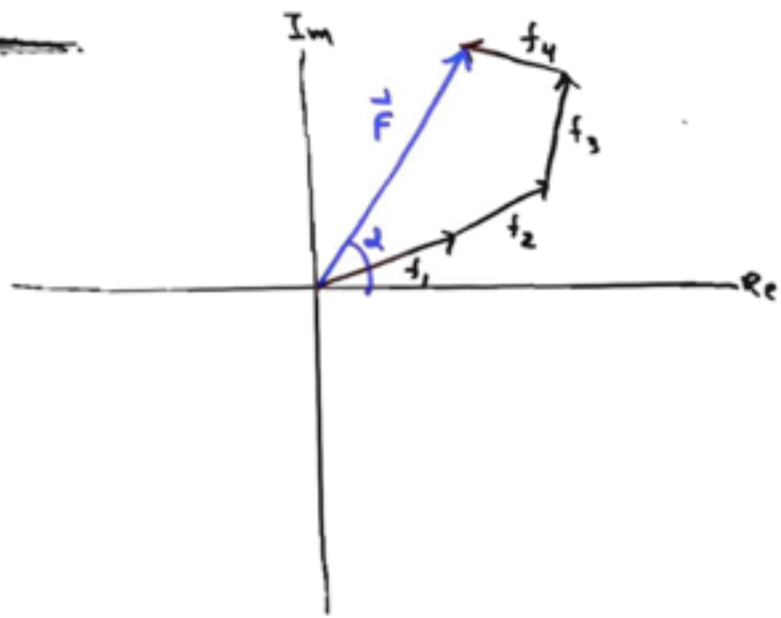
$$\boxed{\vec{A} = A\cos\alpha + i\,A\sin\alpha}$$

(The i denotes the imaginary axis and specifies a phase shift of 90°).

So... to be clear:

① This means a wave with amplitude A and phase α and angular velocity ωt where ω is given by the wavelength.

② Two waves can be added by standard vector addition to give a new amplitude and phase. Angular velocity never changes if the wavelength does not change.



Two more useful things:

① We are about to add a lot of waves! So we produce an even simpler notation for our waves:

we said $\vec{A} = A\cos\alpha + iA\sin\alpha$

Now Euler's theorem tells us that this wave can be written as a complex exponential:

$$\boxed{A\cos\alpha + iA\sin\alpha = Ae^{i\alpha} \quad \text{[Euler's theorem]}}$$

Nothing special... this is sometimes called the phasor representation of a wave. It has amplitude A and phase α.

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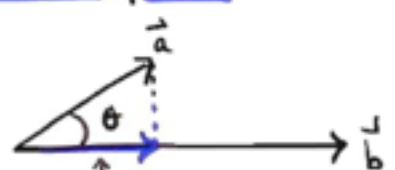
② The dot product:

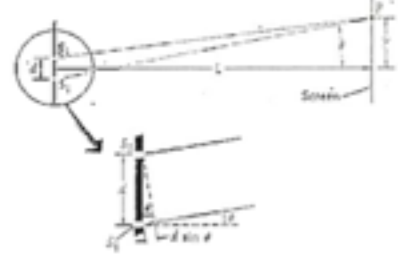


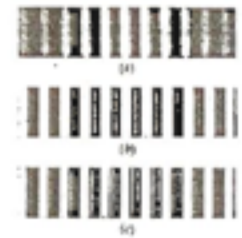
$$\boxed{a \cdot b \equiv |a||b|\cos\theta}$$

This is the projection of $\vec{a}$ onto $\vec{b}$.

Now, for diffraction... a quick example from optical diffraction

Two slit diffraction





Interference patterns for (a) two, (b) three, and (c) four coherent sources. In (b) there is a secondary maximum between each pair of principal maxima, and in (c) there are two such secondary maxima.

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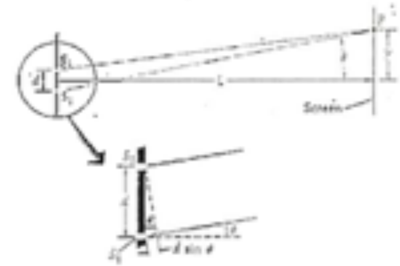

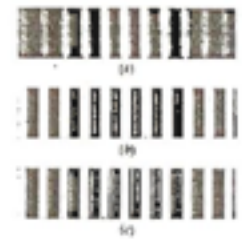

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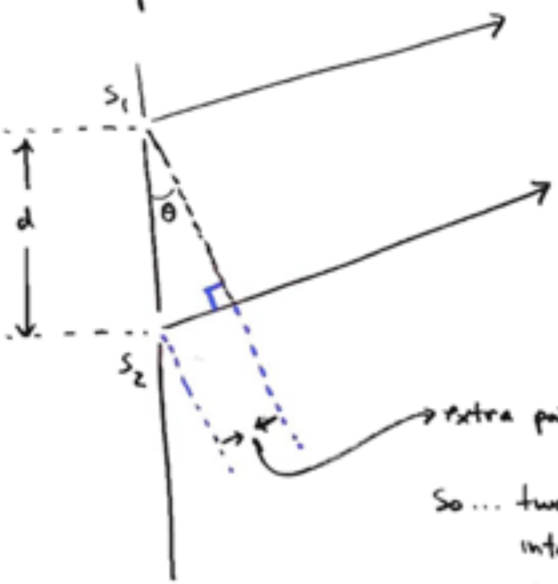
Blow up...



extra path length for the source at S_2 is $d \sin\theta$

So... two diffracted rays of light will constructively interfere whenever the extra path length is equal to some integer multiple of the wavelength.

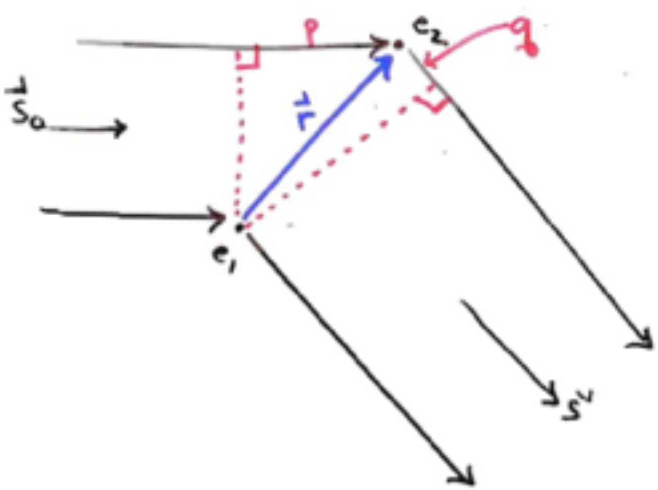
$$d \sin\theta = m\lambda$$

They will destructively interfere when the path length is half of an integer multiple:

$$d \sin\theta = \frac{m\lambda}{2}$$

x-ray diffraction...

① A system of two electrons.



X rays traveling along unit vector $\vec{S}_o$ are scattered in all directions. Let's just focus for now on one direction ... $\vec{s}$.

$$|S_o| = |s| = \frac{1}{\lambda}$$

so... $\lambda |S_o| = 1$.

x-ray diffraction...

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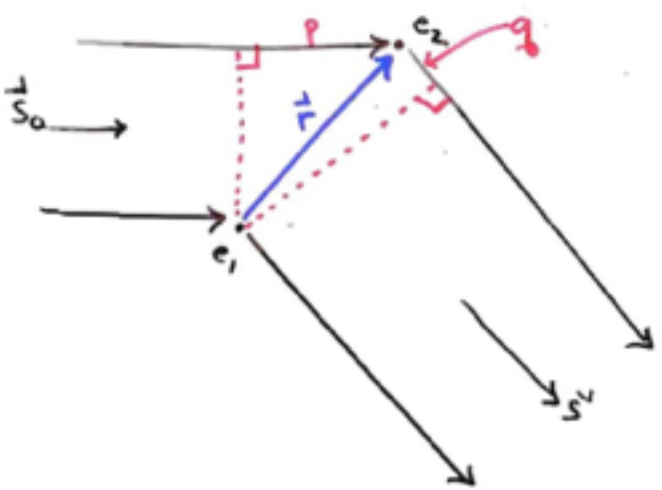


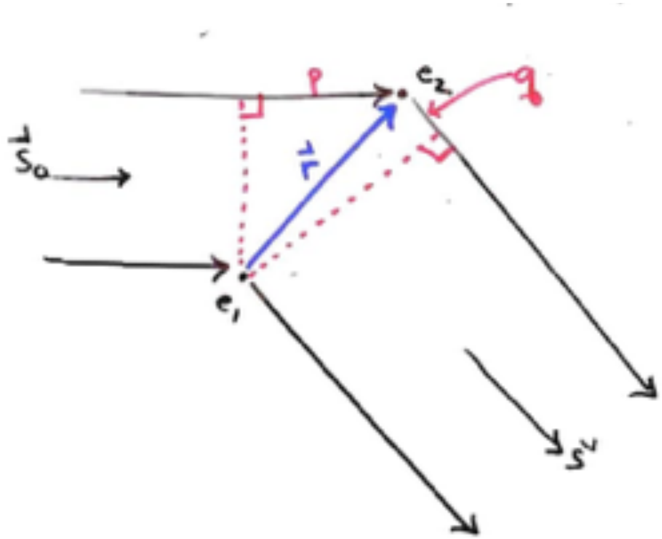
X rays traveling along unit vector $\vec{S}_0$ are scattered in all directions. Let's just focus for now on one direction ... $\vec{s}$.

$$|S_0| = |s| = \frac{1}{\lambda}$$

so... $\lambda |S_0| = 1$.

X rays scattered from e_2 travel further than those scattering from e_1. Thus, scattered xrays from e_2 will lag in phase compared to those from e_1. Obvious ... but how much? And what will the net scattering in direction $\vec{s}$ be?

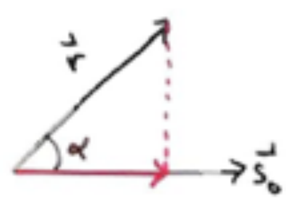
A system of two electrons...



well, the longer path length for e_2 is $p+q$.

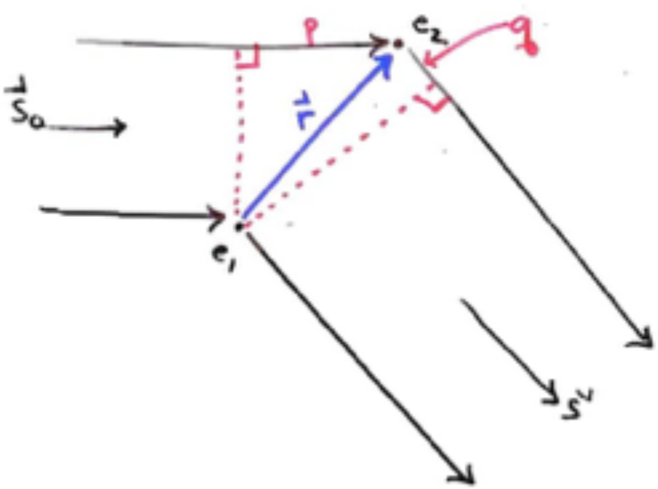
$\boxed{p = \lambda(\vec{r}\cdot\vec{s}_0)}$ [The extra distance traveled in the s_0 direction]

$= \lambda|\vec{s}_0||\vec{r}|\cos\alpha$

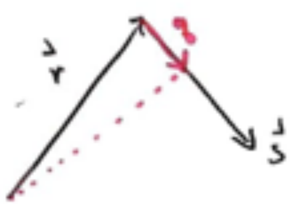


$\Rightarrow$ p is the fraction of 1λ traveled extra by the xray scattering from e_2 in the $\vec{s}_0$ direction.

A system of two electrons...



What about q?

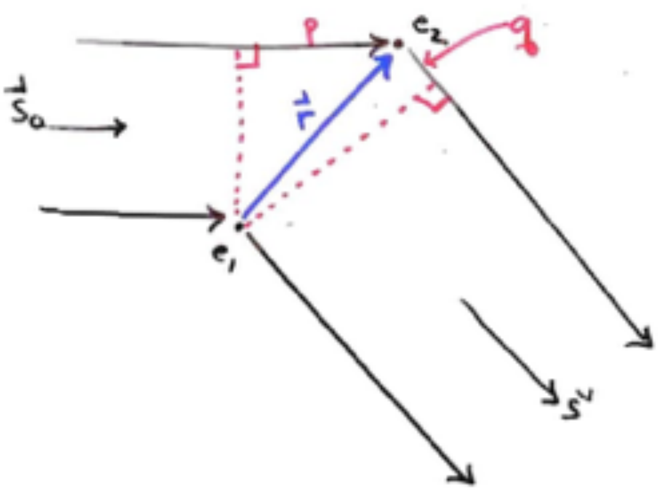


$$q = \lambda(-\vec{r} \cdot \vec{s})$$

(note minus sign on $\vec{r}$!)

q is the fraction of 1λ travelled extra in the $\vec{s}$ direction.

A system of two electrons...



$$p = \lambda(\vec{r} \cdot \vec{s}_0)$$

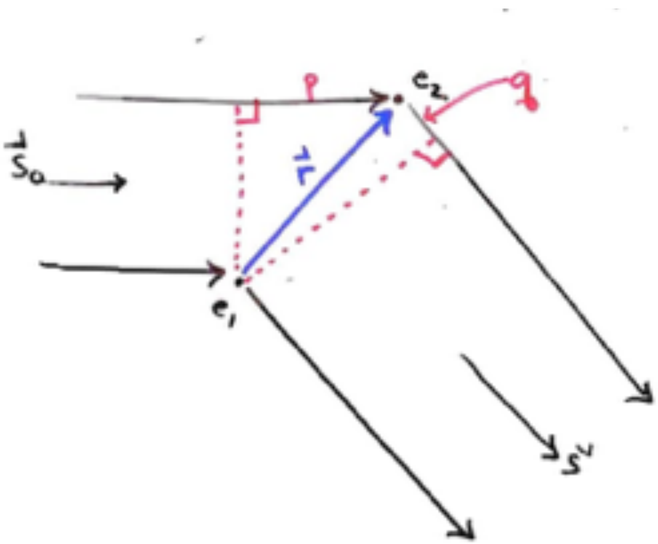
$$q = \lambda(-\vec{r} \cdot \vec{s})$$

What is $p+q$?

$$\boxed{p+q = \lambda \cdot \vec{r} \cdot (\vec{s}_0 - \vec{s})}$$

$p+q$ is the total extra distance traveled by the scattered x-ray from e_2 relative to e_1.

A system of two electrons...



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We can write this as:

$$\boxed{p+q = -\lambda\,\vec{r}\cdot\vec{S}}$$

where $\vec{S} = \vec{s} - \vec{s}_0$ and is called the scattering vector.

The **scattering vector**...

We can write this as:

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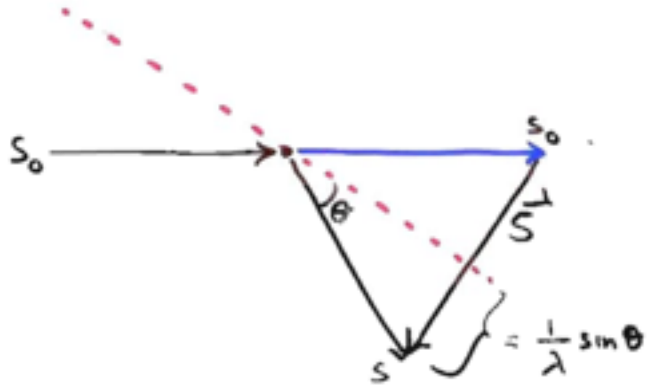
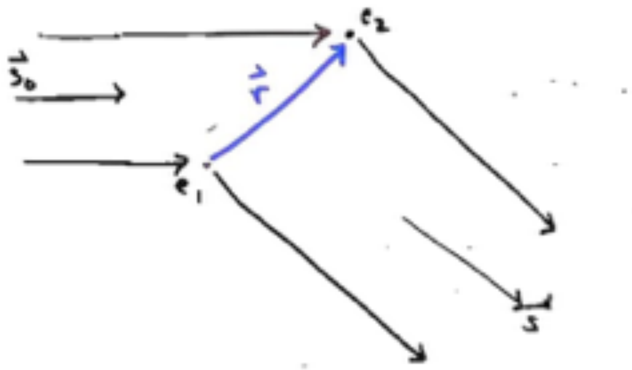
Note:



So... scattering from the e^- in a direction $\vec{S}$ can be seen as a reflection from a plane, and $|\vec{S}| = \frac{2\sin\theta}{\lambda}$

There are S vectors in every direction.

The phase shift due to the extra path length...



So what is the phase difference of the scattered ray from e_2 relative to e_1?

$$p + q = -\lambda \cdot \vec{r} \cdot \vec{s}$$

This is path length in units of λ.

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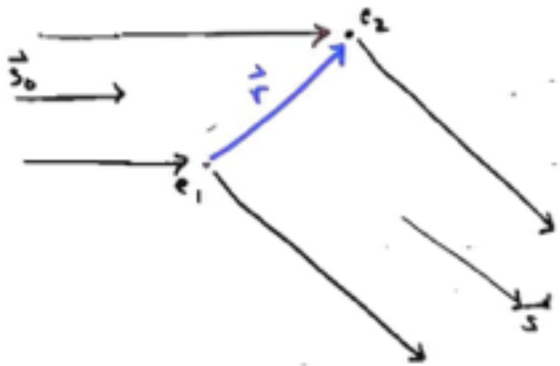

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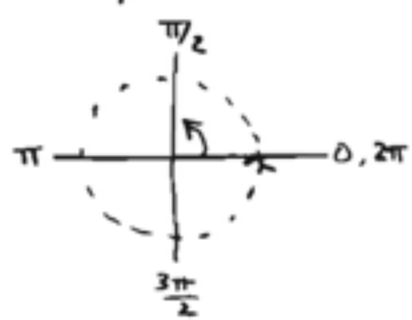
By definition a wave goes through one cycle every 2π rotations....



So...

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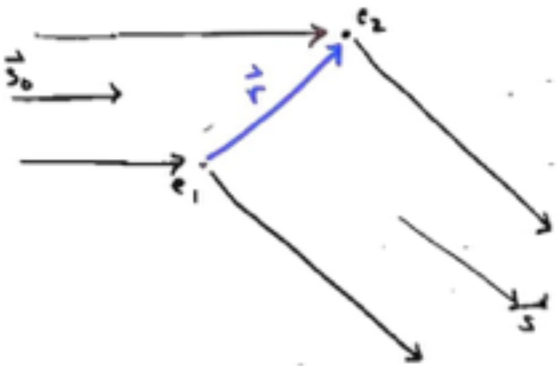

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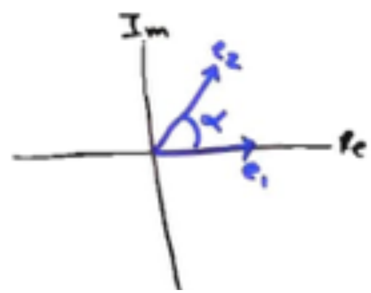
This is path length in units of λ.

So... phase shift of e_2 (taking e_1 as the reference) is:

$$\alpha = +\frac{2\pi \text{ radians}}{\lambda} \cdot \lambda \cdot \vec{r} \cdot \vec{S}$$

$$\boxed{\alpha = +2\pi\, \vec{r} \cdot \vec{S}}$$



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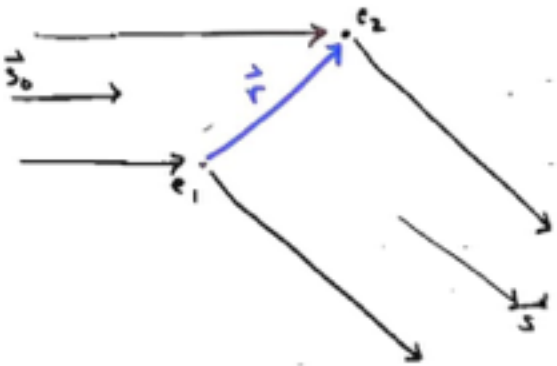

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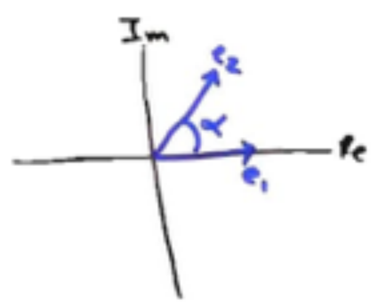
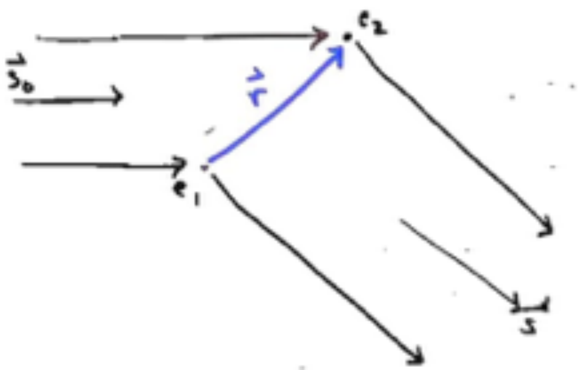


Key concept... magnitude of α depends on:

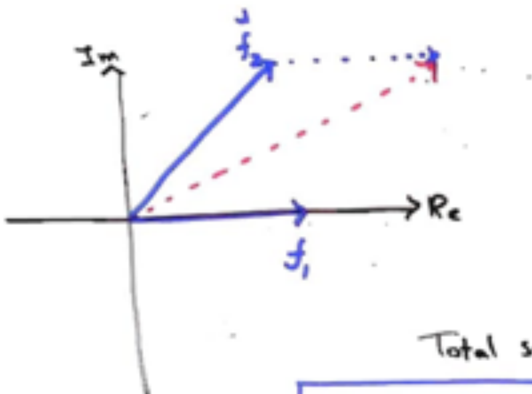
① $\vec{r}$ .... ~~[illegible]~~ what is that?

② $\vec{S}$ .... what is that?

The **structure factor** equation...



So ... to complete our little system of two e^-:

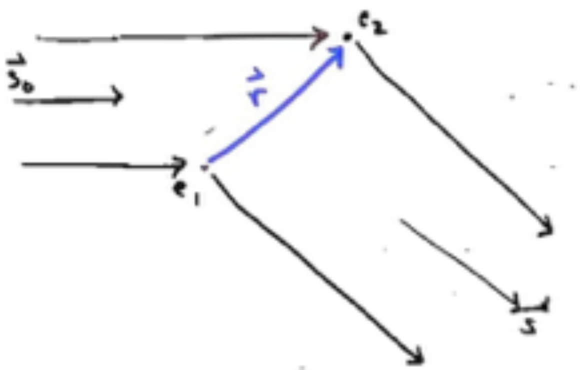


Total scattering in direction $\vec{S}$ is:

$$\boxed{F(s) = f_1 e^{+2\pi i r_1 \cdot s} + f_2 e^{+2\pi i r_2 \cdot s}}$$

where f_1 and f_2 is the magnitude of scattering for each electron, $\vec{r}_1$ and $\vec{r}_2$ are the vectors connecting the position of electron 1 and 2 respectively to the origin, and $\vec{S}$ is the scattering direction we are looking at.

The **structure factor** equation...



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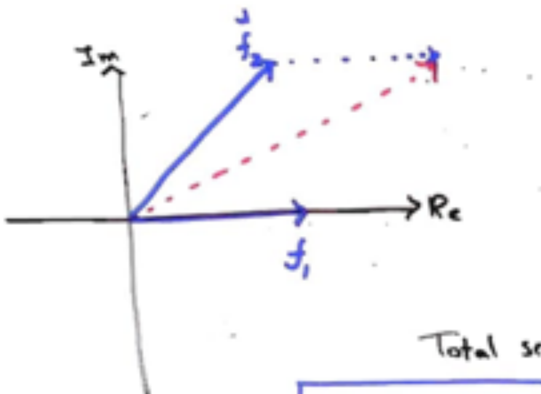

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Since we defined the origin (in our example) to be at e_1:

$$F(s) = f_1 + f_2 e^{+2\pi i r \cdot S}$$

This is called the “structure factor” equation for our little system of two electrons...

The **structure factor** equation...

This also solves the case of n arbitrary electrons located at positions $\vec{r}_n$:

$$F(s) = \sum_n f_n e^{+2\pi i \vec{r}_n \cdot \vec{s}}$$

The sum of all diffracted rays along direction $\vec{S}$.

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The structure factor depends on two things for each electron : $\vec{r}$, the distance and direction from the origin , and $\vec{S}$, the scattering angle. These go into changing the phase of the scattered ray.

What about the structure factor amplitude ?

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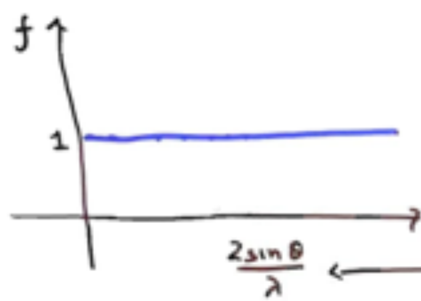
What about the structure factor amplitude ?

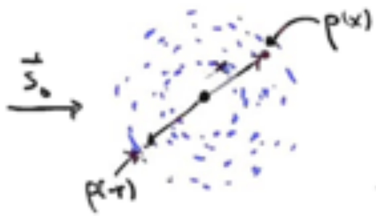
well... for a free electron, it is constant ... that is scattering is equal in intensity at all angles.



⟵⟶ magnitude of scattering vector. What does this axis mean?

Real atoms are more complex....

Of course... atoms are more complex. They have clouds of e^- density surrounding the nucleus... and have different numbers of e^- if different types of atoms.



So... scattering from an atom is more complicated in only one way we need to worry about now... that is the scattering intensity is not constant with scattering angle. It depends like this...

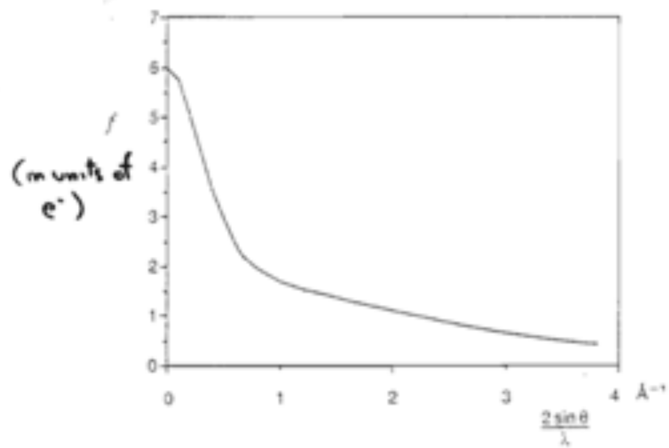


Figure 4.11. The scattering factor f for a carbon atom as a function of $2(\sin\theta/\lambda)$. f is expressed as electron number and for the beam with $\theta = 0$, $f = 6$.

Such graphs are available for all atoms in standard tables.

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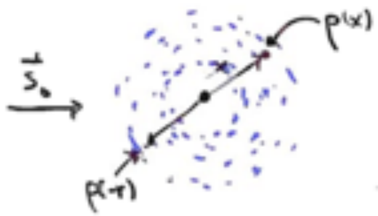

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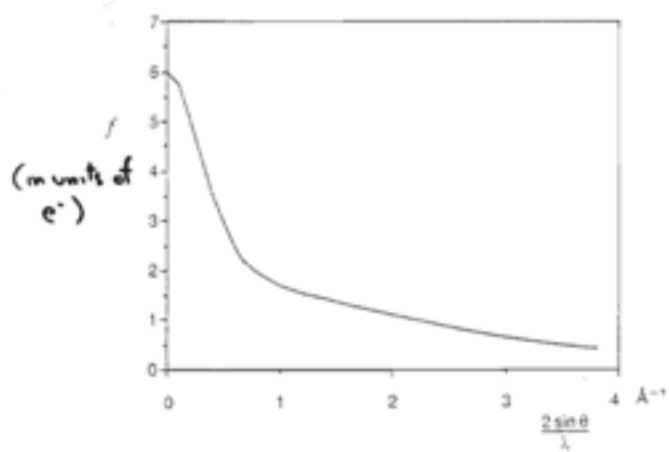

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So for atom i:

$$\vec{F}_i(s) = f_i\, e^{+2\pi i\, \vec{r}_i \cdot \vec{S}}$$

where now f_i itself depends on the scattering vector $\vec{S}$.

The **molecular structure factor**...

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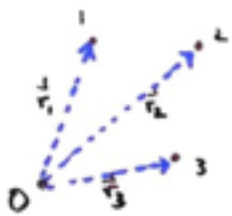
What about a more complex molecule of 3 atoms?



well, each atom will scatter as above, and the net result is:

$$\vec{F}(s) = f_1 e^{+2\pi i r_1 \cdot S} + f_2 e^{+2\pi i r_2 \cdot S} + f_3 e^{+2\pi i r_3 \cdot S}$$

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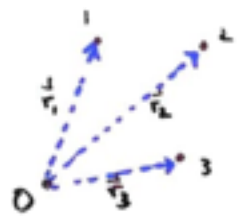

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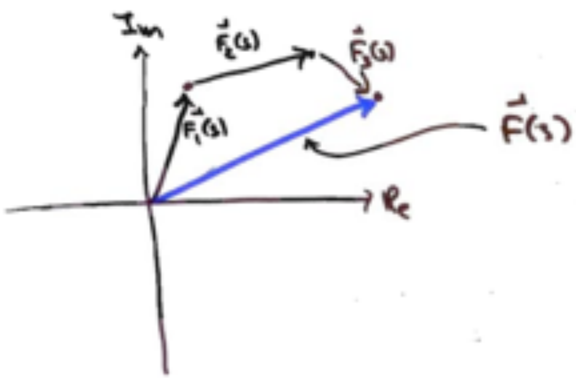
In an Argand diagram:



$$\boxed{\vec{F}(s) = \sum_i f_i \, e^{+2\pi i \, \vec{r}_i \cdot \vec{s}}}$$

This is the <u>molecular structure factor</u>

The **molecular structure factor**...

$$\boxed{\vec{F}(s) = \sum_i f_i \, e^{+2\pi i \, \vec{r}_i \cdot \vec{S}}}$$

This is the molecular structure factor

This is what we have been going for ... the mathematical relationship that gives us the scattering intensity at any direction given the structure of the molecule!

It is mathematically identical to the Fourier Transform.

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i x \xi}\, dx$$

and the spatial **Fourier transform**....

$$\boxed{\vec{F}(s) = \sum_i f_i \, e^{+2\pi i \, \vec{r}_i \cdot \vec{s}}}$$

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This is what we have been going for ... the mathematical relationship that gives us the scattering intensity at any direction given the structure of the molecule!

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...it means that if we can get amplitudes and phase angles for the scattering in all directions, we can mathematically reconstruct the original image by taking the inverse transform!

and the spatial **Fourier transform**....

To see this ... we write the structure factor equation in a slightly different way:

$$\vec{F}(s) = \sum_{\substack{\text{points } j \\ \text{in space}}} \rho(j)\, e^{2\pi i\, \vec{r}_j \cdot \vec{s}}$$

$\rho(j)$ is the electron density at the j^{th} point in space.

Then the inverse relationship is this:

$$\boxed{\rho(j) = \sum_{\substack{\text{points } k \\ \text{in S space}}} F_k(s)\, e^{-2\pi i\, \vec{r}_k \cdot \vec{s}}}$$

So... if we know the amplitude of scattering at every point in "S space", and if we know each associated phase angle, then we can reconstruct the electron density at every point j in real space.

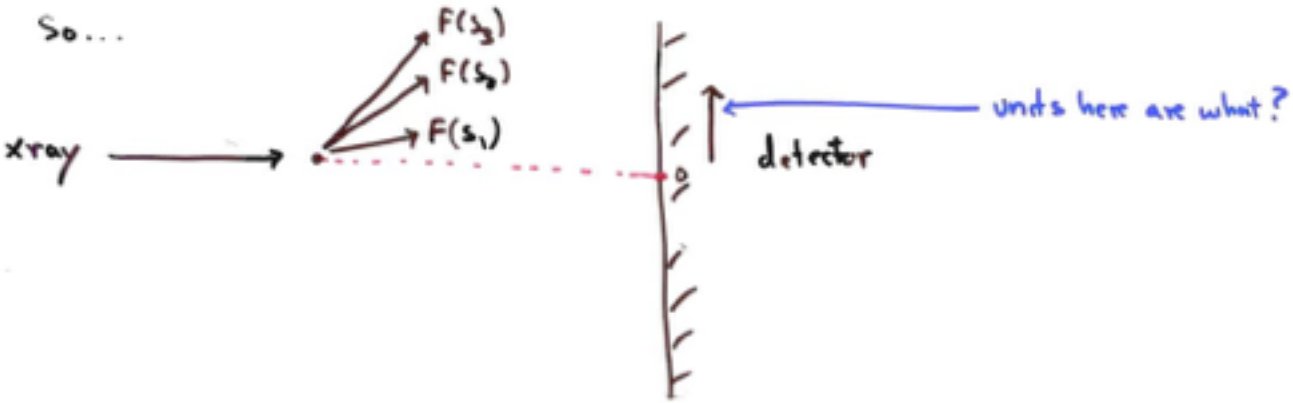
Now, what is "S space"? We need some intuition about this...

Reciprocal Space

What is S space?

Well, $\vec{S}$ is the scattering vector. It has magnitude $\frac{2\sin\theta}{\lambda}$ where θ is the scattering angle. As we vary S, we are varying the angle of scattering.

So...



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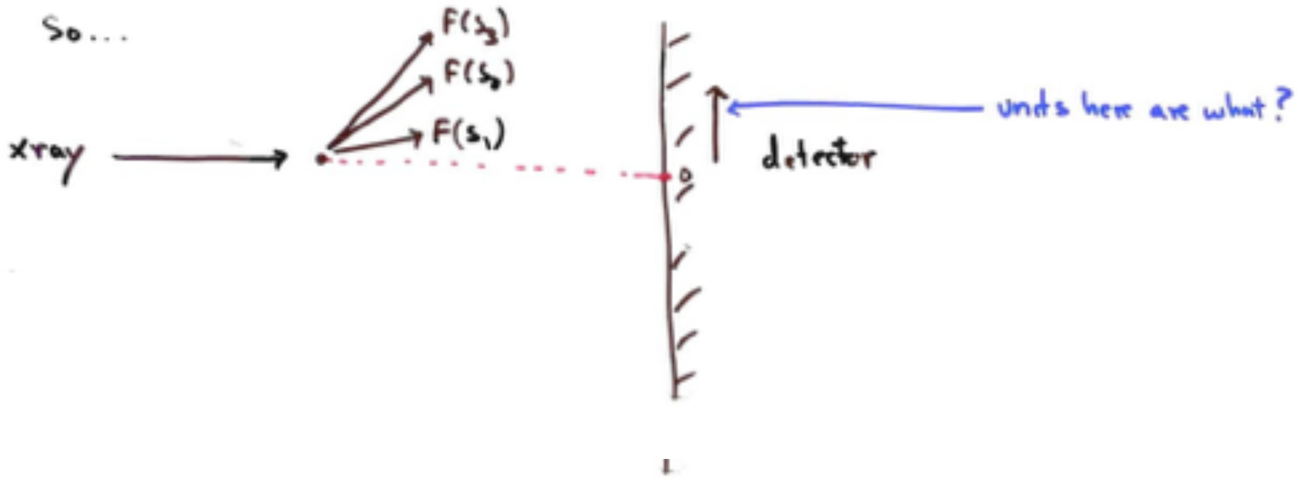


So, at the detector low-angle diffraction ends up near the center (the origin) and high-angle diffraction ends up near the periphery

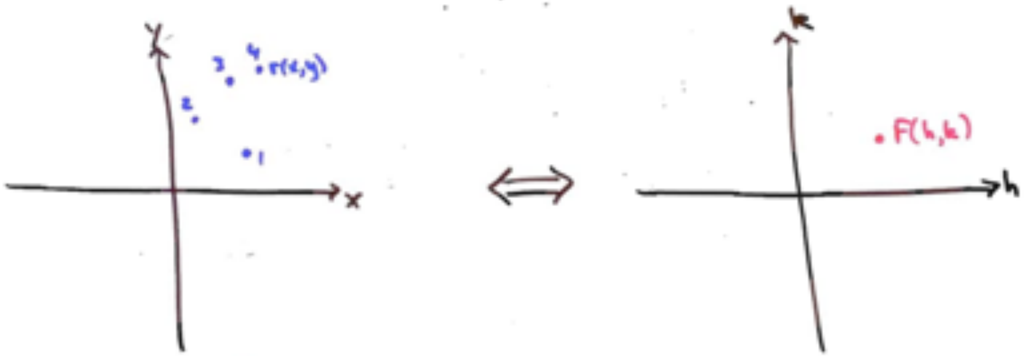
This correlates with low-resolution features of our object near the center, and high-resolution features of our object near the periphery.

⟹ As the spatial dimension gets smaller, the scattering angle gets bigger.

Reciprocal Space

7.

So now we can understand the diffraction pattern space (<u>or</u> S space,
<u>or</u> Fourier space,
<u>or</u> reciprocal space)



[real space]

dimensions are distance

[reciprocal space]

dimensions are spatial frequency

$$F(h,k) = \sum_{\substack{\text{real space}\\ x,y}} \rho(x,y)\, e^{2\pi i\, \vec{r}(x,y)\cdot \vec{S}}$$

same as before!

Each point in reciprocal space, say $F(h,k)$, comes from where in real space?

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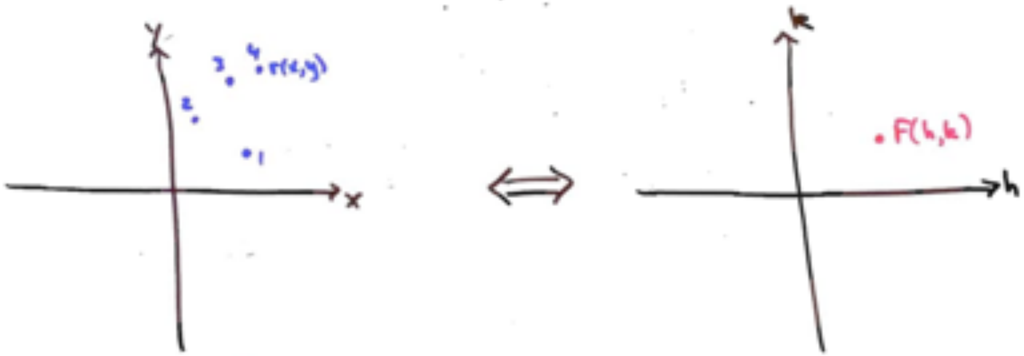

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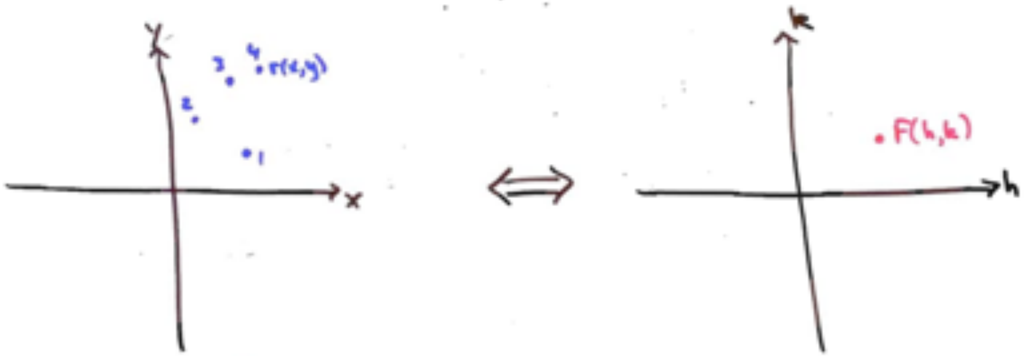

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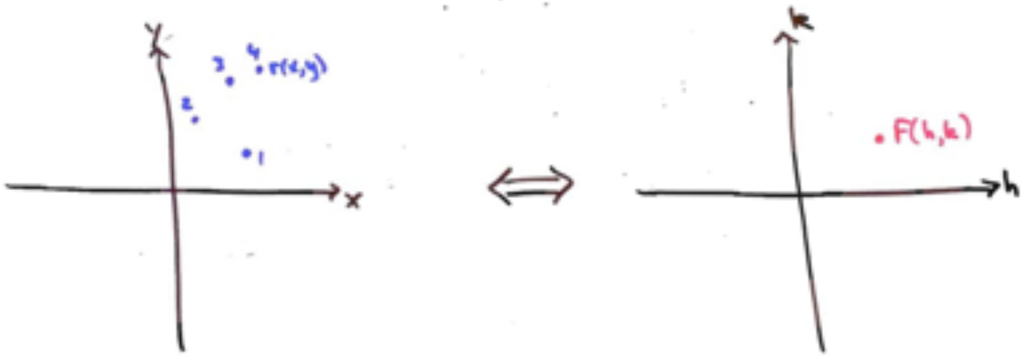
Each point in reciprocal space contains the summed contribution from all atoms (all points) in real space.

What do different points in reciprocal space mean then?

Reciprocal Space

So now we can understand the diffraction pattern space (or S space,
or Fourier space,
or reciprocal space)



[real space]

dimensions are distance

[reciprocal space]

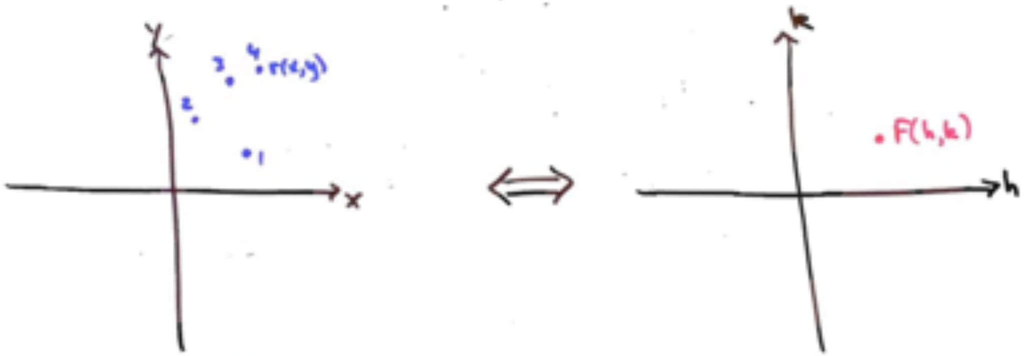
dimensions are spatial frequency

Now...

Each point in real space, say r(x,y), comes from where in reciprocal space?

Reciprocal Space

So now we can understand the diffraction pattern space (or S space,
or Fourier space,
or reciprocal space)



[real space]

dimensions are distance

[reciprocal space]

dimensions are spatial frequency

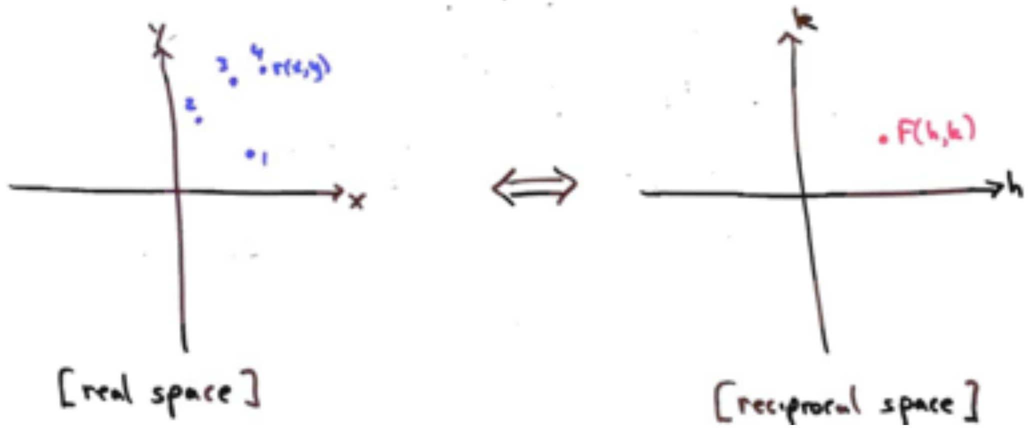
Now...

Each point in real space, say r(x,y), comes from where in reciprocal space?

Each point in real space comes from the summed contribution of all points in reciprocal space!

$$\rho(x,y) = \sum_{\substack{\text{reciprocal} \\ \text{space} \\ h,k}} F(h,k)\, e^{-2\pi i \vec{r}(x,y) \cdot \vec{S}} \qquad \text{(the inverse transform)}$$

A Demo....

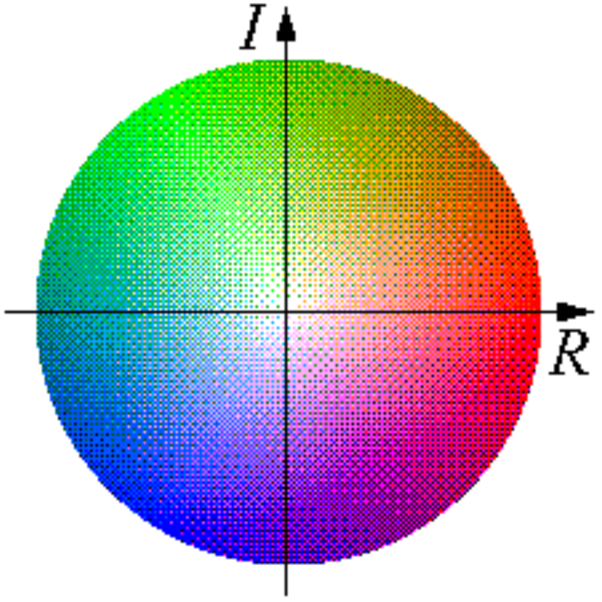


Two goals of this:

1. understand the relationship of real and reciprocal space
2. what's more important ... phase angles or amplitudes ?

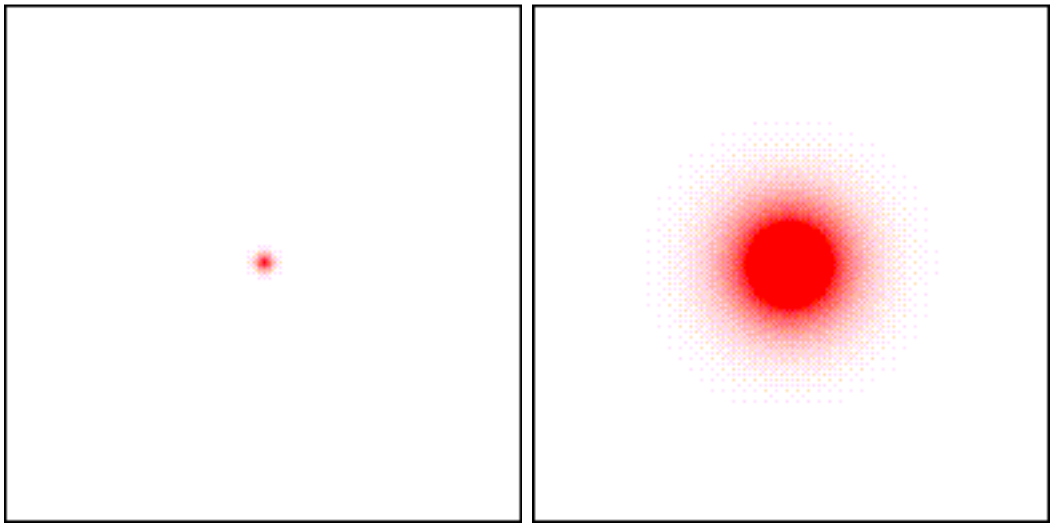
$$\rho(x,y) = \sum_{\substack{\text{reciprocal}\\ \text{space}\\ h,k}} F(h,k)\, e^{-2\pi i\, \vec{r}_{(x,y)} \cdot \vec{S}} \qquad \text{(the inverse transform)}$$

Reciprocal Space



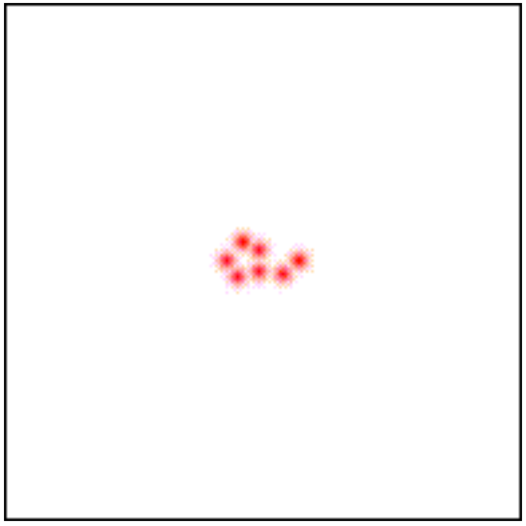
An atom....

Real space Fourier space

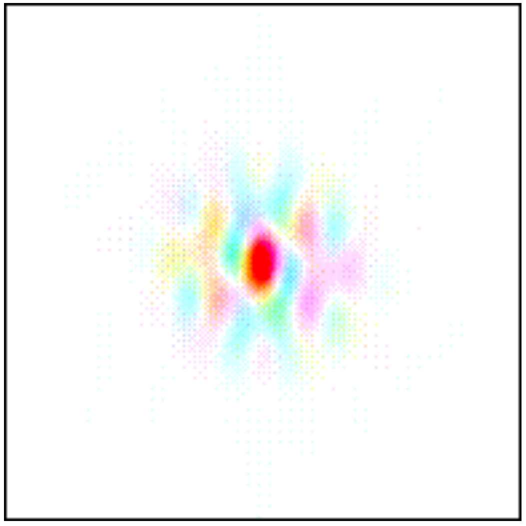


A molecule....

Real space

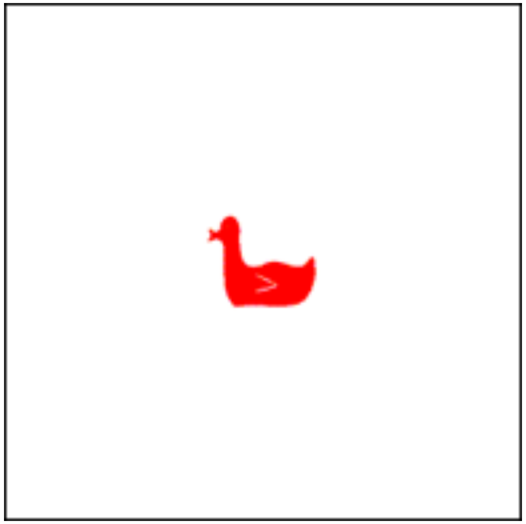


Fourier space

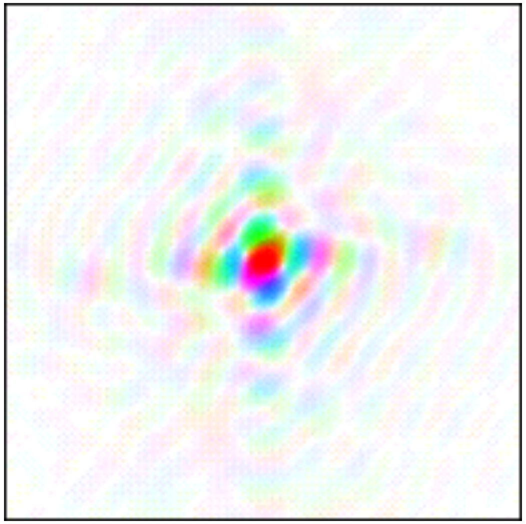


A duck....

Real space



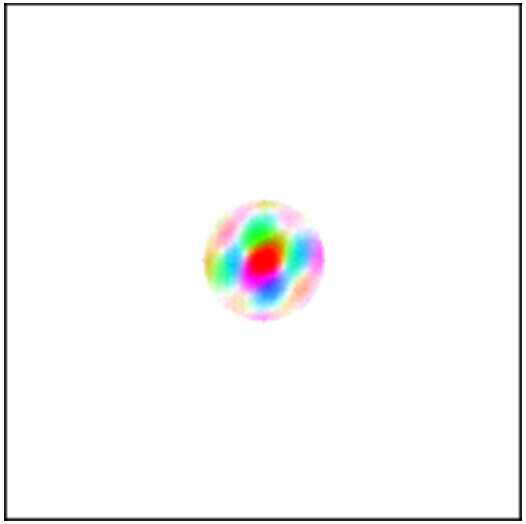
Fourier space



The low scattering angle information from the duck....

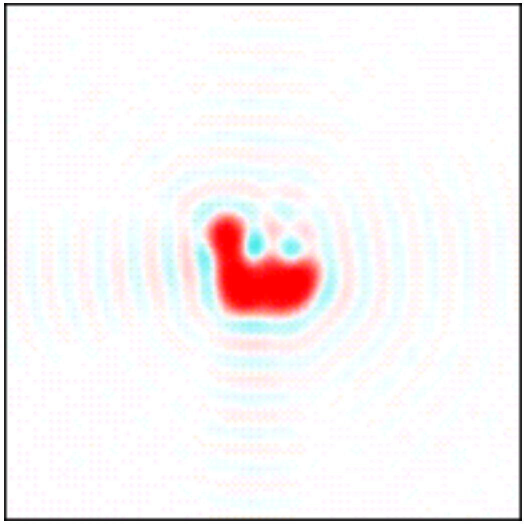
Real space

Fourier space

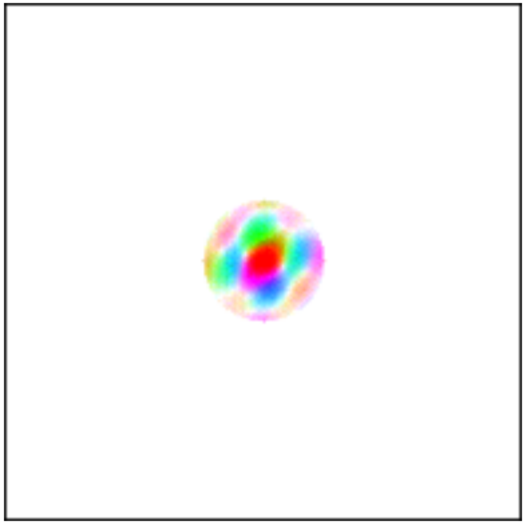


A low-resolution duck....

Real space



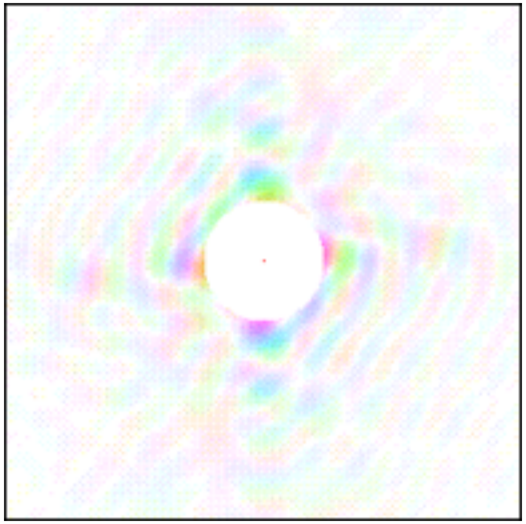
Fourier space



The high scattering angle information from the duck....

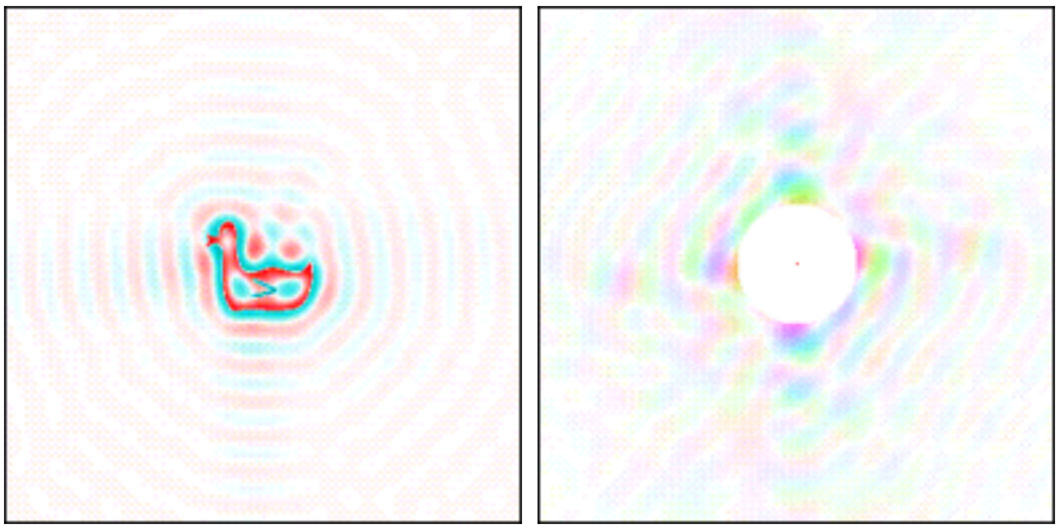
Real space

Fourier space



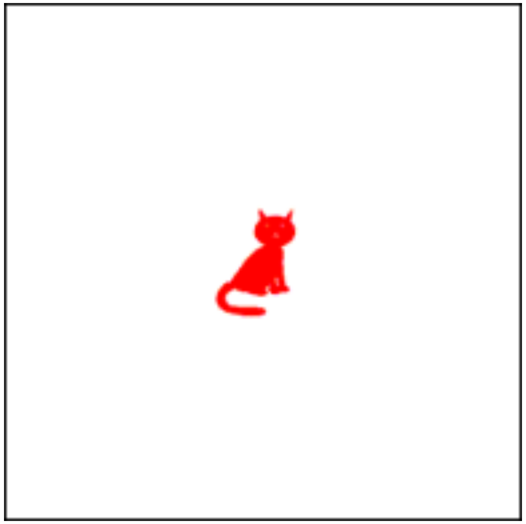
High spatial frequency duck....

Real space Fourier space

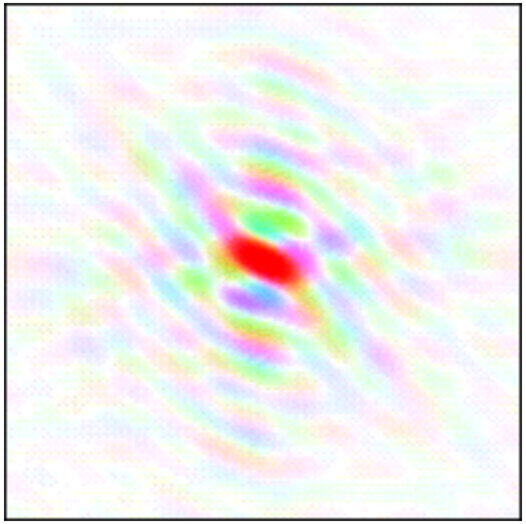


A cat....

Real space

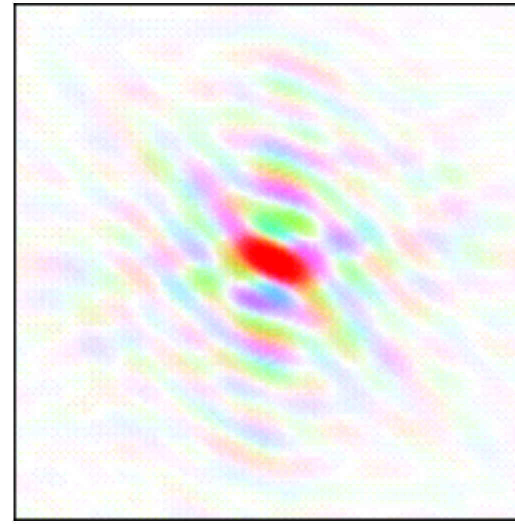


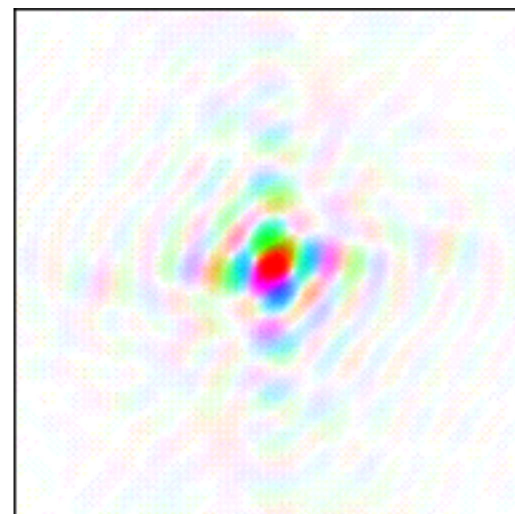
Fourier space



The cat and duck reciprocal spaces....

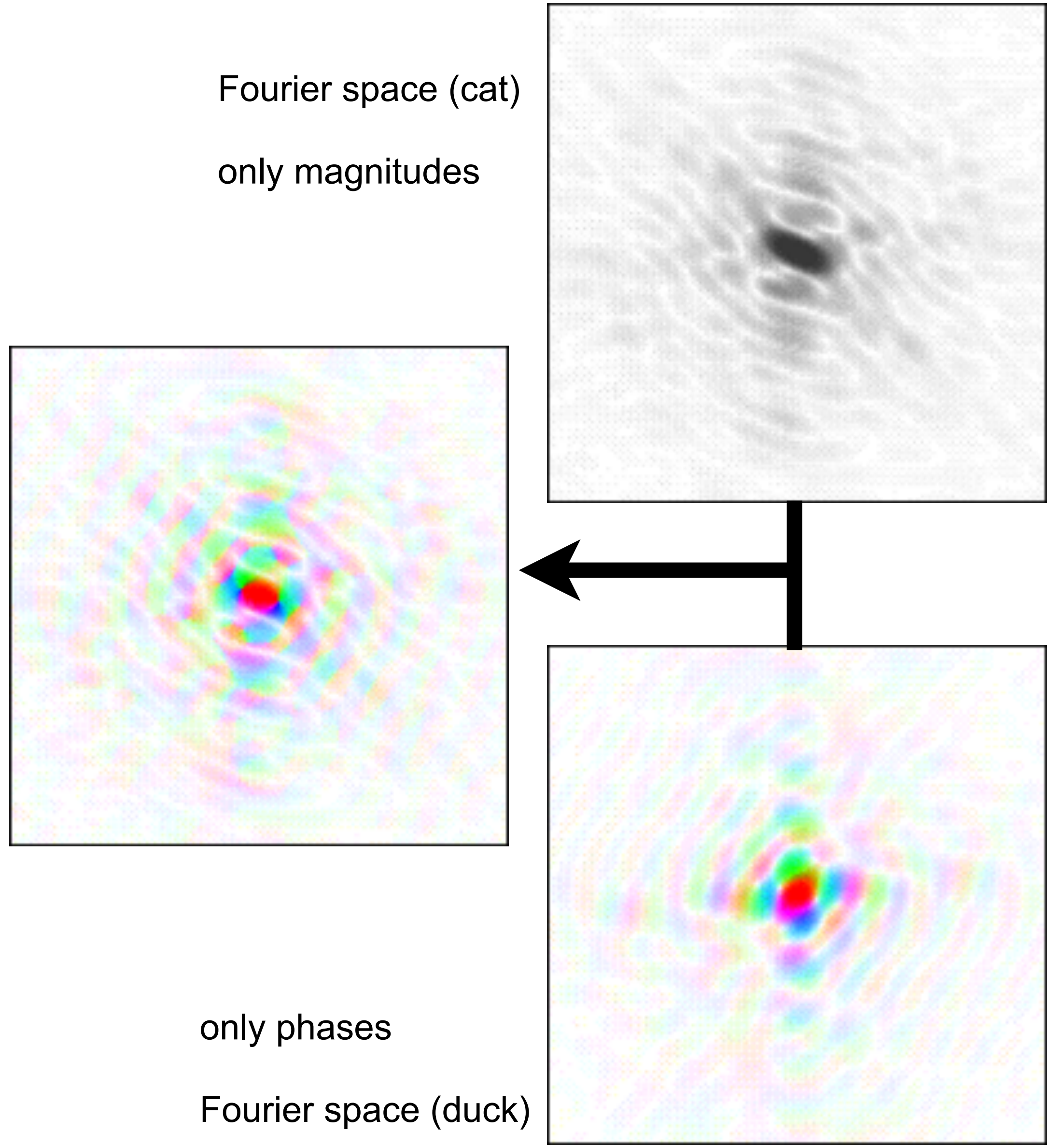
Fourier space (cat)



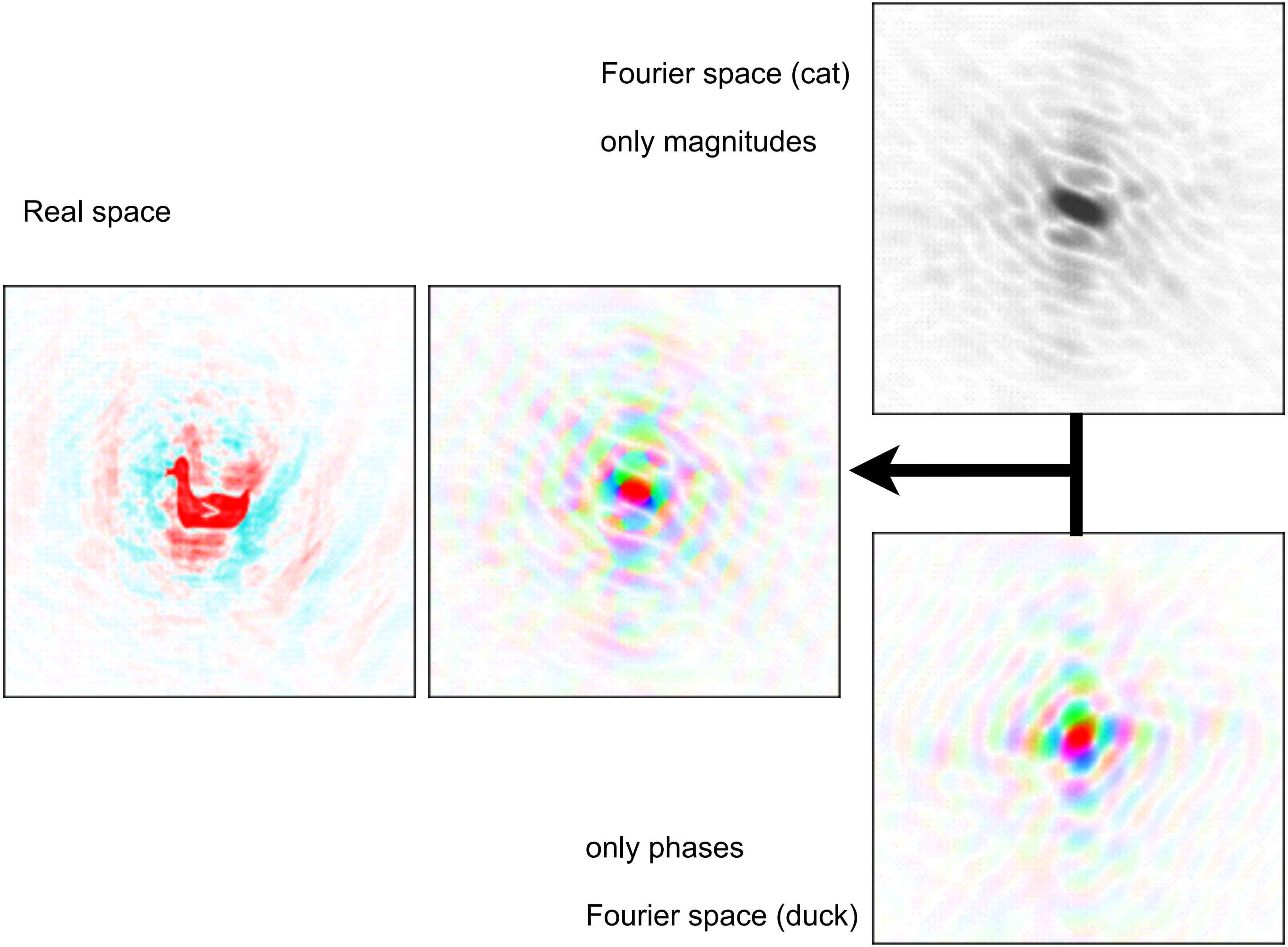


Fourier space (duck)

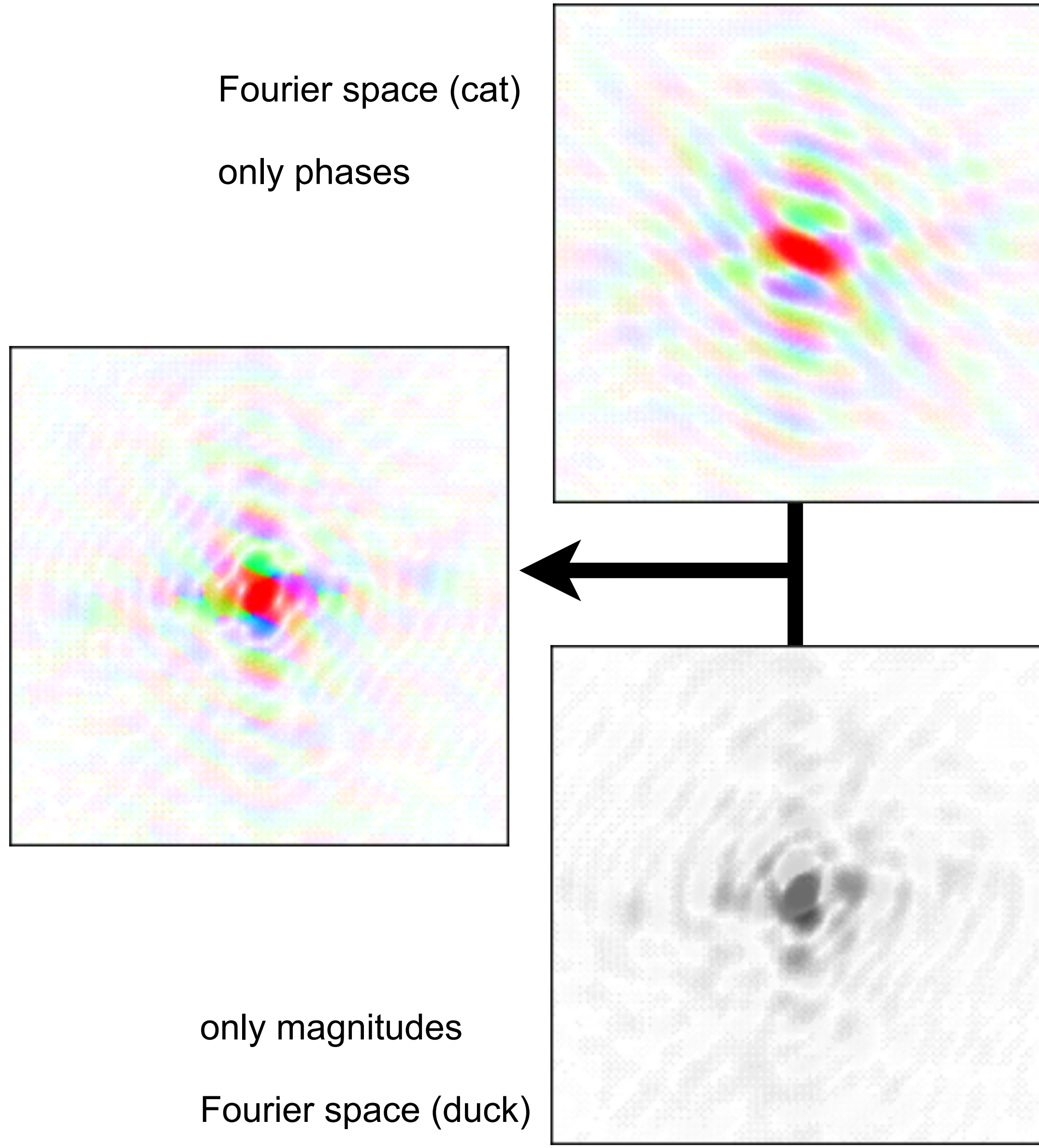
Magnitude from the cat and phases from the duck?



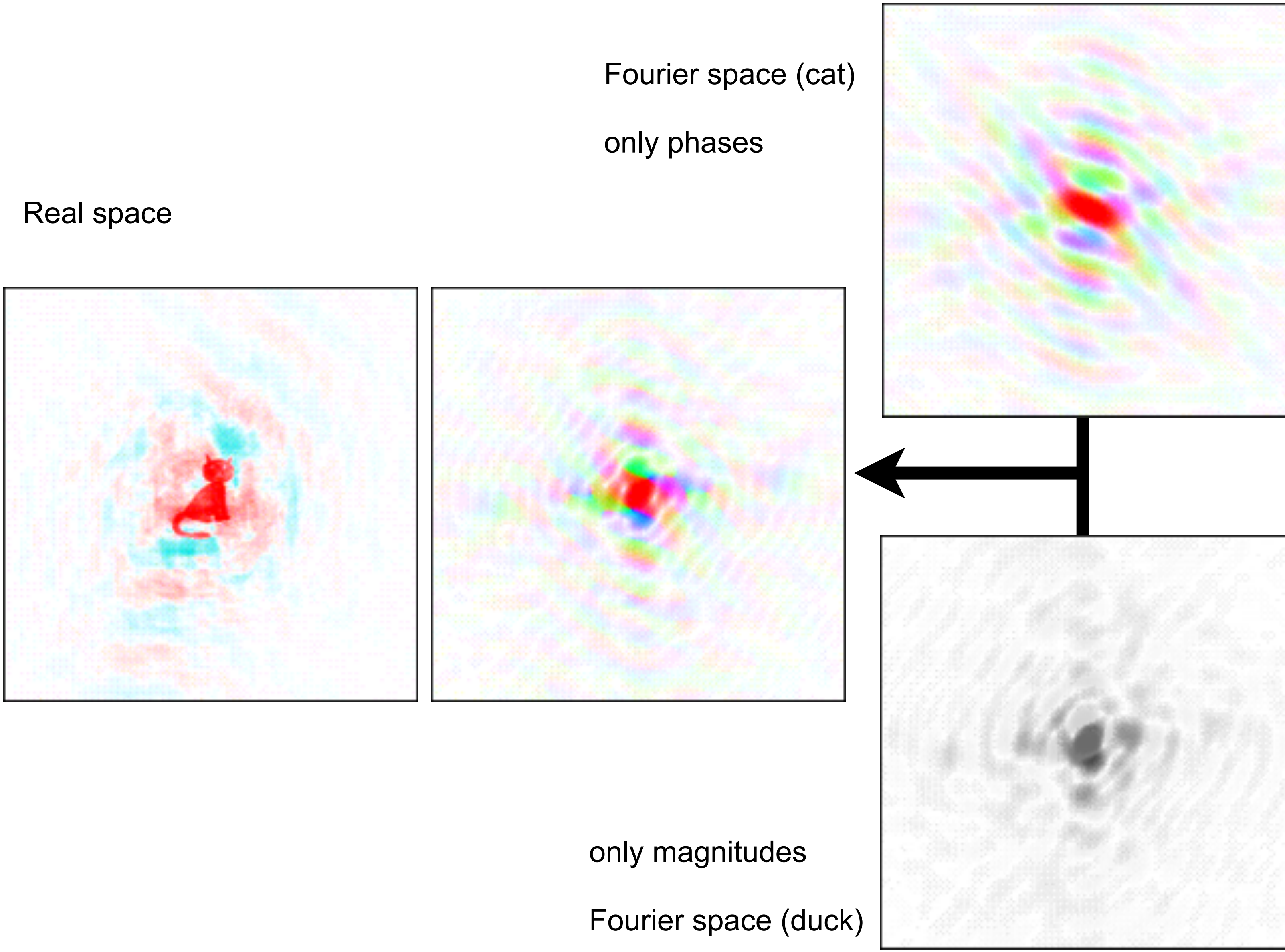
We get back the duck...



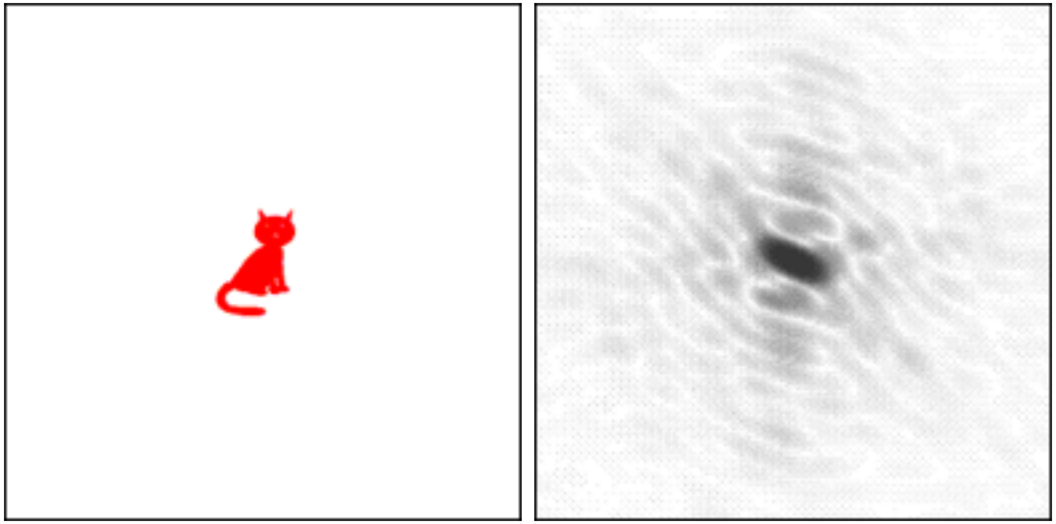
Now, mag from duck and phases from cat...



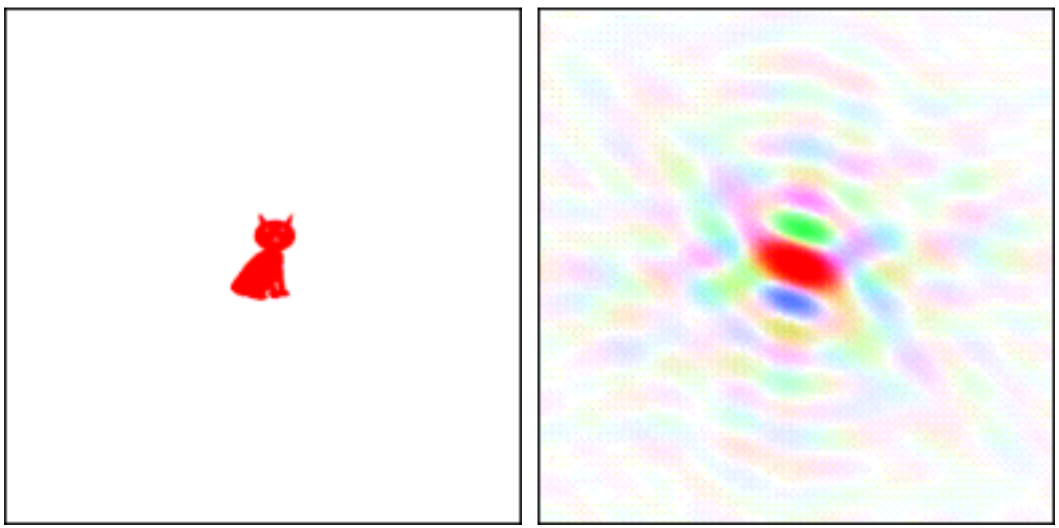
Now, mag from duck and phases from cat...



But magnitudes do have information...



A cat and fourier space magnitudes



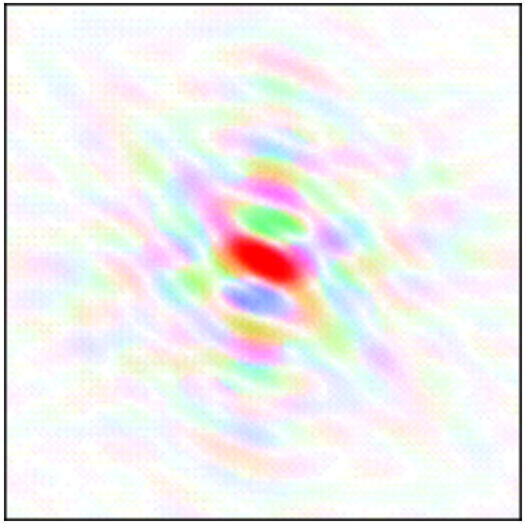
A manx cat and fourier space

So what if we get mag from the cat and phases from the manx cat?

So, phases from manx and mags from complete cat....

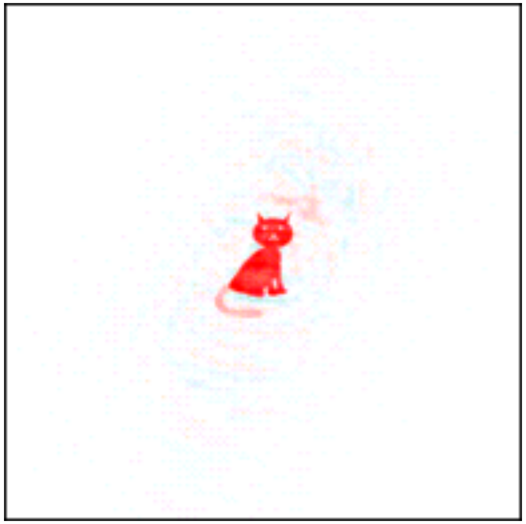
Real space

Fourier space

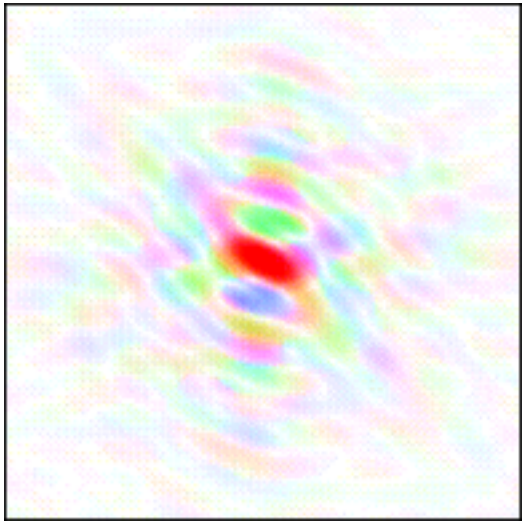


We get back the tail, sort of....

Real space



Fourier space



Now... for two big depressing problems ...

① we cannot practically collect the diffraction pattern of a single molecule. Too weak.... so how can we solve structures?

② we do not directly get any phases in protein crystallography. All we get are amplitudes!

forward…

$$\vec{F}(s) = \sum_{\substack{\text{points } j \\ \text{in space}}} \rho(j)\, e^{2\pi i\, \vec{r}_j \cdot \vec{s}}$$

reverse…

$$\rho(j) = \sum_{\substack{\text{points } k \\ \text{in S space}}} F_k(s)\, e^{-2\pi i\, \vec{r}_k \cdot \vec{s}}$$

Next, we continue our discussion of diffraction theory….

	n = 1	n = 2 or 3	n >> 1	continuum
Linear	exponential growth and decay single step conformational change fluorescence emission pseudo first order kinetics	second order reaction kinetics linear harmonic oscillators simple feedback control sequences of conformational change	electrical circuits molecular dynamics systems of coupled harmonic oscillators equilibrium thermodynamics diffraction, Fourier transforms	Diffusion Wave propagation quantum mechanics viscoelastic systems
Nonlinear	fixed points bifurcations, multi stability irreversible hysteresis overdamped oscillators	anharmonic oscillators relaxation oscillations predator-prey models van der Pol systems Chaotic systems	systems of non-linear oscillators non-equilibrium thermodynamics protein structure/ function neural networks the cell ecosystems	Nonlinear wave propagation Reaction-diffusion in dissipative systems Turbulent/chaotic flows

adapted from S. Strogatz