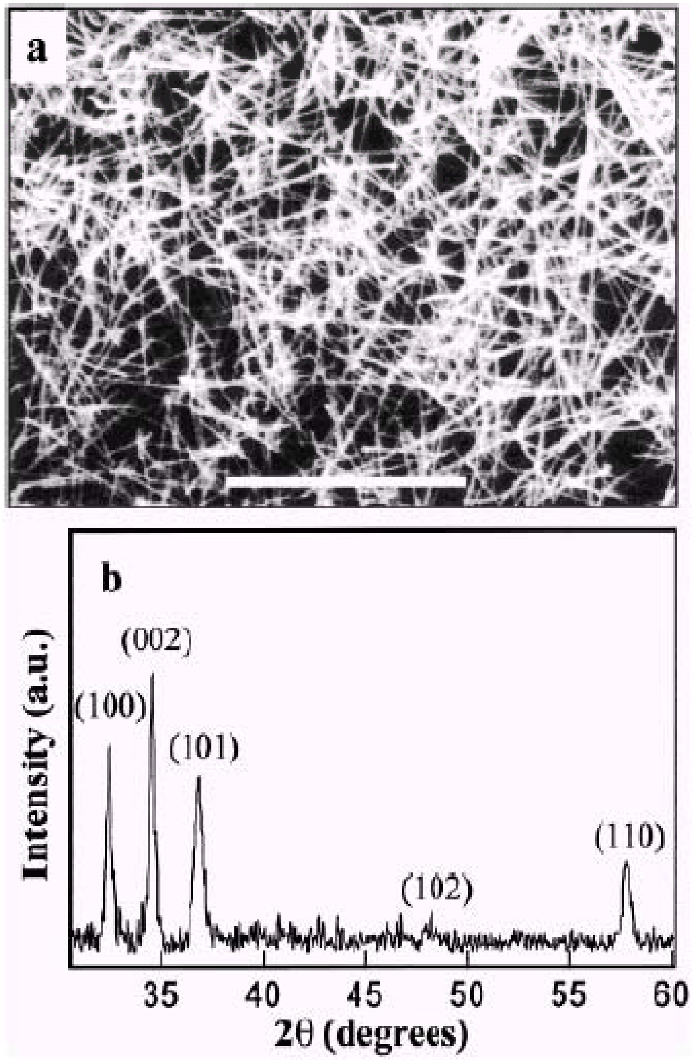
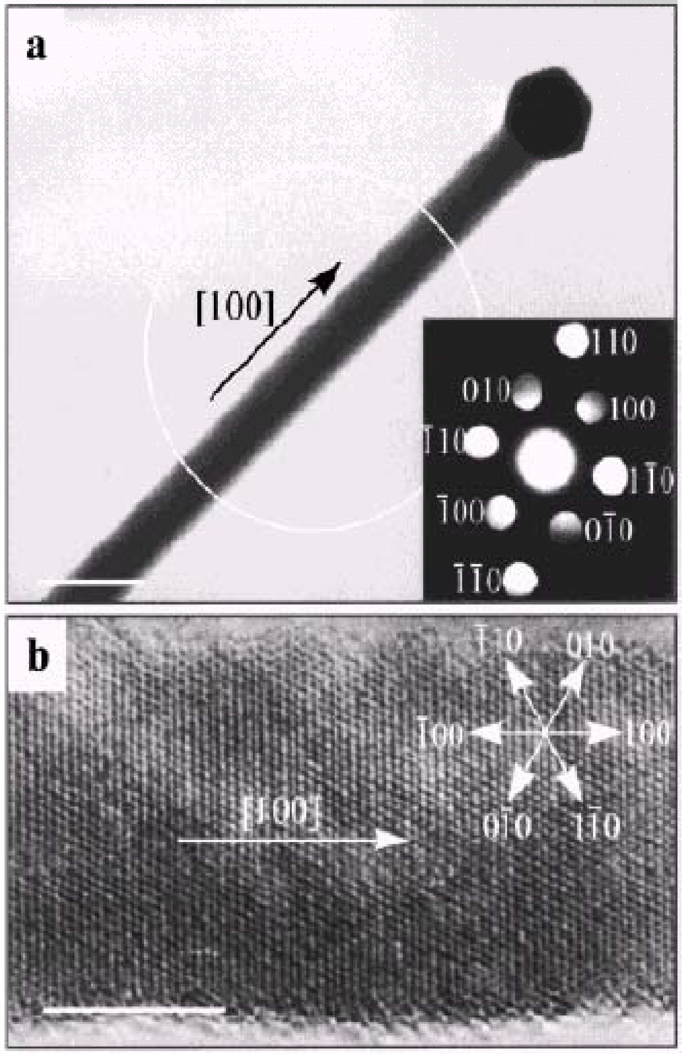
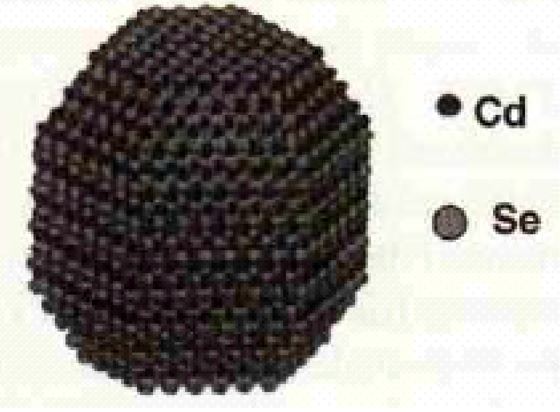
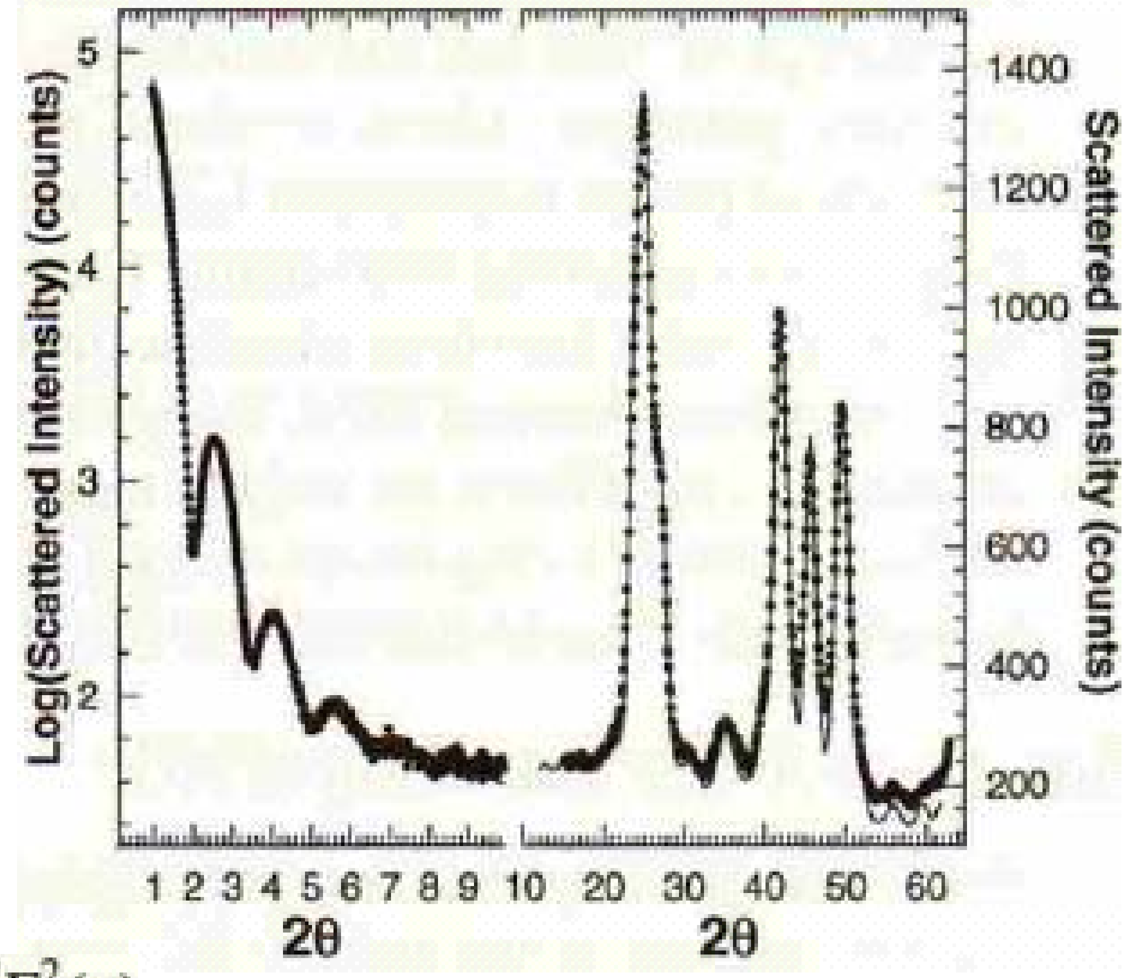
Overview on Scattering


a
b
Intensity (a.u.)
(100)
(002)
(101)
(102)
(110)
35
40
45
50
55
60
2θ (degrees)


a
[100]
1̄10
010
100
1̄10
11̄0
1̄00
01̄0
1̄1̄0
b
[100]
1̄10
010
1̄00
100
01̄0
11̄0

Scattering pattern of nanocrystal

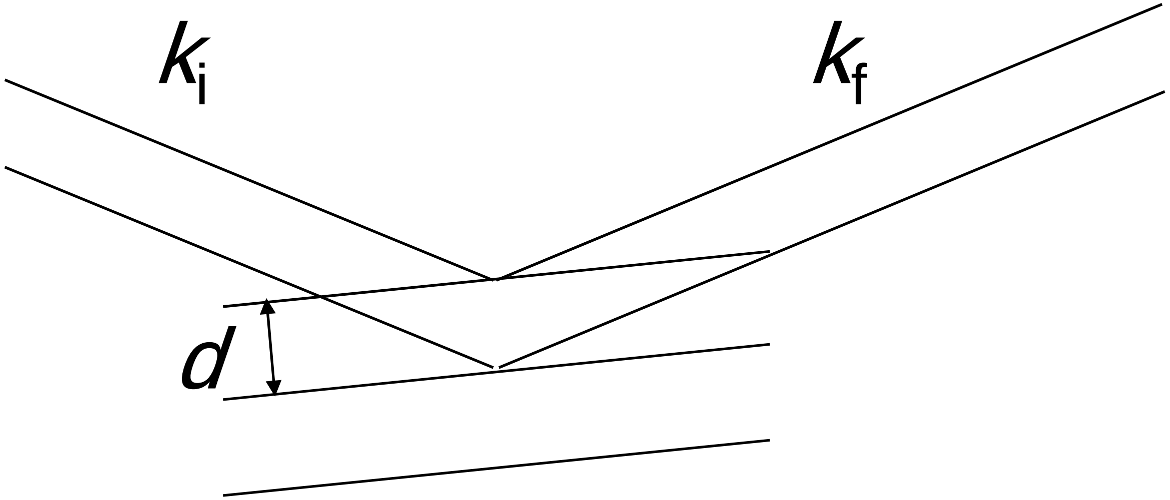




$$I(q) = I_o N(\rho - \rho_o)^2 F^2(q)$$

$$F(q) = \frac{4}{3}\pi R^3 \left[3\frac{\sin(qR) - qR\cos(qR)}{(qR)^3}\right]$$

elastic scattering: $k_i = k_f$



for constructive interference: $2\vec{k} \cdot \vec{s} = \left|\vec{k}\right|^2$

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

Properties of x-rays and neutrons

x-rays:

electromagnetic radiation

$$c = \lambda v$$

$$E = hv$$

$$p = h / v$$

$$1/\nu = \tau = 10^{-19}\mathrm{s}$$

neutron:

an uncharged elementary particle

v depends on λ

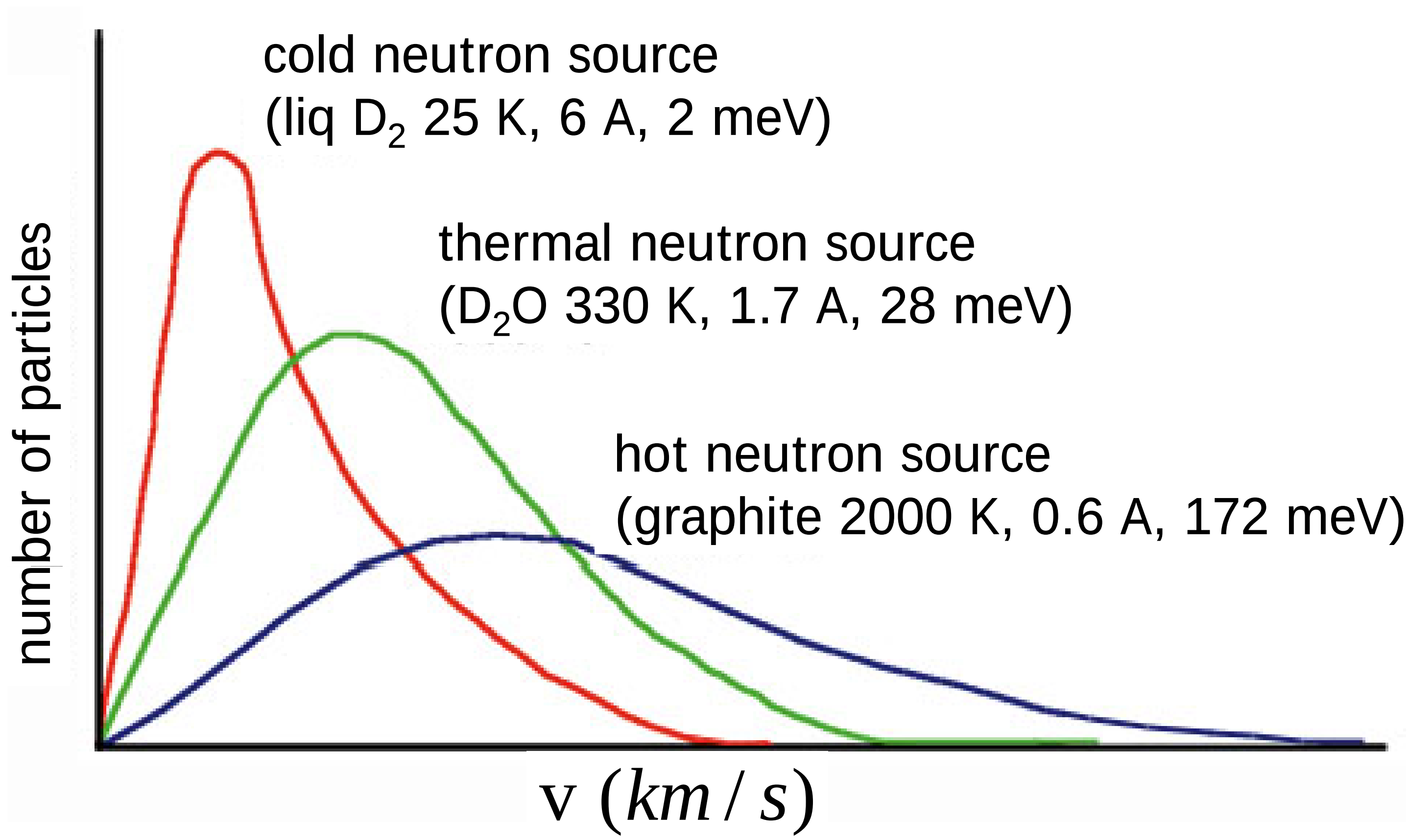
$$E = m\mathrm{v}^2 / 2$$

$$p = m\mathrm{v}$$

$$1/\nu = \tau = 10^{-13}\mathrm{s}$$

magnetic moment

v distribution from reactor:-dep. on moderator
Maxwell-Boltzmann distribution



-kT (at RT) ~ 20 meV
investigation on dyanamics is also availabe.

$$J = |A|^2 = AA^*$$

$$\frac{J}{J_0} = \frac{d\sigma}{d\Omega}$$

- differential scattering cross-section:

the probability that a photon or a neutron impinging on the sample into a unit solid angle in the given direction

$$\frac{J}{J_0} = \frac{d\sigma}{d\Omega}$$

$$= \frac{\text{number of particles scattered into a unit solid angle per second}}{\text{flux of incident beam}}$$

$$\sigma_{\text{tot}} = \frac{\text{total number of particles scattered in all direction per second}}{\text{flux of incident beam}}$$

$$A(\vec{q}) = \int \rho(\vec{r}) e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$

SLDD

$$\rho(\vec{r}) = \rho_{\mathrm{u}}(\vec{r}) * z(\vec{r})$$

FT

IFT

Scattering amplitude

$$A(\vec{q}) = F(\vec{q}) Z(\vec{q})$$

Form factor

lattice factor

autocorrelation

$$\Gamma_\rho(\vec{r}) = V\langle \rho(\vec{u})\rho(\vec{u}\,')\rangle = \int \rho(\vec{r})\rho(\vec{u}+\vec{r}) d\vec{u}$$

X

squaring

$$I(\vec{q}) = A(\vec{q}) \cdot A^*(\vec{q})$$

$$\Gamma_\rho(\vec{r})$$

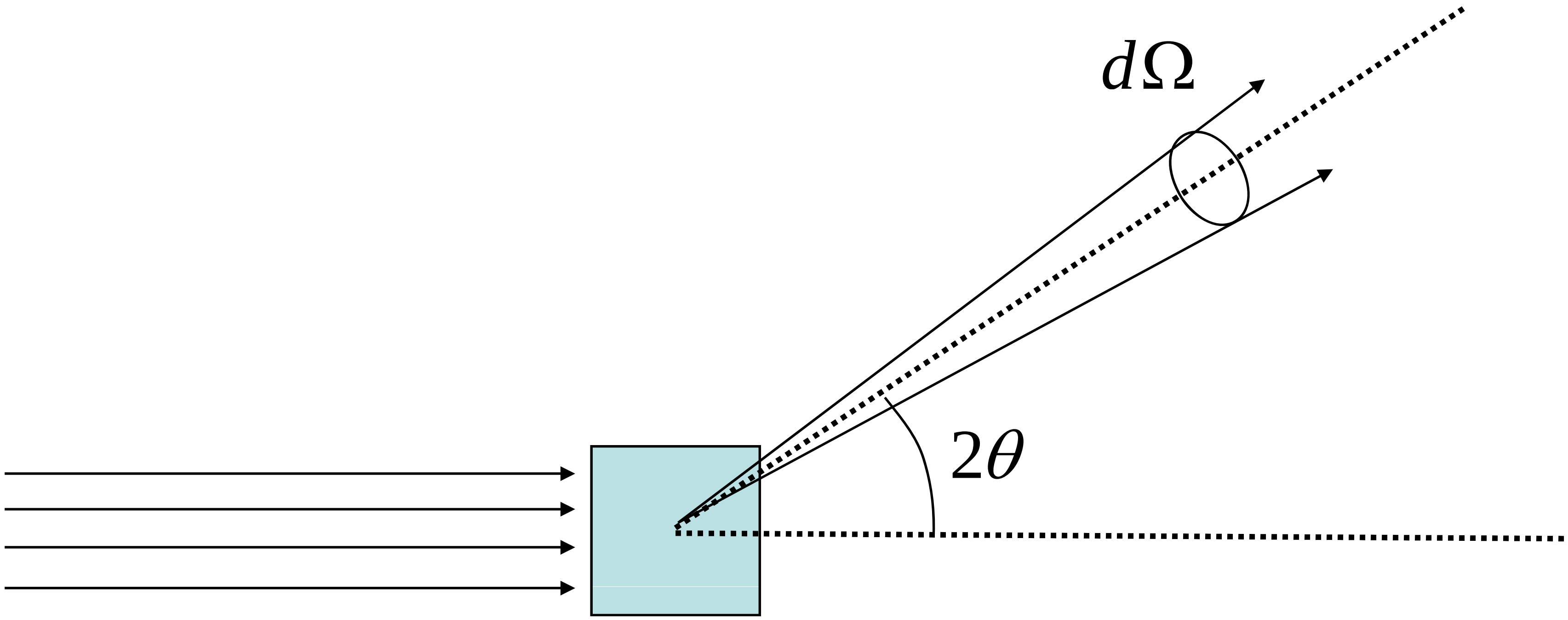
Autocorrelation ftn

FT

IFT

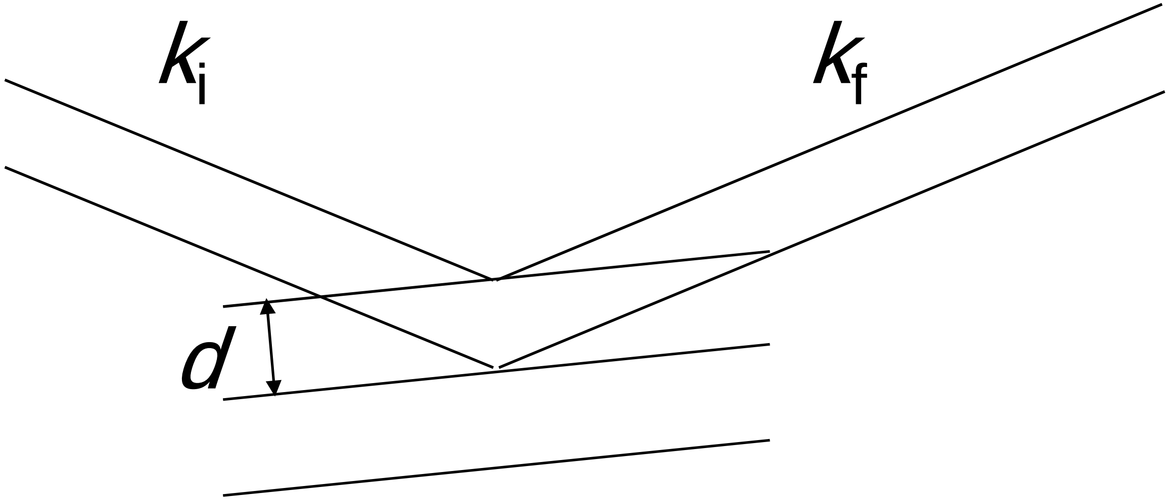
$$I(\vec{q})$$

$$I(\vec{q}) = \int \Gamma_\rho(\vec{r}) e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$



dΩ
2θ

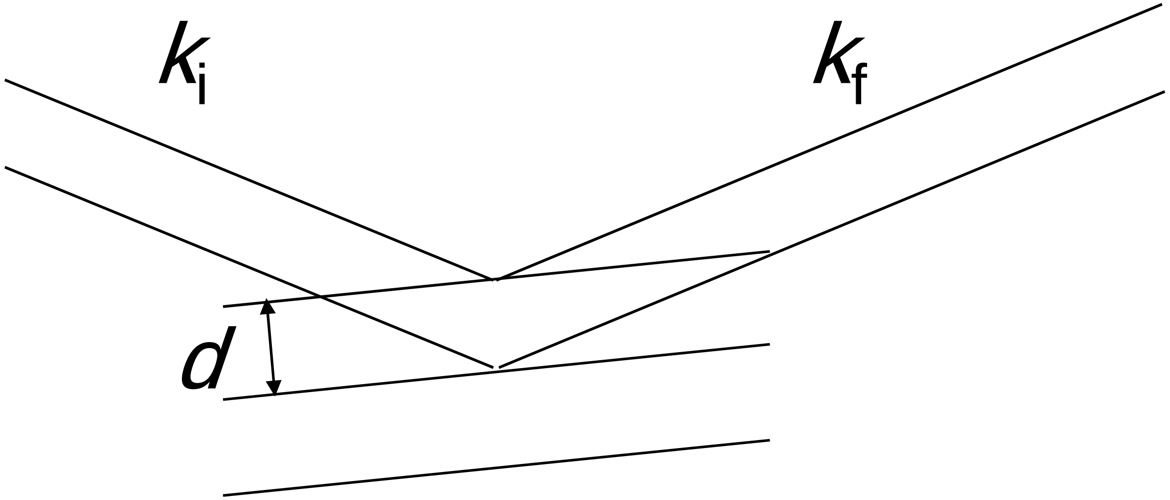
elastic scattering: $k_i = k_f$



for constructive interference: $2\vec{k} \cdot \vec{s} = \left|\vec{k}\right|^2$

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

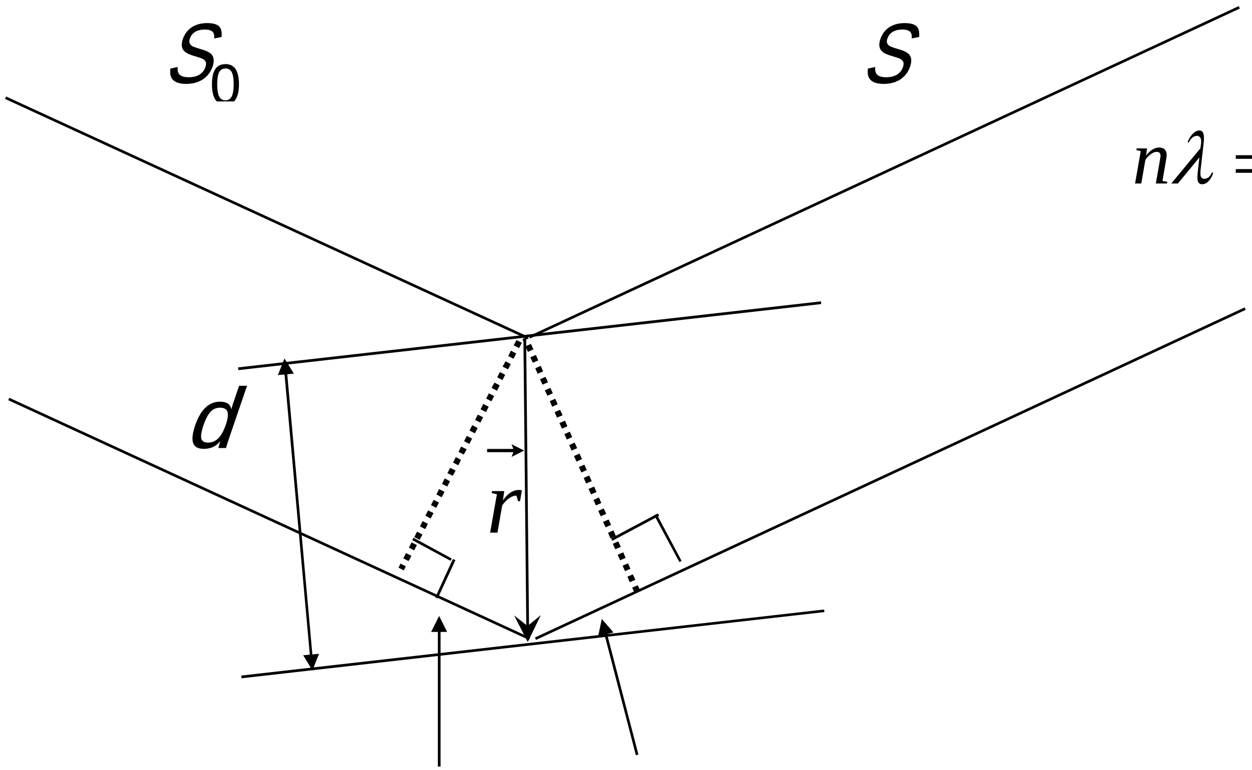
elastic scattering: $k_i = k_f$



for constructive interference: $2\vec{k} \cdot \vec{s} = \left|\vec{k}\right|^2$

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

coherent scattering:



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

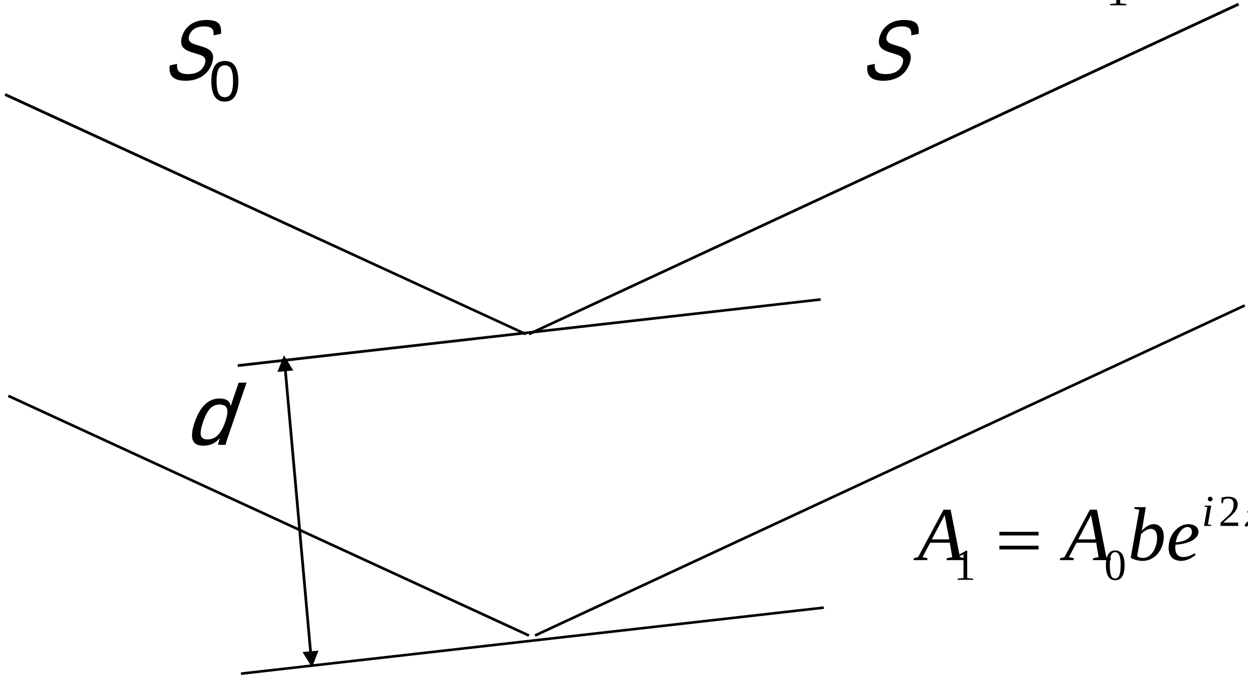
$$\Delta\phi = \frac{2\pi\delta}{\lambda} = \frac{2\pi}{\lambda}(\vec{S}_0 \cdot \vec{r} - \vec{S} \cdot \vec{r})$$

$$= -2\pi\vec{s} \cdot \vec{r}$$

$$\vec{s} = \frac{\vec{S} - \vec{S}_0}{\lambda}$$

$$A_2 = A_1 b e^{i\Delta\phi}$$

$$= A_1 b e^{i2\pi(\nu t - x/\lambda)} e^{-i2\pi \vec{s}\cdot\vec{r}}$$



$$A_1 = A_0 b e^{i2\pi(\nu t - x/\lambda)}$$

at the detector:

$$A = A_1 + A_2 = A_0 b e^{i2\pi(\nu t - x/\lambda)}\left(1 + e^{-i2\pi \vec{s}\cdot\vec{r}}\right)$$

Ewald sphere and reciprocal scattering

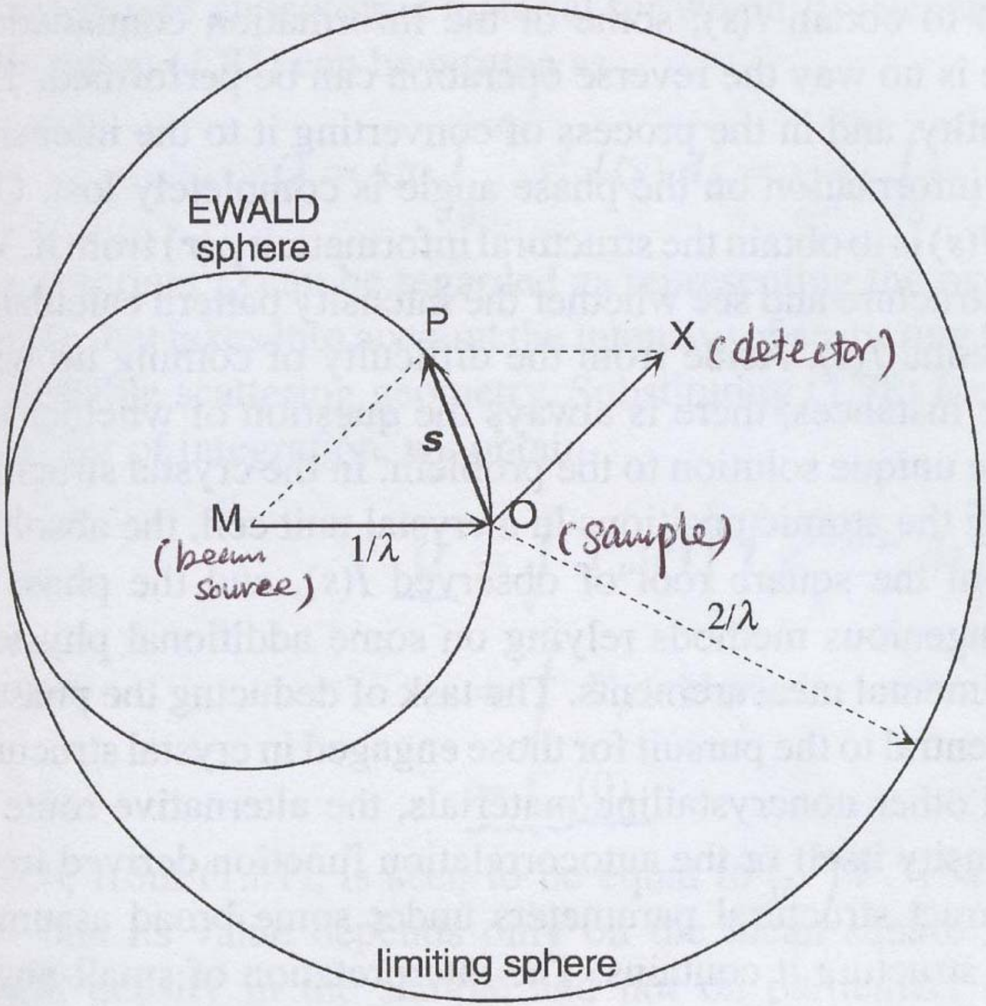


Figure 1.11 Ewald sphere construction.

at the detector:

$$A = A_1 + A_2 = A_0 b e^{i2\pi(vt - x/\lambda)} (1 + e^{-i2\pi\vec{s}\cdot\vec{r}})$$

$$J = AA^* = A_0^2 b^2 (1 + e^{i2\pi\vec{s}\cdot\vec{r}})(1 + e^{-i2\pi\vec{s}\cdot\vec{r}})$$

$$A = A_0 b \ (1 + e^{-i2\pi\vec{s}\cdot\vec{r}})$$

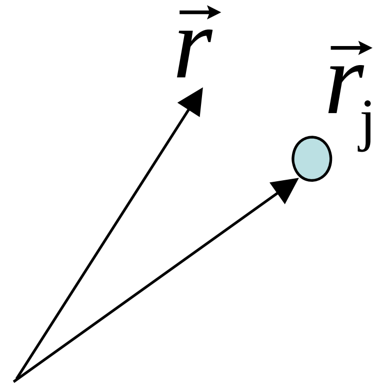
when there are N identical scatteres,

$$A = A_0 b \sum_{j=1}^{N} e^{-i2\pi\vec{s}\cdot\vec{r}_j} = A_0 b \sum_{j=1}^{N} e^{-i\vec{q}\cdot\vec{r_j}}$$

$$A = A_0 b \int_V n(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} d\vec{r}$$

Unitcell Structure factor or form factor

$$A(q) \sim F(q) \qquad \rho(\vec{r}) = \sum_j \rho_{\mathrm{j}}(\vec{r} - \vec{r}_{\mathrm{j}})$$



$$F(q) = \int \rho(\vec{r}) \exp(-i\vec{r} \cdot \vec{q}) d\vec{r}$$

$$\Rightarrow \sum_j \int \rho(\vec{r} - \vec{r}_{\mathrm{j}}) \exp(-i\vec{r} \cdot \vec{q}) d\vec{r}$$

$$= \sum_j \left[\int_V \rho(\vec{r} - \vec{r}_{\mathrm{j}}) \exp[-i\vec{q} \cdot (\vec{r} - \vec{r}_{\mathrm{j}})] d\vec{r} \exp(-i\vec{q} \cdot \vec{r}_{\mathrm{j}}) \right]$$

$$= \sum_j f_{\mathrm{j}} \exp(-i\vec{q} \cdot \vec{r}_{\mathrm{j}})$$

Atomic form factor:
intensity determination

lattice sum
Position determination

for n atomic crystal,

$$F(q) = \sum_j f_j \exp(-i\vec{q}\cdot\vec{r}_j) \sum_n \exp(-i\vec{q}\cdot\vec{R}_n)$$

unit cell structure factor

lattice sum
Position determination

$$\vec{q}\cdot\vec{R}_n = 2\pi \times \text{integer}$$

since $\sum_n \exp(-i\vec{q}\cdot\vec{R}_n) \sim N$

otherwise, $\sum_n \exp(-i\vec{q}\cdot\vec{R}_n) \sim 1$

Real and inverse lattice

$$\vec{r} \cdot \vec{q} = 2\pi \times \text{integer}$$ (Laue condition ~ Bragg Law)

$$\vec{r} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3 \qquad \vec{q} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$$

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_2 \cdot a_3 \times a_1}$$

$$b_2 = 2\pi \frac{a_3 \times a_1}{a_3 \cdot a_1 \times a_2}$$

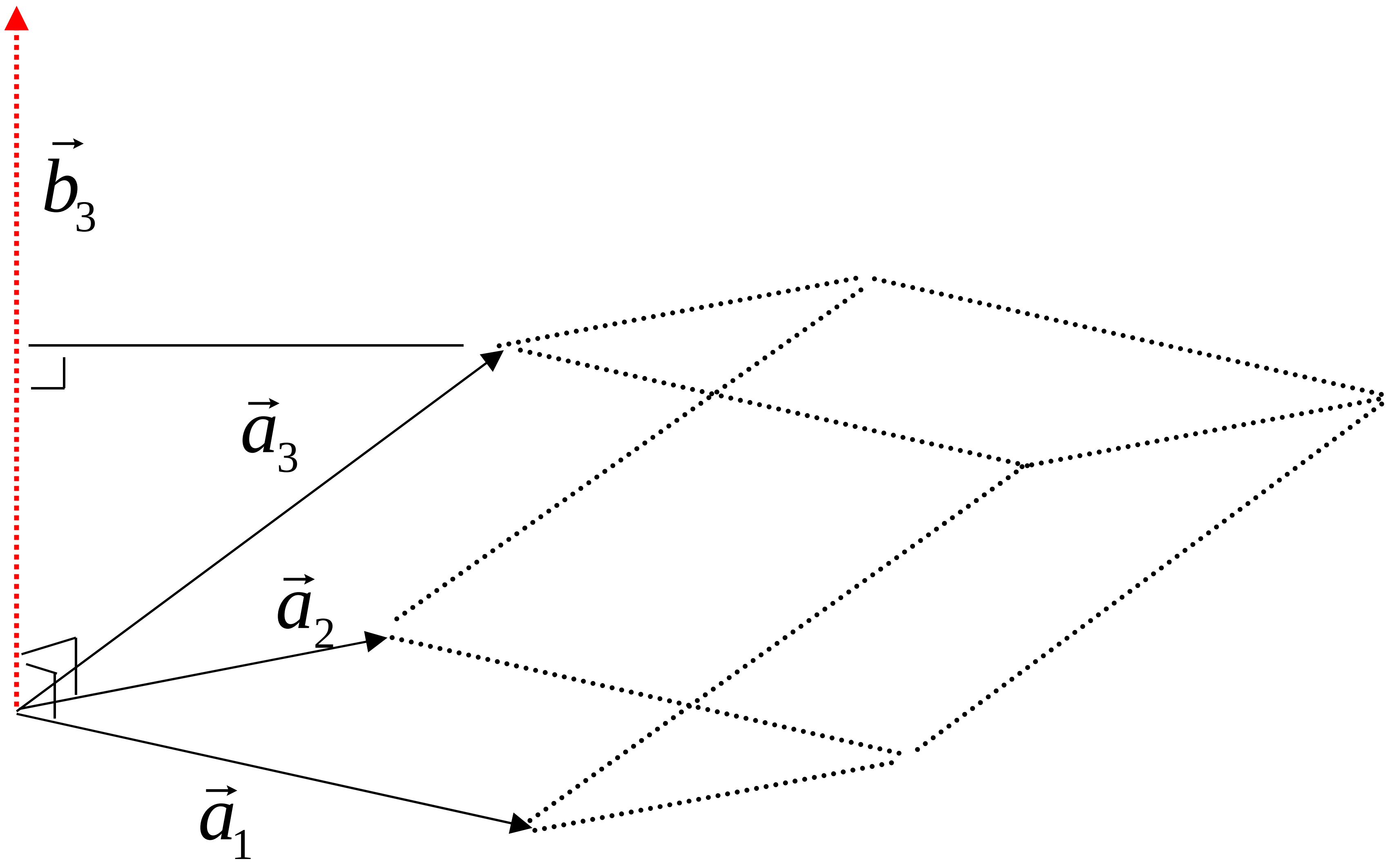
$$b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot a_2 \times a_3}$$

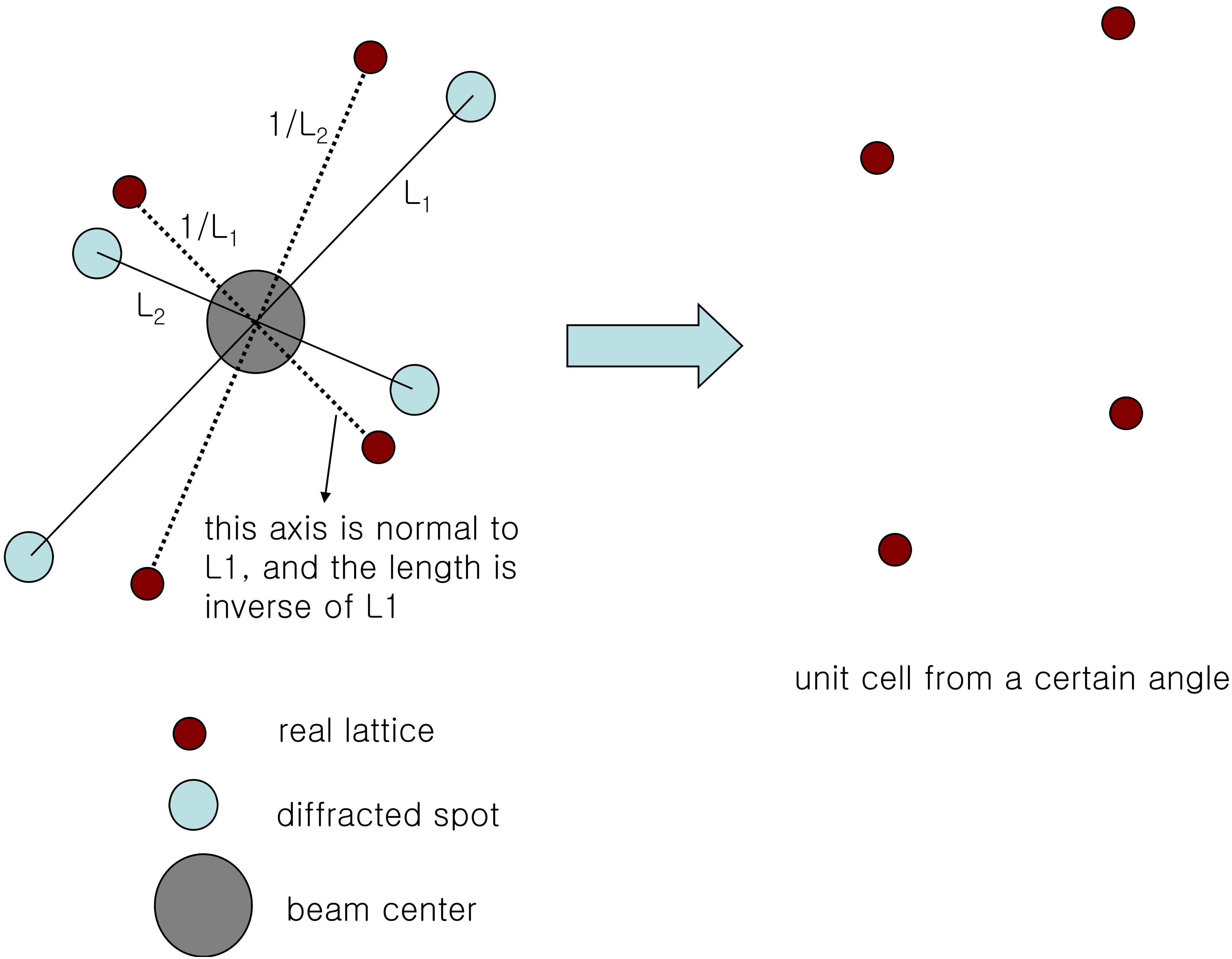
$$b_{\mathrm{i}} \cdot a_{\mathrm{j}} = 2\pi\delta_{\mathrm{ij}}$$

when $i \neq j$, 0

when $i = j$, 2π

$$\Rightarrow \quad \vec{r} \cdot \vec{q} = 2\pi \times \left(u_1 v_1 + u_2 v_2 + u_3 v_3\right)$$


$\vec{b}_3$
$\vec{a}_3$
$\vec{a}_2$
$\vec{a}_1$


1/L2
L1
1/L1
L2
this axis is normal to L1, and the length is inverse of L1
unit cell from a certain angle
real lattice
diffracted spot
beam center

Structure factor or form factor

$$A(q) \sim F(q) \qquad \rho(\vec{r}) = \sum_j \rho_{\mathrm{j}}(\vec{r} - \vec{r}_{\mathrm{j}})$$

$$F(q) = \int \rho(\vec{r}) \exp(-i\vec{r} \cdot \vec{q}) d\vec{r}$$

assuming spherical symmetry,

$$= \int 4\pi r^2 \rho(r) \frac{\sin(\vec{r} \cdot \vec{q})}{\vec{r} \cdot \vec{q}} dr$$

see Fig 1.6

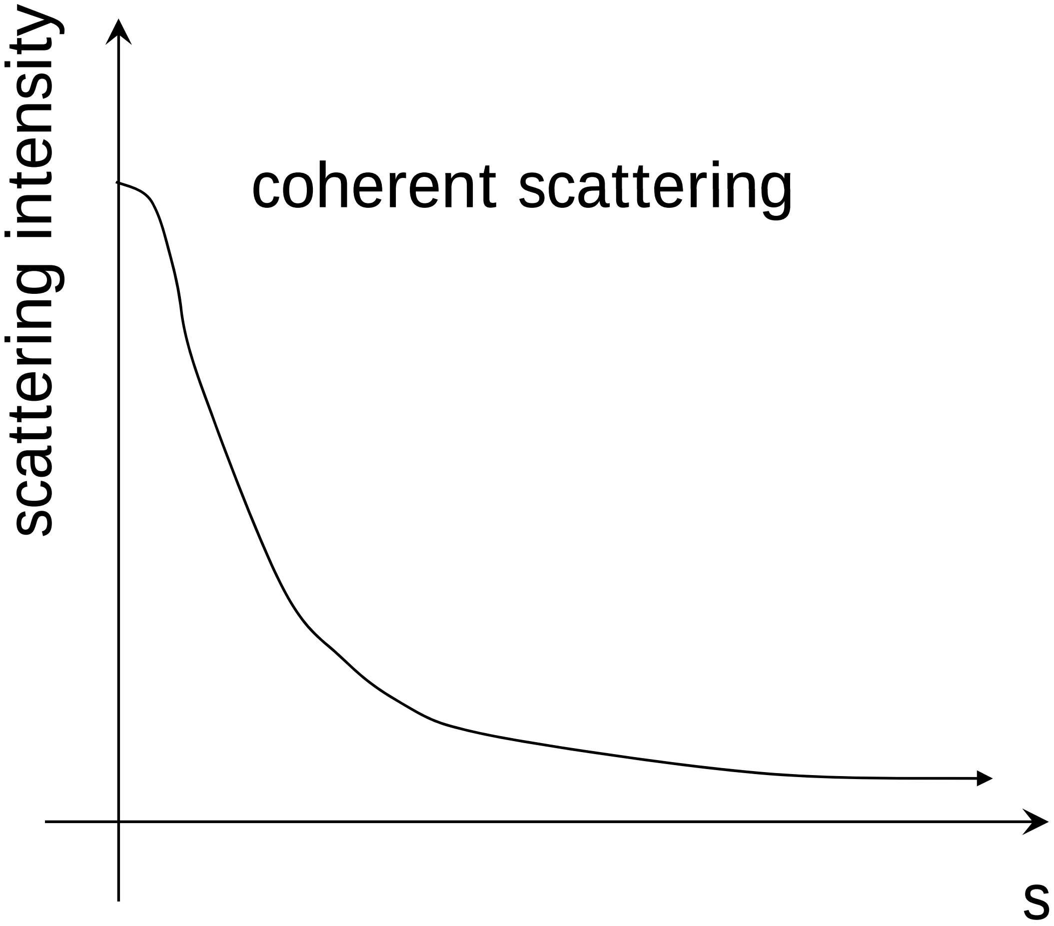
•Scattering length of a single nucleus

-interaction w/ nucleus:
highly penetrating

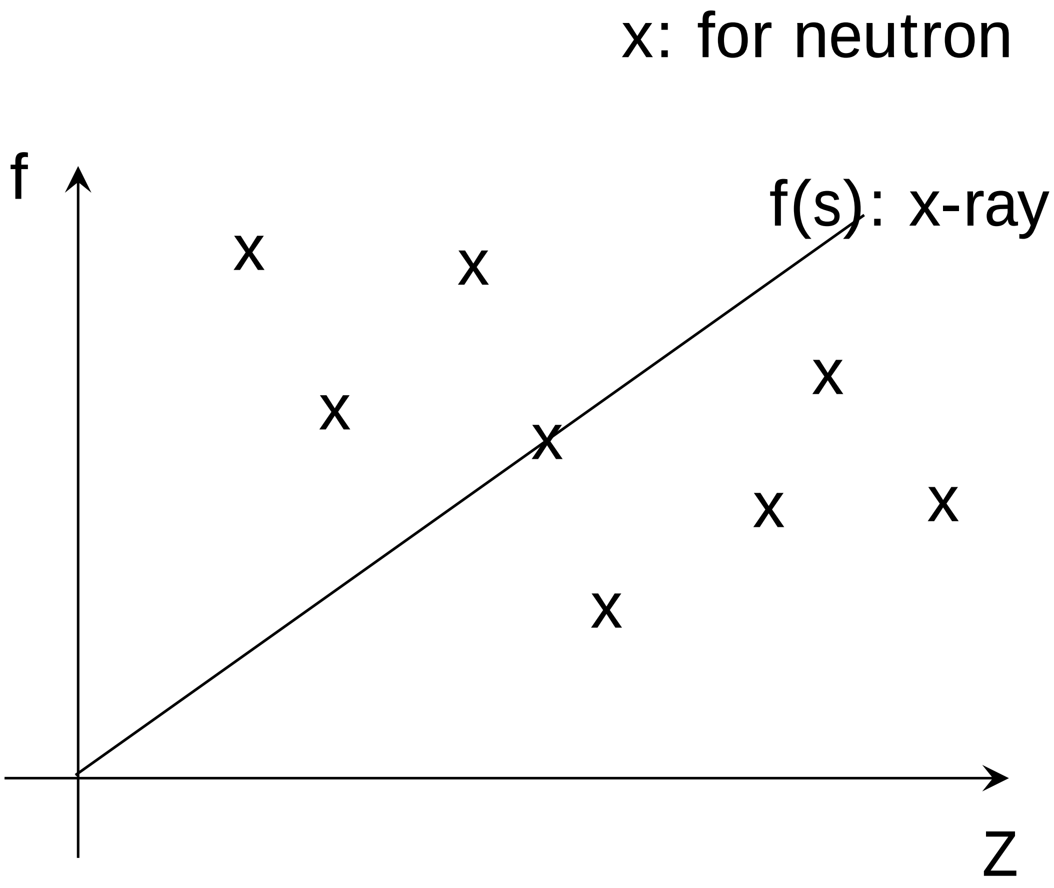
-scattering occurs due to

1. structure
2. randomness of spin state
   and distribution of isotope

scattering intensity for C atom as a function of q



atomic scattering factor



•Coherent and incoherent scattering length

random variability in scattering lengths
~ due to isotopes or non-zero nuclear spin

Structural info. + incoherent background

-when neutron (spin 1/2) interacts with a nucleus of spin *i*

total spin	spin multiplicity -associated w/ total spin	probability
$i+1/2$	$2(i+1/2)+1=2i+2$	$f^{+}=\frac{2i+2}{4i+2}=\frac{i+1}{2i+1}$
$i-1/2$	$2(i-1/2)+1=2i$	$f^{-}=\frac{2i}{4i+2}=\frac{i}{2i+1}$

$$A(q) = A_0 \sum_j b_j e^{-i\vec{r}\cdot\vec{q}}$$

$$\frac{d\sigma}{d\Omega} = \sum_{j,k} \left\langle b_j b_k \right\rangle e^{-i(\vec{r}_j - \vec{r}_k)\cdot\vec{q}}$$

$$\left\langle b_j b_k \right\rangle \quad \text{when } j = k,\ \left\langle b_j b_k \right\rangle = \left\langle b_j^2 \right\rangle = \left\langle b^2 \right\rangle$$

$$\text{when } j \neq k,\ \left\langle b_j b_k \right\rangle_{j\neq k} = \left\langle b_j \right\rangle \left\langle b_k \right\rangle = \left\langle b \right\rangle^2$$

$$\left\langle b_j b_k \right\rangle = \left\langle b \right\rangle^2 + \delta_{j,k} \left(\left\langle b^2 \right\rangle - \left\langle b \right\rangle^2 \right)$$

$$\frac{d\sigma}{d\Omega} = \sum_{j,k} \left\langle b_j b_k \right\rangle e^{-i(\vec{r}_j - \vec{r}_k)\cdot\vec{q}}$$

$$\Rightarrow \quad \frac{d\sigma}{d\Omega} = \left\langle b \right\rangle^2 \sum_{j,k} e^{-i(\vec{r}_j - \vec{r}_k)\cdot\vec{q}} + N\left(\left\langle b^2 \right\rangle - \left\langle b \right\rangle^2\right)$$

$$b_{coh} = \left\langle b \right\rangle$$

$$b_{inc} = \left(\left\langle b^2 \right\rangle - \left\langle b \right\rangle^2\right)^{1/2}$$

see Table 1.2
note on H and D

$$\sigma_{coh} = 4\pi \left\langle b \right\rangle^2$$

$$\sigma_{inc} = 4\pi\left(\left\langle b^2 \right\rangle - \left\langle b \right\rangle^2\right)$$

(since $\sigma_{tot} \sim 4\pi b^2$)

Q. what does negative b means?

A. scattering from the nucleus
undergoes a 180º phase shift

$$A(\vec{q}) = \int \rho(\vec{r}) e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$

SLDD

$$\rho(\vec{r}) = \rho_{\mathrm{u}}(\vec{r}) * z(\vec{r})$$

FT

IFT

Scattering amplitude

$$A(\vec{q}) = F(\vec{q}) Z(\vec{q})$$

Form factor

lattice factor

autocorrelation

$$\Gamma_{\rho}(\vec{r}) = V \langle \rho(\vec{u}) \rho(\vec{u}') \rangle = \int \rho(\vec{r}) \rho(\vec{u} + \vec{r}) d\vec{u}$$

X

squaring

$$I(\vec{q}) = A(\vec{q}) \cdot A^{*}(\vec{q})$$

$$\Gamma_{\rho}(\vec{r})$$

Autocorrelation ftn

FT

IFT

$$I(\vec{q})$$

$$I(\vec{q}) = \int \Gamma_{\rho}(\vec{r}) e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$

$$A(\vec{q}) = \int \rho(\vec{r}) e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$

SLDD

$$\rho(\vec{r}) = \rho_{\mathrm{u}}(\vec{r}) * z(\vec{r})$$

FT

IFT

Scattering amplitude

$$A(\vec{q}) = F(\vec{q}) Z(\vec{q})$$

Form factor

lattice factor

X

squaring

$$I(\vec{q}) = A(\vec{q}) \cdot A^{*}(\vec{q})$$

$$I(\vec{q})$$

SLDD

$$\rho(\vec{r}) = \rho_{\mathrm{u}}(\vec{r}) * z(\vec{r})$$

FT →

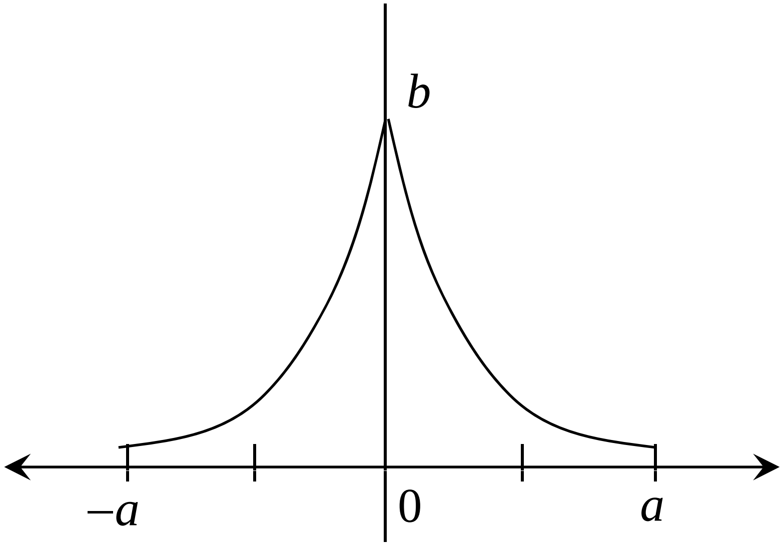
← IFT

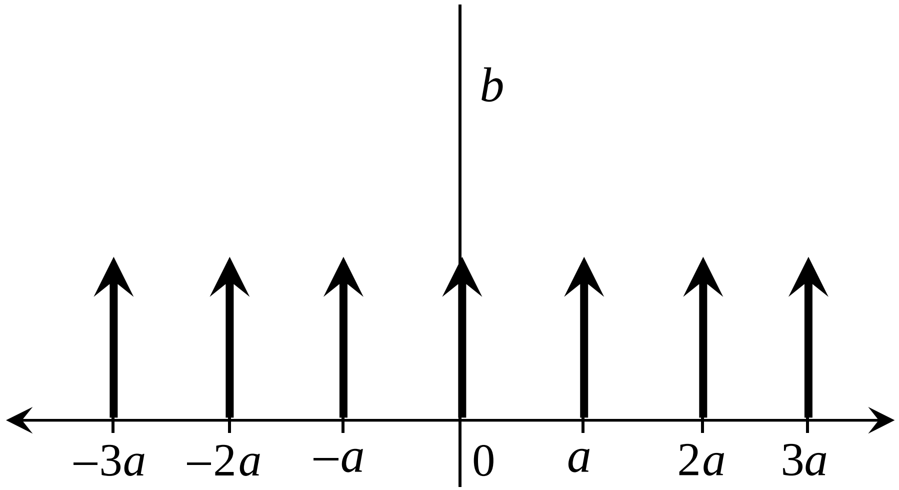
Scattering amplitude

$$A(\vec{q}) = F(\vec{q})Z(\vec{q})$$

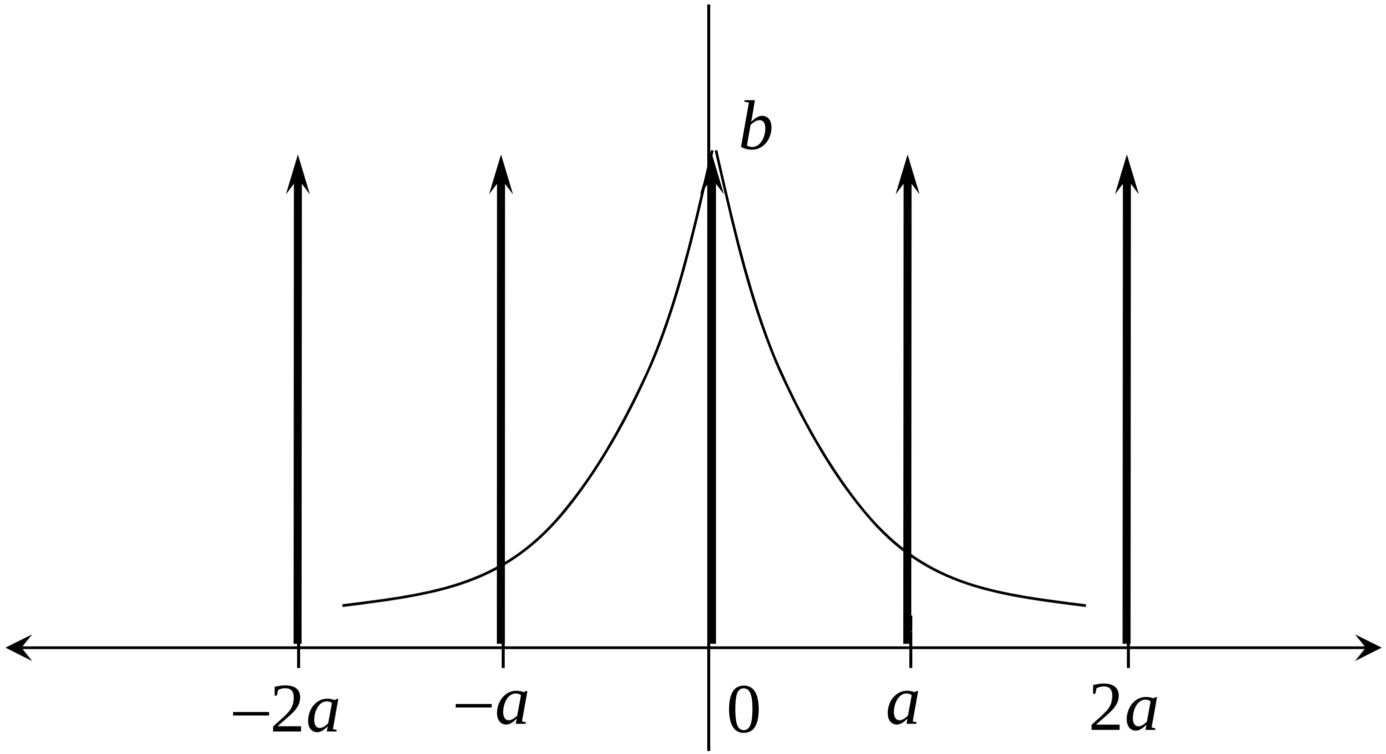
Form factor → $F(\vec{q})$

lattice factor → $Z(\vec{q})$





$$\rho_{\mathrm{u}}(\vec{r}) \times z(\vec{r})$$



$$\rho(\vec{r}) = \rho_{\mathrm{u}}(\vec{r}) * z(\vec{r})$$

$$\rho(x) * z(x)$$

$$= \sum_{n=-\infty}^{\infty} \rho(x) * \delta(x - na)$$

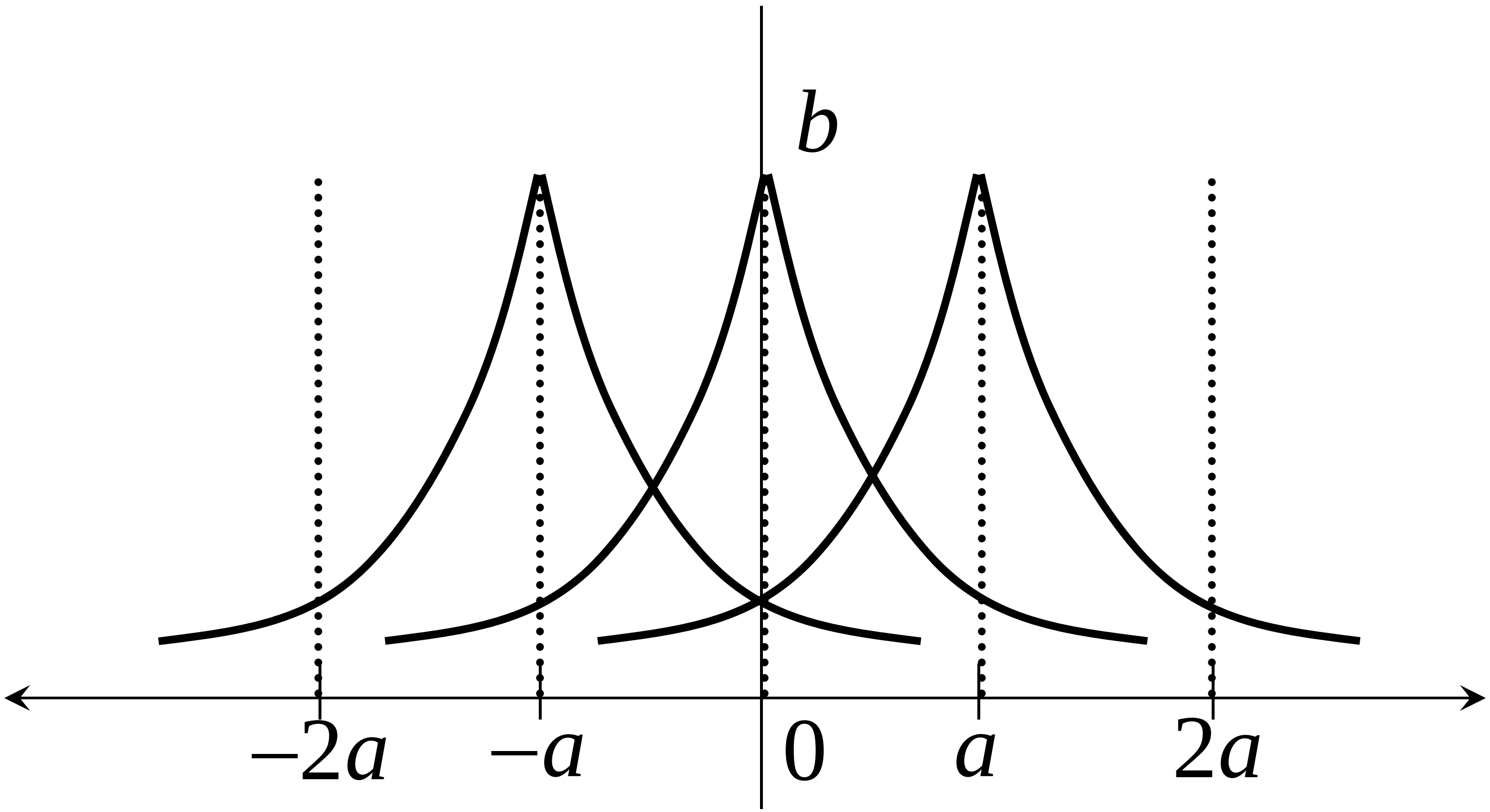
$$= \sum_{n=-\infty}^{\infty} \int_{0}^{x-na} \rho(u)\delta((x-na)-u)du$$

$$\left[\text{since} \int_{0}^{x-na} \rho(u)\delta((x-na)-u)du = f(x-na), \right]$$

$$= \sum_{n=-\infty}^{\infty} \rho(x-na)$$

$$\rho(\vec{r}) = \rho_{\mathrm{u}}(\vec{r}) * z(\vec{r})$$

$$= \sum_{n=-\infty}^{\infty} \rho(x - na)$$



SLDD

$$\rho(\vec{r}) = \rho_{\mathrm{u}}(\vec{r}) * z(\vec{r})$$

autocorrelation

$$\Gamma_\rho(\vec{r}) = V\left\langle \rho(\vec{u})\rho(\vec{u}\,')\right\rangle = \int \rho(\vec{r})\rho(\vec{u}+\vec{r})d\vec{u}$$

$$\Gamma_\rho(\vec{r})$$

Autocorrelation ftn

FT →

← IFT

$$I(\vec{q})$$

$$I(\vec{q}) = \int \Gamma_\rho(\vec{r})e^{-i\vec{r}\cdot\vec{q}}d\vec{r}$$

$$I(\vec{q})$$

$$= \left\langle \left| A(\vec{q}) \right|^2 \right\rangle = A(\vec{q}) \cdot A^*(\vec{q})$$

$$= \left\langle \left| \int \rho(\vec{r}) e^{i\vec{r}\cdot\vec{q}} d\vec{r} \right|^2 \right\rangle = A^*(\vec{q}) \cdot A(\vec{q})$$

$$= \left[\int \rho(\vec{u}) e^{i\vec{u}\cdot\vec{q}} d\vec{u} \right] \left[\int \rho(\vec{u}') e^{-i\vec{u}'\cdot\vec{q}} d\vec{u}' \right]$$

$$\vec{u}' = \vec{r} + \vec{u}$$

$$d\vec{u}' = d\vec{r}$$

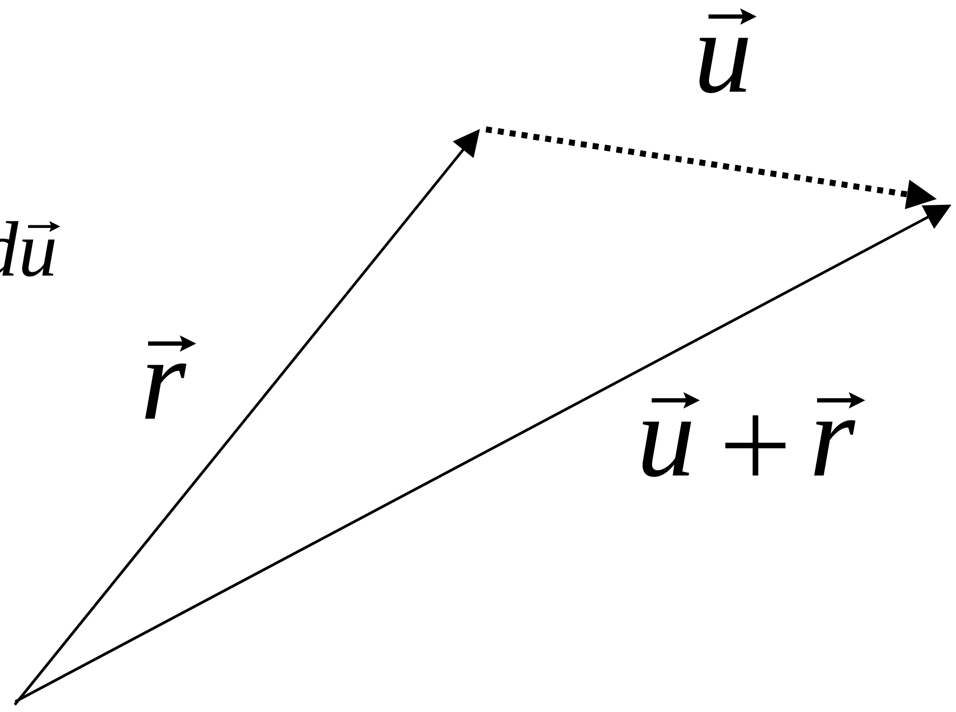
$$= \left[\int \rho(\vec{u}) e^{i\vec{u}\cdot\vec{q}} d\vec{u} \right] \left[\int \rho(\vec{r} + \vec{u}) e^{-i(\vec{r}+\vec{u})\cdot\vec{q}} d\vec{r} \right]$$

$$= \int \left[\int \rho(\vec{u}) \rho(\vec{r} + \vec{u}) d\vec{u} \right] e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$

$$= \int \Gamma_\rho(\vec{r}) e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$

Physical meaning of auto correlation ftn

$$\Gamma_{\rho}(\vec{r})$$
$$= V\langle \rho(\vec{u})\rho(\vec{u}\,')\rangle$$
$$= \int \rho(\vec{u})\rho(\vec{u}+\vec{r})d\vec{u}$$



see also p.96

Invariant $$Q = \int I(\vec{s})d\vec{s} = \frac{1}{(2\pi)^3}\int I(\vec{q})d\vec{q}$$

for isotropic materials,

$$Q = 4\pi\int s^2 I(s)ds = \frac{1}{2\pi^2}\int q^2 I(q)dq$$

$$Q = \int \Gamma_\rho(\vec{r})\left[\int e^{-i\vec{s}\cdot\vec{r}}\right]d\vec{r}$$

$$= \int \Gamma_\rho(\vec{r})\delta(\vec{r})d\vec{r}$$

$$= \Gamma_\rho(0)$$

$$\eta(\vec{r}) = \rho(\vec{r}) - \langle \rho \rangle$$

$$\Gamma_\rho(\vec{r})$$

$$= V\left\langle \rho(\vec{u})\rho(\vec{u}\,')\right\rangle$$

$$= \int \rho(\vec{r})\rho(\vec{u}+\vec{r})d\vec{u}$$

$$= \int \left[\eta(\vec{u}) + \langle \rho \rangle\right]\left[\eta(\vec{u}+\vec{r}) + \langle \rho \rangle\right] d\vec{u}$$

$$= \int \eta(\vec{u})\eta(\vec{u}+\vec{r})d\vec{u} + \langle \rho \rangle^2 \int d\vec{u} + \langle \rho \rangle \int \eta(\vec{u})d\vec{u} + \langle \rho \rangle \int \eta(\vec{u}+\vec{r})d\vec{u}$$

=0

macroscopic dimension

$$\sim \int \eta(\vec{u})\eta(\vec{u}+\vec{r})d\vec{u} + \langle \rho \rangle^2 V$$

$$\sim \Gamma_\eta(\vec{r})$$

null scattering or scattering at q=0
Experimentally unobservable

$$A(\vec{q}) = \int \rho(\vec{r}) e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$

SLDD

$$\rho(\vec{r}) = \rho_{\mathrm{u}}(\vec{r}) * z(\vec{r})$$

FT →

← IFT

Scattering amplitude

$$A(\vec{q}) = F(\vec{q}) Z(\vec{q})$$

Form factor

lattice factor

autocorrelation ↓

$$\Gamma_\rho(\vec{r}) = V\langle \rho(\vec{u})\rho(\vec{u}\,')\rangle = \int \rho(\vec{r})\rho(\vec{u}+\vec{r})d\vec{u}$$

squaring ↓

X (no inverse)

$$I(\vec{q}) = A(\vec{q}) \cdot A^{*}(\vec{q})$$

$$\Gamma_\rho(\vec{r})$$

Autocorrelation ftn

FT →

← IFT

$$I(\vec{q})$$

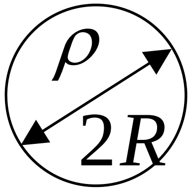
$$I(\vec{q}) = \int \Gamma_\rho(\vec{r}) e^{-i\vec{r}\cdot\vec{q}} d\vec{r}$$

Structure factor for a uniform sphere

$$2\pi\vec{s} = \vec{q}$$

$$\rho \sim 0$$

$$P(q) \sim \left[F(q)\right]^2$$



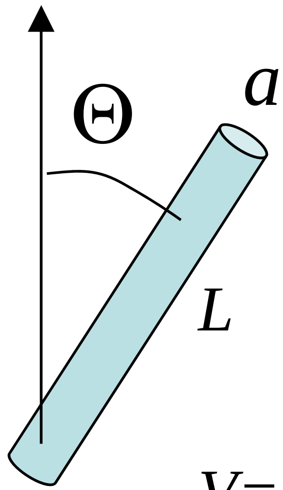
$$F(q) = \int \rho(\vec{r})\exp(-i\vec{q}\cdot\vec{r})d\vec{r}$$

Structure factors for several structures

Thin rod

At a certain orientations,

$$F(q) = \frac{4}{qL\cos\Theta}\sin\left(\frac{qL\cos\Theta}{2}\right)$$



$V=aL$

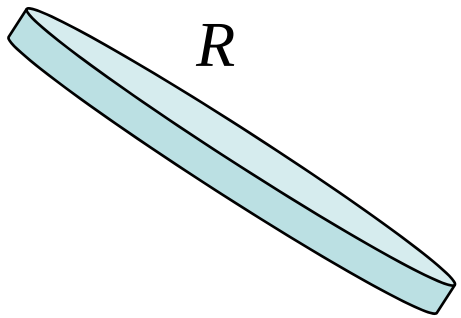
Random orientations,

$$P(q) = \frac{2}{qL}\left[\int_0^{qL}\frac{\sin u}{u}du - \frac{1-\cos qL}{qL}\right]$$

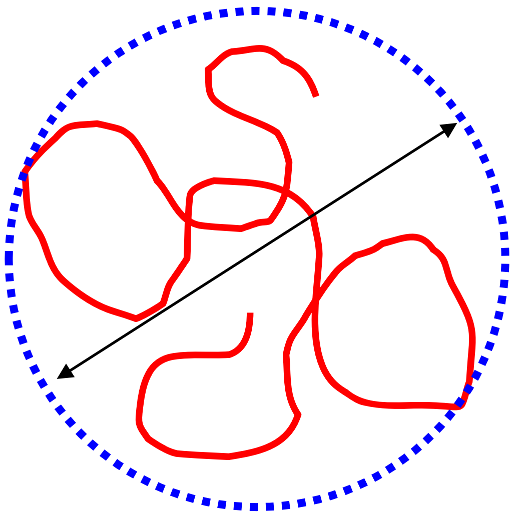
Structure factors for several structures

Circular disk

$$P(q) = \frac{2}{q^2 R^2}\left[1 - \frac{J_1(2qR)}{qR}\right]$$



Size of chain molecules
-synthetic polymer, DNA, protein...



Number of repeat unit

Charateristic ratio

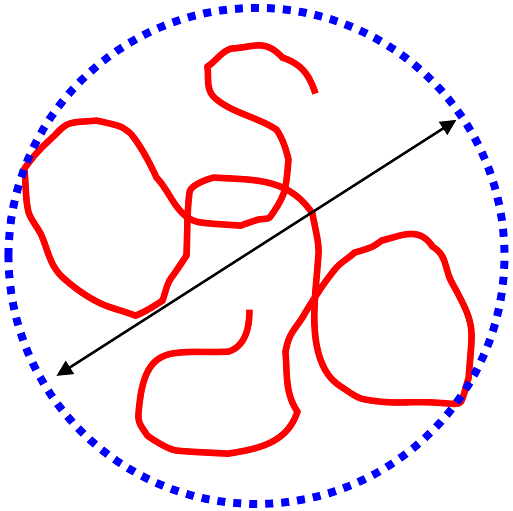
$$R_g^2 = C_\infty n l^2 / 6$$

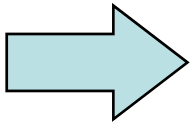
$$R_0^2 = 6R_g^2 = Nb^2$$

Number of Kuhn segment

Kuhn segment length

How about this?





$$P(q) \sim [F(q)]^2$$

constant form factor?

Random coil
Or Gaussian coil

$$P(q) \sim 2\frac{\exp(-q^2R_g^2) - 1 + q^2R_g^2}{q^4R_g^4}$$

http://www.ncnr.nist.gov/programs/sans/pdf/polymer_tut.pdf

Not only lattice scattering but also shape of the single object is important

$$I(q) = I_o N(\rho - \rho_o)^2 F^2(q)$$

$$F(q) = \frac{4}{3}\pi R^3 \left[3\frac{\sin(qR) - qR\cos(qR)}{(qR)^3}\right]$$