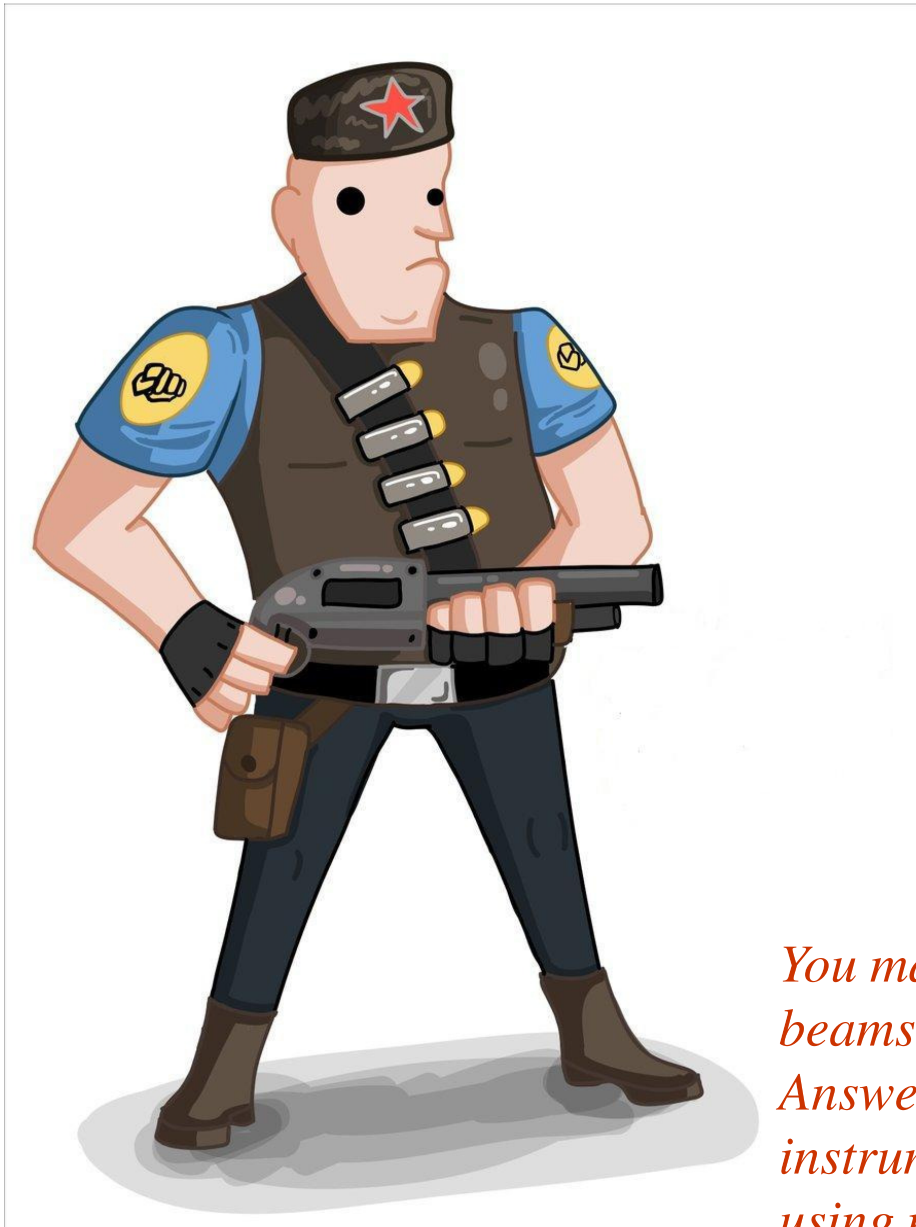
Introduction to Neutron Scattering (in 3 ways)

1. Bragg's Law (Warning: not easy)
2. Laue formalism
3. Kinematic Scattering Theory

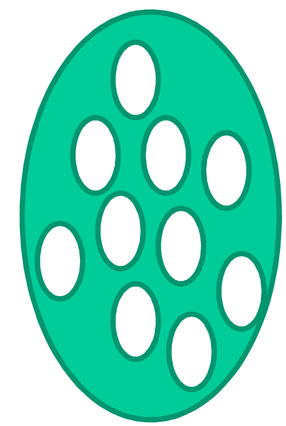
One approximation shared by all three: scattering must be weak, i.e. only a small fraction of the incident beam is scattered.

The 4th way we will not talk about: Dynamical Scattering Theory (needed only for Reflectometry)

What is scattering?



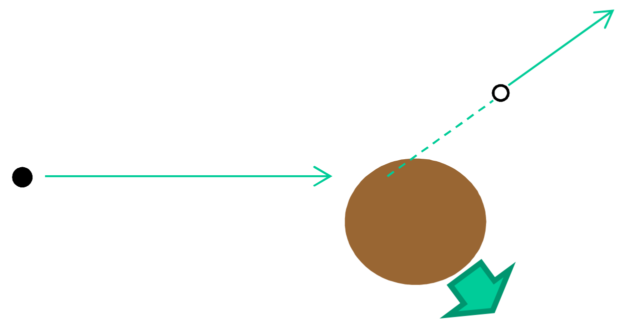
Target with
full of holes



You may ask why don't we focus neutron beams instead of this shot-gun approach. Answer: focused beams on C5 and D3 instruments. Also, there are other ways of using neutrons more effectively (talk by Ron Rogge)

1. Bragg's Law (Warning: not easy) 2. Laue formalism 3. Kinematic Scattering Theory

Two particle collision - classical picture



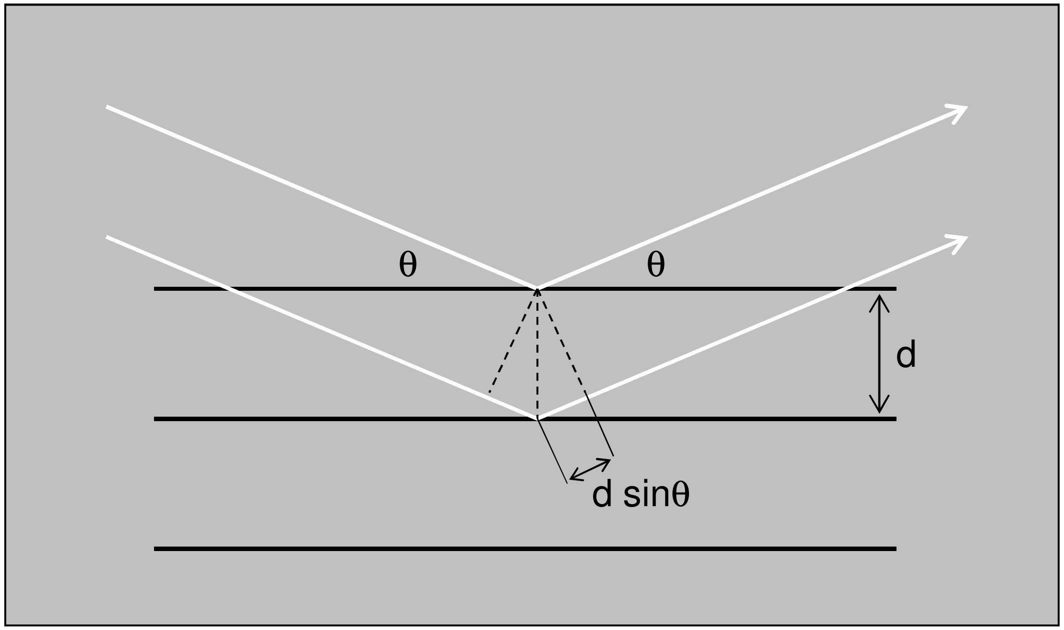
Concepts to recall:
(still thinking classically in macroscopic world)

Momentum conservation (always holds)
KE conservation (if elasticity e=1)
Recoil of the target

Modifications for microscopic world:

1) KE is always conserved (e is always 1)
2) Recoil of the whole target or just a few of the atoms (elastic or inelastic)
3) Wave nature is ubiquitous (de Broglie's wavelength ~> 1 Å)
4) Elastic scattering of neutrons where "recoil = 0" is a very good approximation.

Method 1: Bragg's Law



$$2d \sin\theta = n\lambda$$

Note the reciprocal relationship between d and sinθ

d-spacing and stress measurement talk by Michael Gharghouri

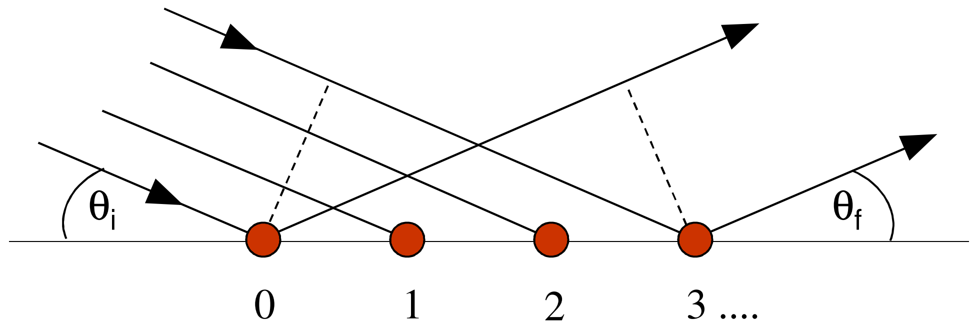
First, there are no Bragg planes. We have atoms (or nuclei).

Second, atoms give rise to isotropic wavelets.

Then, how could it be that Bragg planes act like mirrors?

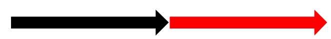
Circular wavelets from a reed

1D array of atoms



Think pictorially
with arrows

Constructive

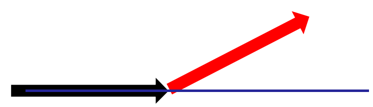


Resultant = 2 × original
(intensity = 4 times)

Destructive

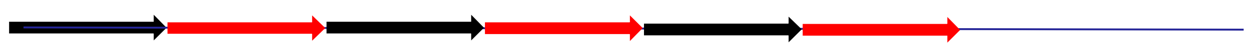
Resultant = 0

Partial

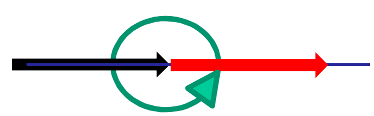


Resultant = between 2 and 0

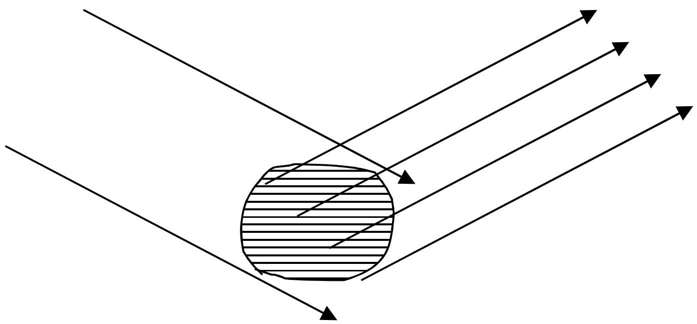
For a long 1-D array



Higher order constructive interference



Real space



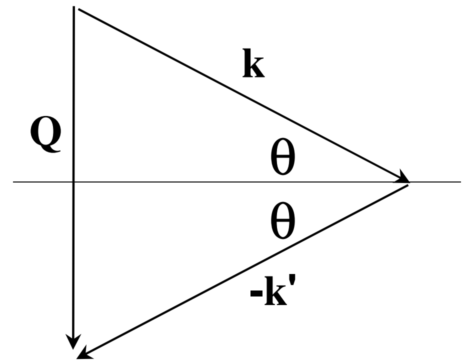
A crystal in Bragg reflecting position.

Ignore the possibility of being reflected by the back-side of the same planes (weak scattering).

Normal to the Bragg planes bisects the angle between incident and diffracted beam.

Reciprocal space

(or Momentum space, or Q space)



Change of neutron momentum or, momentum transfer

$$\mathbf{Q} = \mathbf{k} - \mathbf{k'}$$

While in Bragg condition, $\mathbf{Q}$ is perpendicular to the Bragg planes and coincides with the reciprocal lattice vector $\boldsymbol{\tau}$ of magnitude $2\pi/d$. From the figure, we get

$$Q/2 = \pi/d = k \sin\theta$$

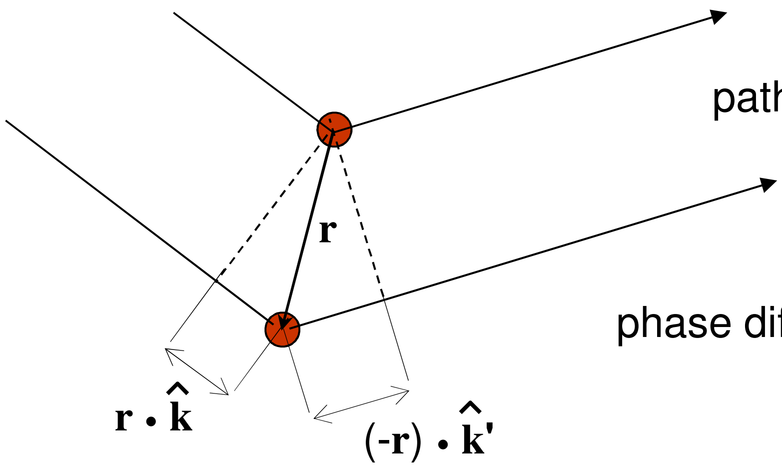
or $Q = 2\pi/d = 2k \sin\theta$

Method 2: The structure factor F(Q)

Consider the incident beam as a coherent wave train.

When the beam strikes a set of points that scatter the beam coherently, the net diffracted intensity can be calculated from path differences.

Consider two scattering centers, one at the origin and the other at the position **r**.



path difference = $\mathbf{r} \cdot \hat{\mathbf{k}} - \mathbf{r} \cdot \hat{\mathbf{k}}'$

phase difference = path difference $\times$ $(2\pi/\lambda)$

$= \mathbf{r} \cdot \mathbf{k} - \mathbf{r} \cdot \mathbf{k}' = \mathbf{Q} \cdot \mathbf{r} \qquad (\mathbf{Q} \equiv \mathbf{k} - \mathbf{k}')$

Disturbance by a wave = (Amplitude) $\exp\{i \text{ (phase)}\}$

$\therefore$ net scattering amplitude = $b_1 + b_2 \exp(i\, \mathbf{Q} \cdot \mathbf{r})$

(Ignoring the wavelet from Particle 1 scattered by Particle 2, i.e. weak scattering)

Amplitude of the wavelet from j^{th} scattering centre → b_j = scattering length (fm = 10^{-13} cm)

Scattering lengths for Neutrons

Neutron-nucleus interaction can be repulsive or attractive (+ or –b).
Probability of interaction is given by cross-section, in units of barn (10^{-24} cm^2)

Examples:

Isotope	b(neutron)	Z	b(X-ray)
H	-3.741	1	r_o
D	+6.671	1	r_o
O	5.803	8	$8r_o$

Isotopic substitution instead of isomorphous replacement
(used extensively for structural work, SANS, reflectometry)

Scattering from light atoms is comparable to that from heavy atoms

The structure factor of a system containing N particles (N can be very large, ~ 10^{23})

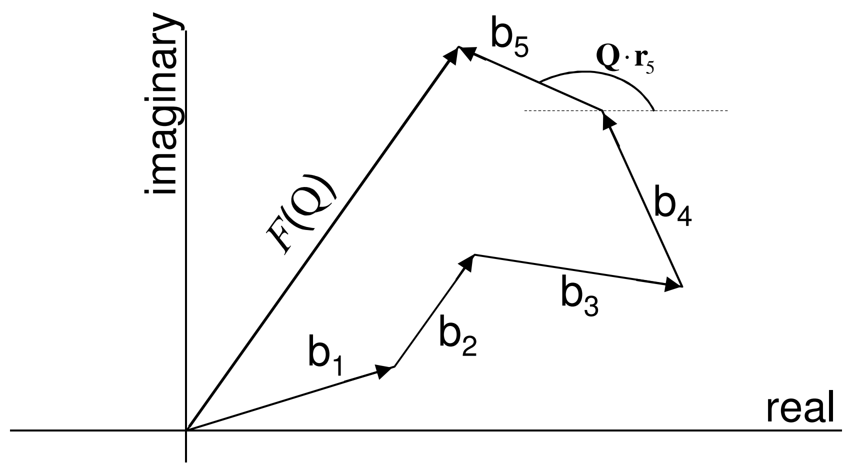
$$F(\mathbf{Q}) = \sum_{j=1}^{N} b_j \exp(i\mathbf{Q}\cdot\mathbf{r}_j)$$

Avogadro number

$F(\mathbf{Q})$ is the Fourier transform of the distribution of $b(\mathbf{r})$, and

Diffracted intensity = $|F(\mathbf{Q})|^2$

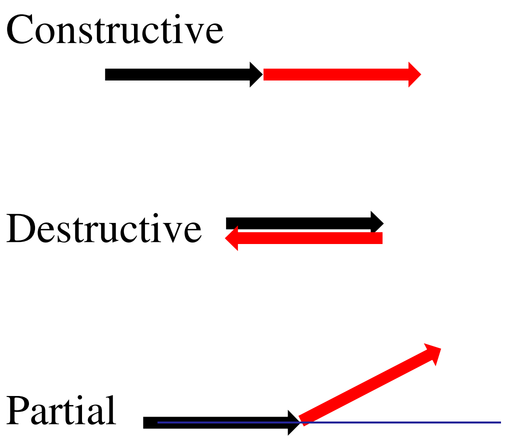
Geometrical interpretation of the sum on a complex plane.



If N particles belong to identical cells,
Fourier sum is needed only for one cell.

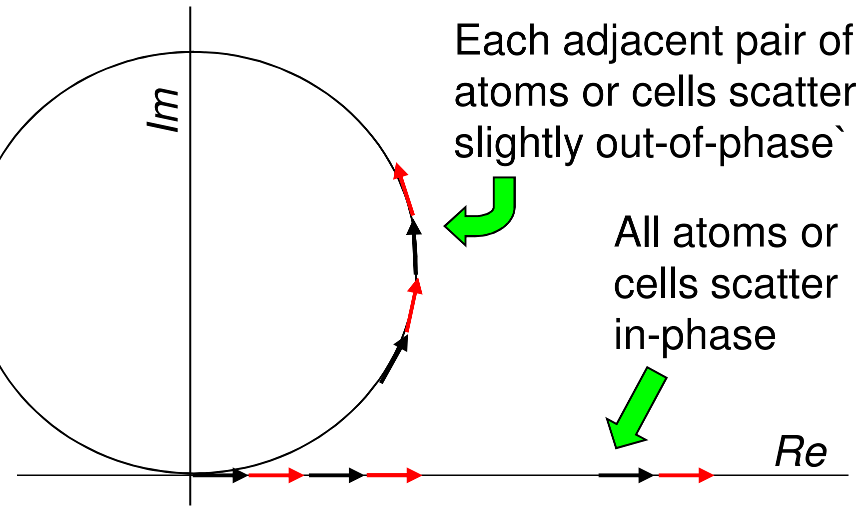
The difference between few and many

Two as the example for “few”



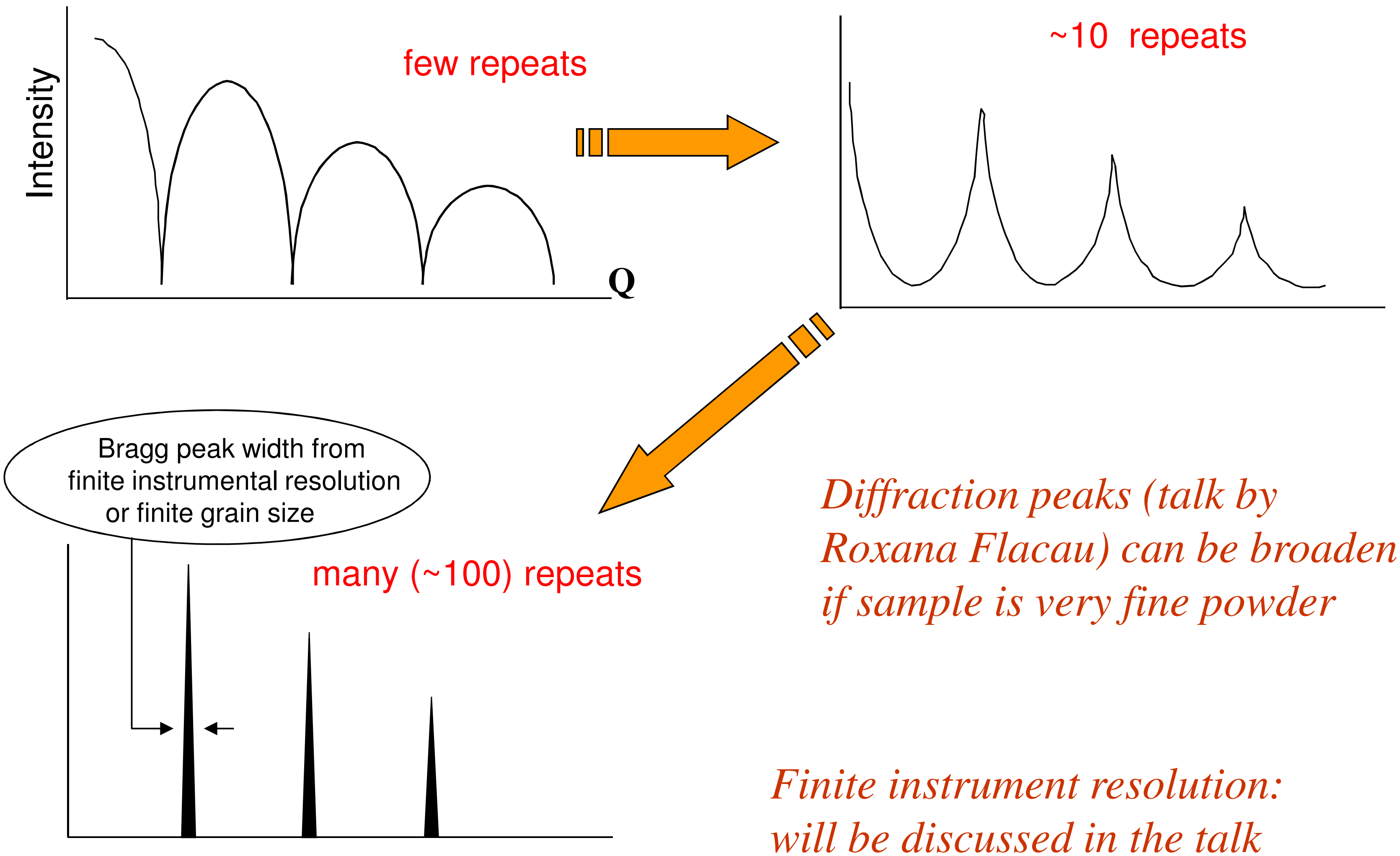
Broad maxima and sharp minima

“Many” means many!



Sharp maxima and broad minima

Fourier sum of many identical particles (atoms of a mono-atomic crystal or unit cells)



Diffraction peaks (talk by Roxana Flacau) can be broaden if sample is very fine powder

Finite instrument resolution: will be discussed in the talk by Bruce Gaulin

$$F(\mathbf{Q}) = \sum_{j=1}^{N} b_j \exp(i\mathbf{Q}\cdot\mathbf{r}_j)$$

or

$$F(\mathbf{Q}) = \int \rho(\mathbf{r}) \exp(i\mathbf{Q}\cdot\mathbf{r}) d\mathbf{r}$$

Always valid provided scattering is weak, but meaning of $\rho(\mathbf{r})$ depends on the scale the matter is viewed.

At large $\mathbf{Q}$, graininess due to atoms shows, and $\rho(\mathbf{r})$ is made up of discrete points. This is how matter is viewed in the study of crystal structures or lattice vibrations.

Talk by Roxana Flacau

Talk by Young-June Kim

At small $\mathbf{Q}$, matter looks homogeneous and $\rho(\mathbf{r})$ is a continuous function. In that case, $\rho(\mathbf{r})$ is the scattering length density, i.e. sum of b within 1 Å^3.

Talk on SANS by Mu-Ping Nieh

Talk on reflectometry by Helmut Fritzsche

Fourier Transform, named after Joseph Fourier (1768 – 1830)

$$F(\mathrm{Q}) = \int_{-\infty}^{\infty} f(x)\exp(i\mathrm{Q}x)dx$$

General Properties:

1. F (Q) can be calculated if $f(x)$ is known for $(-\infty,+\infty)$.
2. F (Q) is real if $f(x)$ is centrosymmetric.
3. FT of FT is the original function (times constant).

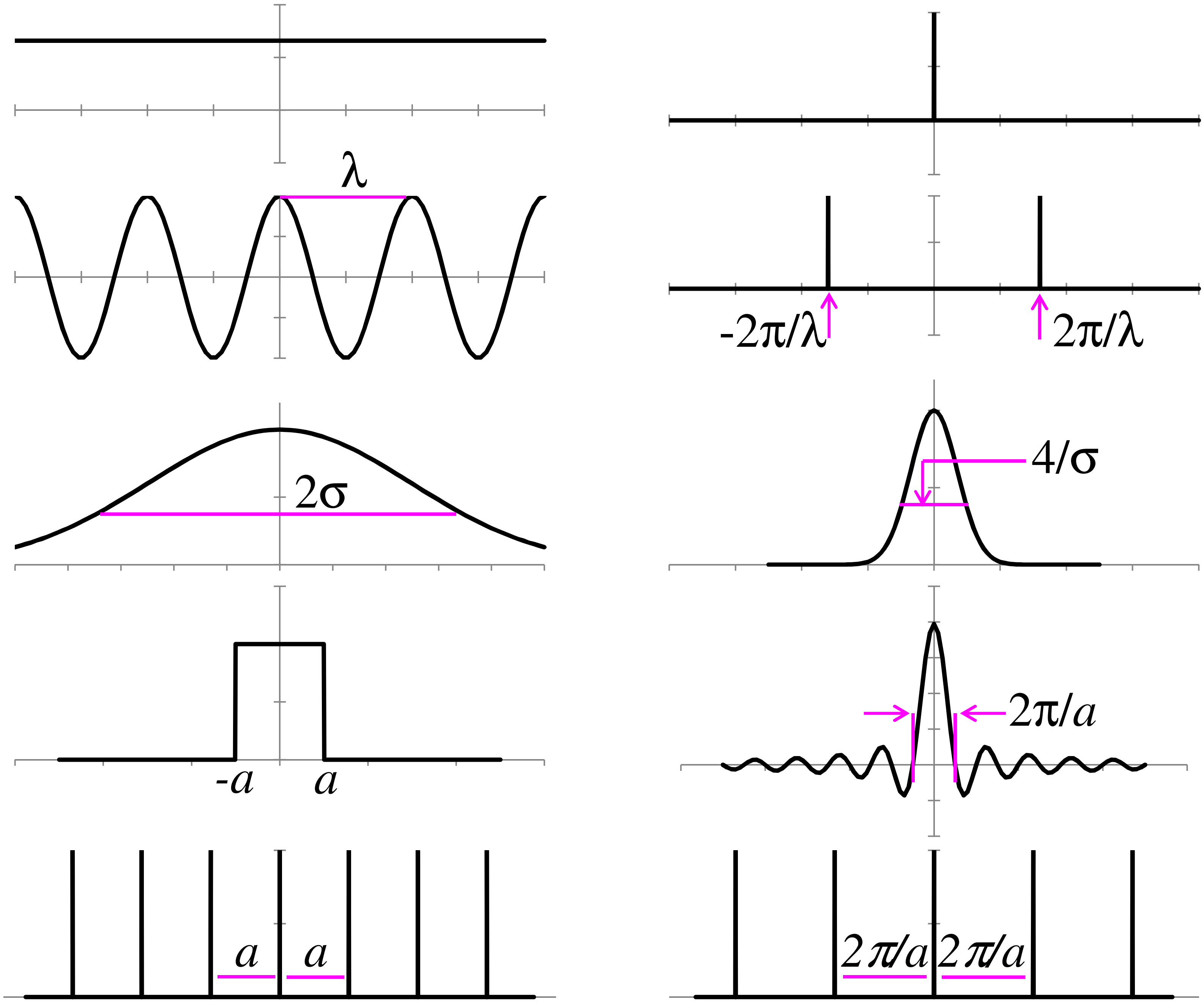
Constant to δ-function

Sine wave to pair of δ-functions

Gaussian (broad) to Gaussian (narrow)

Box to sinc (cardinal sine) function

Comb to comb


λ
-2π/λ
2π/λ
2σ
4/σ
-a
a
2π/a
a
a
2π/a
2π/a

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3. FT of FT is the original function (times constant).

Constant to δ-function — *No contrast means no scattering*

Sine wave to pair of δ-functions — *Growth of charge or mass density waves*

Gaussian (broad) to Gaussian (narrow) — *Thermal motion reduces intensity at large Q*

Box to sinc (cardinal sine) function — *"ringing" due to finite data range*

Comb to comb — *Crystal as convolution of a unit cell with a comb (very intuitive way of understanding diffraction)*

Fourier Theorem:

Any periodic function is a sum of sine or cosine wave of fundamental frequency (or period) plus the higher harmonics.

Adjustables: amplitude and phase of the harmonics

Convolution Theorem:

$$a(x) \; * \; b(x) \; = \; c(x)$$

FT ↓ ↓ ↓

$$A(Q) \quad B(Q) \; = \; C(Q)$$

In real space, unit cell is convoluted with a comb. In Q-space, peaks of a comb are weighted by the FT of the unit cell. This is the basic math for crystallography. Talk by Roxana Flacau

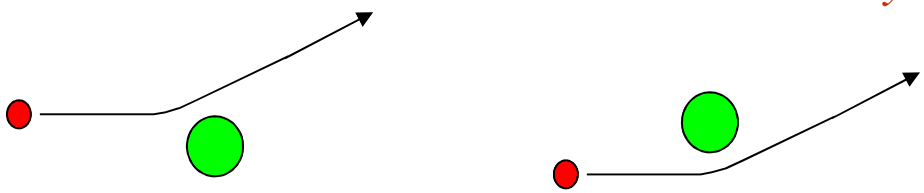
A special case worth remembering:

$$a(x) \; * \; \delta(x) \; = \; a(x) \quad \text{(times constant)}$$

Method 3: Scattering due to "weak" perturbation (Kinematic Approximation)

An equation valid for both elastic and inelastic scattering will be derived.

Talks by Carl Adams and Young-June Kim are mainly to describe this method



Not that weak!

After all, it hold the nucleus.

Very short range makes it look weak.

Squires Eq. (2.59)

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}(\text{constants})\sum_{j,j'} b_j b_{j'} \int \left\langle e^{-i\mathbf{Q}\cdot\mathbf{R}_{j'}(0)} e^{i\mathbf{Q}\cdot\mathbf{R}_j(t)} \right\rangle e^{-i\omega t} dt$$

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}(\text{constants})\, S(\mathbf{Q},\omega)$$

With 3-axis spectrometer, $S(Q,\omega)$ is measured directly (talk by Bruce Gaulin)

Systems and States

Example 1: Free particle

de Broglie wavelength can be any value. $\therefore$ momentum k can be any value.

Since k can be any value, energy continuum with no upper limit.

Wavefunction $\psi_k(x) = e^{ikx} = \cos kx + \imath \sin kx$ extends from -∞ to +∞.

Each ψ_k is an eigenstate, i.e. It satisfies the Schrodinger Eq. $H\psi_k(x) = E_k\psi_k(x)$

Energy of ψ_κ has no uncertainty. A measurement will always yield E_k.

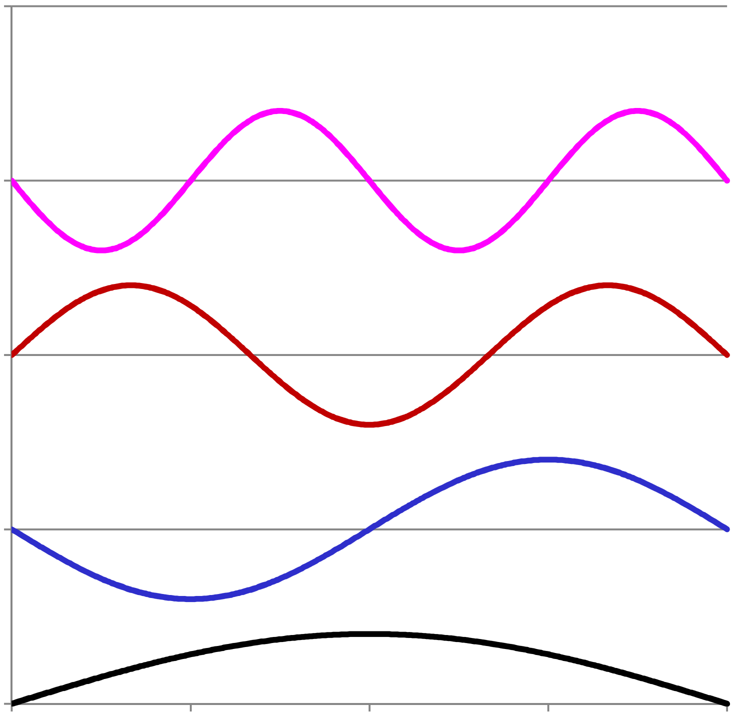
ψ_κ has infinite lifetime.

Linear combination of ψ_κ with different k's is an allowed state but not an eigenstate.

Problem: Normalization condition $\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$ cannot be satisfied.

Systems and States (continued)

Example 2: Particle in a box



Normalization condition $\int_{-a}^{a} \psi^* \psi \, dx = 1$

Normalized wavefunction of an eigenstate $\psi_k(x) = \frac{1}{\sqrt{2a}} e^{ikx}$

Only discrete k's are allowed (n = 1,2,3, ...) $k = n\frac{\pi}{2a}$

For an eigenstate $E_k = \int \psi_k^* H \psi_k \, dx$

For a general state ψ (mixture of eigenstates),

$$\langle H \rangle = \int \psi^* H \psi \, dx$$

Specific example: $\psi = \psi_1 / \sqrt{2} + \psi_2 / \sqrt{2}$

Systems and States (continued)

Example 3: spin ½ in magnetic field

Basis states for magnetic moments are eigenstates of S_z.

Only 2 eigenstates: u and v or $|u\rangle$ and $|v\rangle$.

Discrete states of finite number are written in matrix form:

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |v\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Mixed states are possible. Examples:

$$\begin{pmatrix} \sqrt{0.9} \\ \sqrt{0.1} \end{pmatrix}$$

Partially polarized beam (90% neutrons are spin up)

Polarizing neutrons will be explained by Dominic Ryan

$$\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

Eigenstate with $S_x = +1/2$

Dirac Notations

$$\langle \zeta | A | \zeta \rangle = \langle A \rangle$$

Expectation value of a measurable quantity A while the system is in state $|\zeta\rangle$

bra-c-ket

An example: $|\zeta\rangle = \begin{pmatrix} \sqrt{0.9} \\ \\ \sqrt{0.1} \end{pmatrix}$

A ket describing a general state of a system with two eigenstates

Another example: a system with 4 eigenstates:

$$|\alpha\rangle = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} \qquad |\beta\rangle = \begin{pmatrix} \sqrt{2/3} \\ 0 \\ \sqrt{1/3} \\ 0 \end{pmatrix} \qquad |e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

"bra" is the transpose of "ket". For any state ψ, $\langle \psi | \psi \rangle = 1$

Dirac Notations (continue)

$$\langle H \rangle = \langle \psi | H | \psi \rangle = \int \psi^*(x)\, H(x)\, \psi(x)\, dx$$

(or)

$$= \begin{pmatrix} p & q & r & s \end{pmatrix} \begin{pmatrix} E_1 & & & \\ & E_2 & & 0 \\ & 0 & E_3 & \\ & & & E_4 \end{pmatrix} \begin{pmatrix} p \\ q \\ r \\ s \end{pmatrix}$$

$$= p^2 E_1 + q^2 E_2 + r^2 E_3 + s^2 E_4$$

Closure relation: $$\sum_j^{all} |e_j\rangle\langle e_j| = 1$$

Starting point for deriving the scattering cross-section - Fermi Golden Rule

$$(Transition\ Rate)_{I\rightarrow F} = \frac{2\pi}{\hbar}\left|\langle F\,|V\,|\,I\rangle\right|^2 \rho(E_F)$$

Taken from Baym.
Slightly modified in
Squires' Eq. (2.2)

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\rightarrow\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\langle \mathbf{k}'\lambda'|V\,|\,\mathbf{k}\lambda\rangle\right|^2$$

Squires' Eq. (2.13)
Caution: Dimension of ⟨...⟩
has changed to energy.cm^3

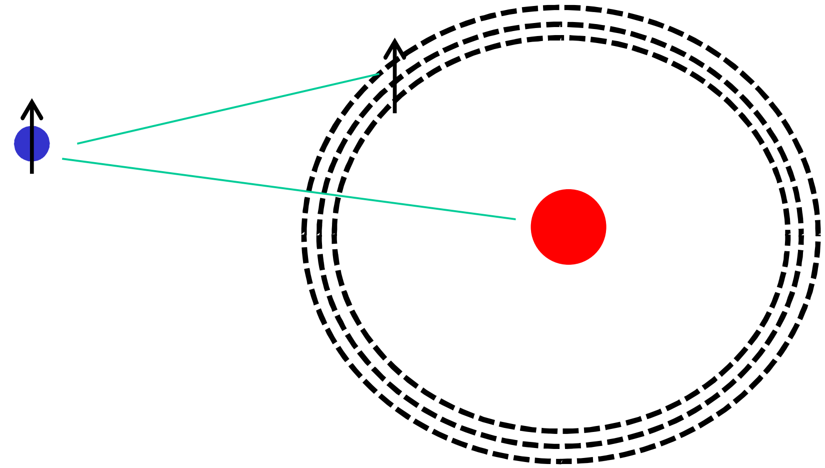
$$\left(\frac{d^2\sigma}{d\Omega\,dE'}\right)_{\lambda\rightarrow\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\langle \mathbf{k}'\lambda'|V\,|\,\mathbf{k}\lambda\rangle\right|^2 \delta(E_{\lambda'} - E_\lambda - \hbar\omega)$$

Squires' Eq. (2.15)

where the δ-function is normalized, i.e. $\int \delta(E)\,dE = 1$

A few words about the perturbation potential V

(1) Nuclear
(2) Magnetic



Magnetic scattering will be discussed by Collin Broholm

1. Both interactions are spin-dependent, i.e. not free of magnetism, but only the dipole-dipole interaction is called "magnetic".
2. Magnetic scattering length, γr_0 = 5.39 fm, is comparable to a typical |b| of nuclear scattering.
3. Caused by a finite-sized object (electronic cloud of an atom), magnetic scattering falls off with a form factor.

Summary

Three approaches for neuron scattering have been presented.
Although the starting points are different:

The three approaches are all inter-related.

Concepts presented in one are covered in the other, at least as a special case.

None should be labelled “too easy” or “too difficult”.
By paying due attention we can learn a lot from all three approaches.