Scattering for dummies?

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Weitz group meeting

5/17/07

motivation

-- Hidden structural information
-- Particle sizing
-- Thermodynamic info, constants
-- Good statistics

-- Often hard to interpret non-trivial cases
-- Great when complimented by images

-> Important to know what you're doing.

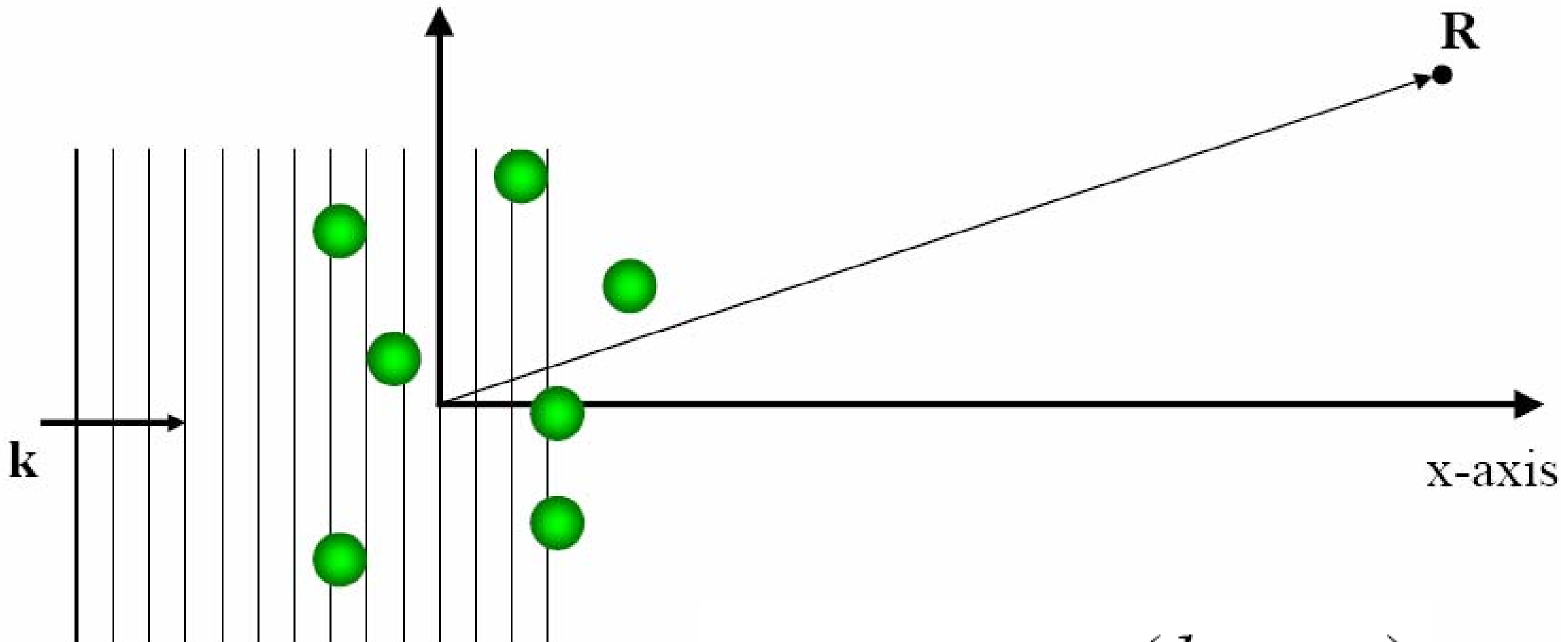
electrons, light, x-rays… they're all the same.

	λ		ε
Light	~100's nm		1's eV's
X-rays	~1's Å		10's keV
Electrons	~1's Å		100's keV

Okay, not really… we'll treat them the same…
neutrons too

Kinematic Scattering

Plane wave, *A,* impinges on particles, detected at **R**.
Single scattering events occur.
Scattering is elastic: |**k**|=|**k**'|



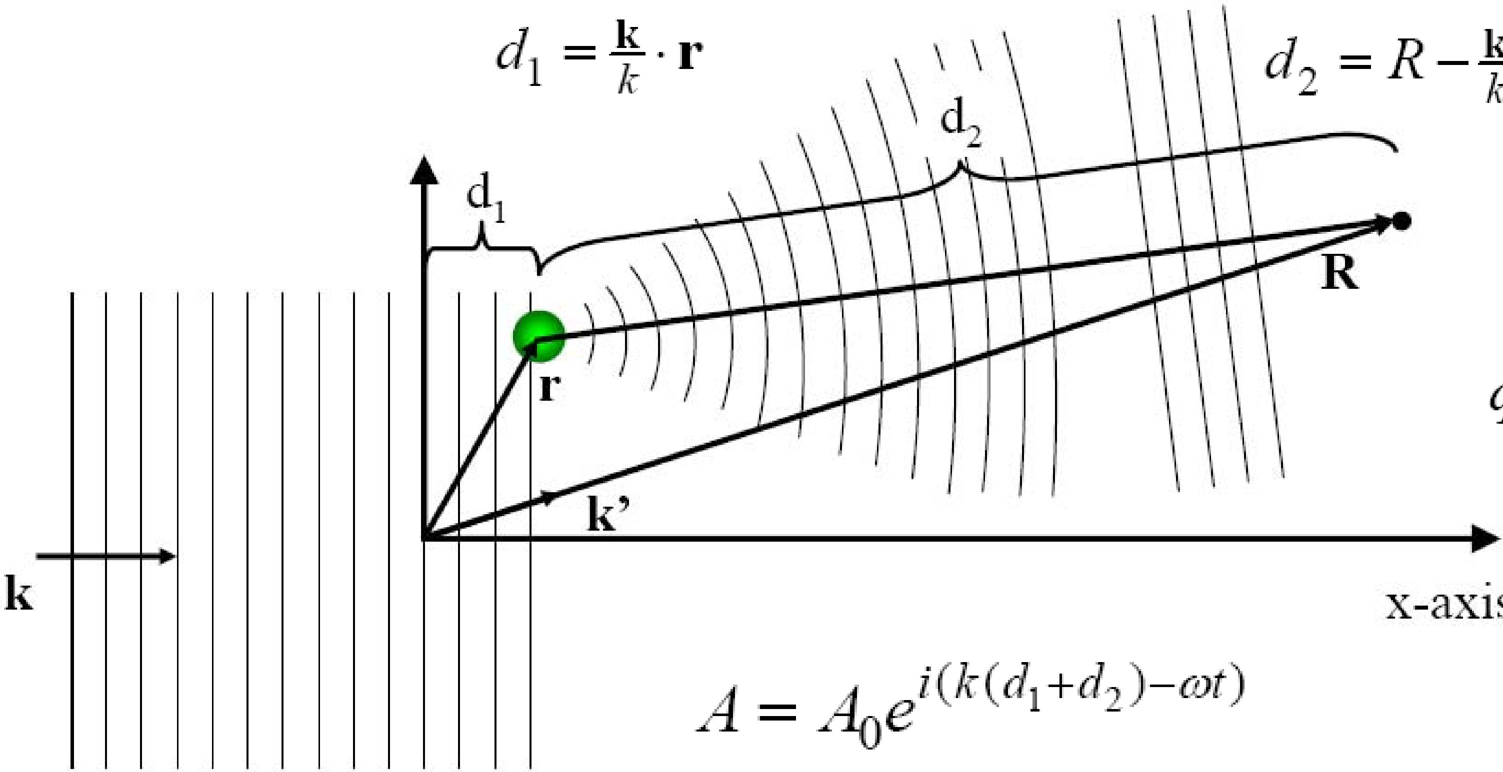
$$A = A_0 e^{i(kx-\omega t)}$$

Kinematic Scattering

Large **R**, scattered wave looks like plane wave.

$$d_1 = \frac{\mathbf{k}}{k} \cdot \mathbf{r}$$

$$d_2 = R - \frac{\mathbf{k}'}{k'} \cdot \mathbf{r}$$



$$q = \frac{4\pi}{\lambda} \sin\theta$$

$$\begin{aligned} A &= A_0 e^{i(k(d_1+d_2)-\omega t)} \\ &= A_0 e^{i(kR+(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}-\omega t)} \\ &= A_0 e^{i(kR-\omega t+\mathbf{q}\cdot\mathbf{r})} \end{aligned}$$

Kinematic Scattering

Many scatterers, add up waves at R.
All waves have kR and ωt… factor out and absorb into A_o

$$A(\mathbf{q}) = A_0 \sum_j e^{i\,\mathbf{q}\cdot\mathbf{r}_j}$$

Let each scatterer have a different scattering strength, f_j

$$A(\mathbf{q}) = A_0 \sum_j f_j e^{i\,\mathbf{q}\cdot\mathbf{r}_j}$$

In the continuum:

$$A(\mathbf{q}) = A_0 \int \rho(\mathbf{r}) e^{i\,\mathbf{q}\cdot\mathbf{r}} d^3 r$$

$$I(\mathbf{q}) = \left| A(\mathbf{q}) \right|^2$$

Ex 1: objects on a lattice

$$\rho(r) = \rho_{mol}(r) \otimes \rho_{lattice}(r)$$

$$I(q) \propto \left|\mathbb{F}[\rho(r)]\right|^2 = \mathbb{F}[\rho_{mol}(r)]^2 \, \mathbb{F}[\rho_{lattice}(r)]^2$$

$$I(q) = \left|f(q)\right|^2 \left|S(q)\right|^2$$

"form factor" **"structure factor"**

Let's look at the 2 pieces one at a time…

1D structure factor

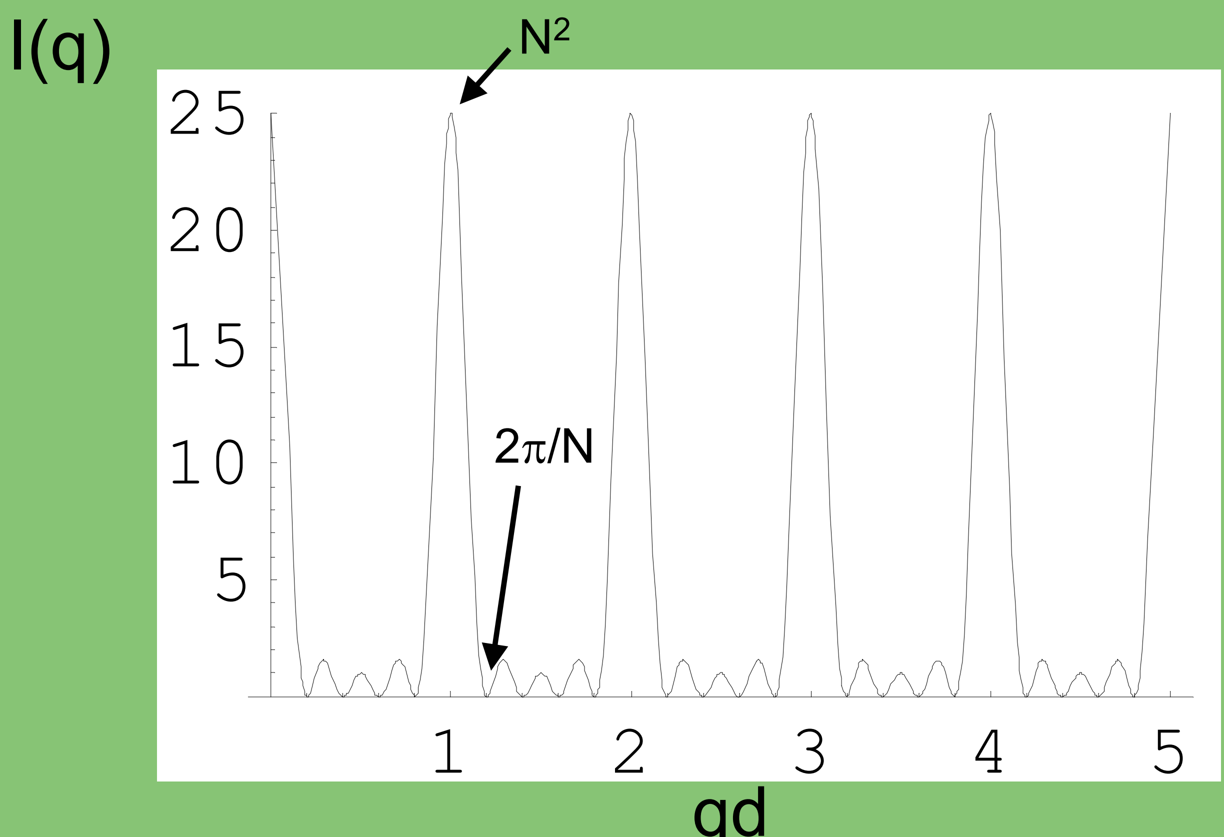
A little 1D crystal of point-like particles:

$$r = dn$$

• • • • •

d 2d 3d 4d 5d

$$A(\mathbf{q}) = A_0 \sum_j f_j e^{i\,\mathbf{q}\cdot\mathbf{r}_j}$$



$$S(q) = \sum_{n=1}^{N} e^{iqdn}$$

$$= \frac{1 - e^{iqdN}}{1 - e^{iqd}}$$

$$I(q) \propto \left| S(q) \right|^2$$

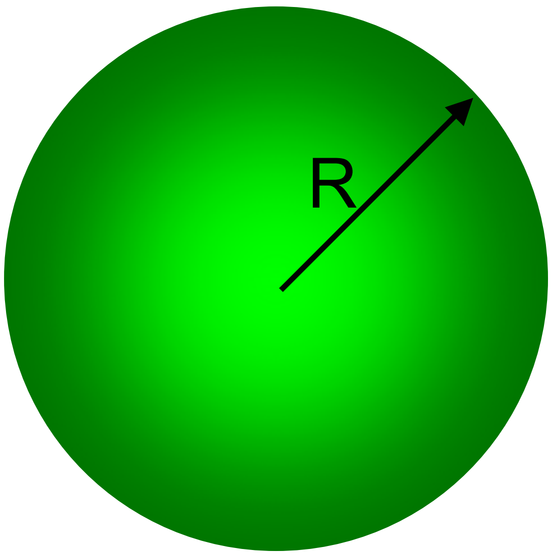
$$= \frac{\sin^2(Nqd/2)}{\sin^2(qd/2)}$$

Spherical form factor

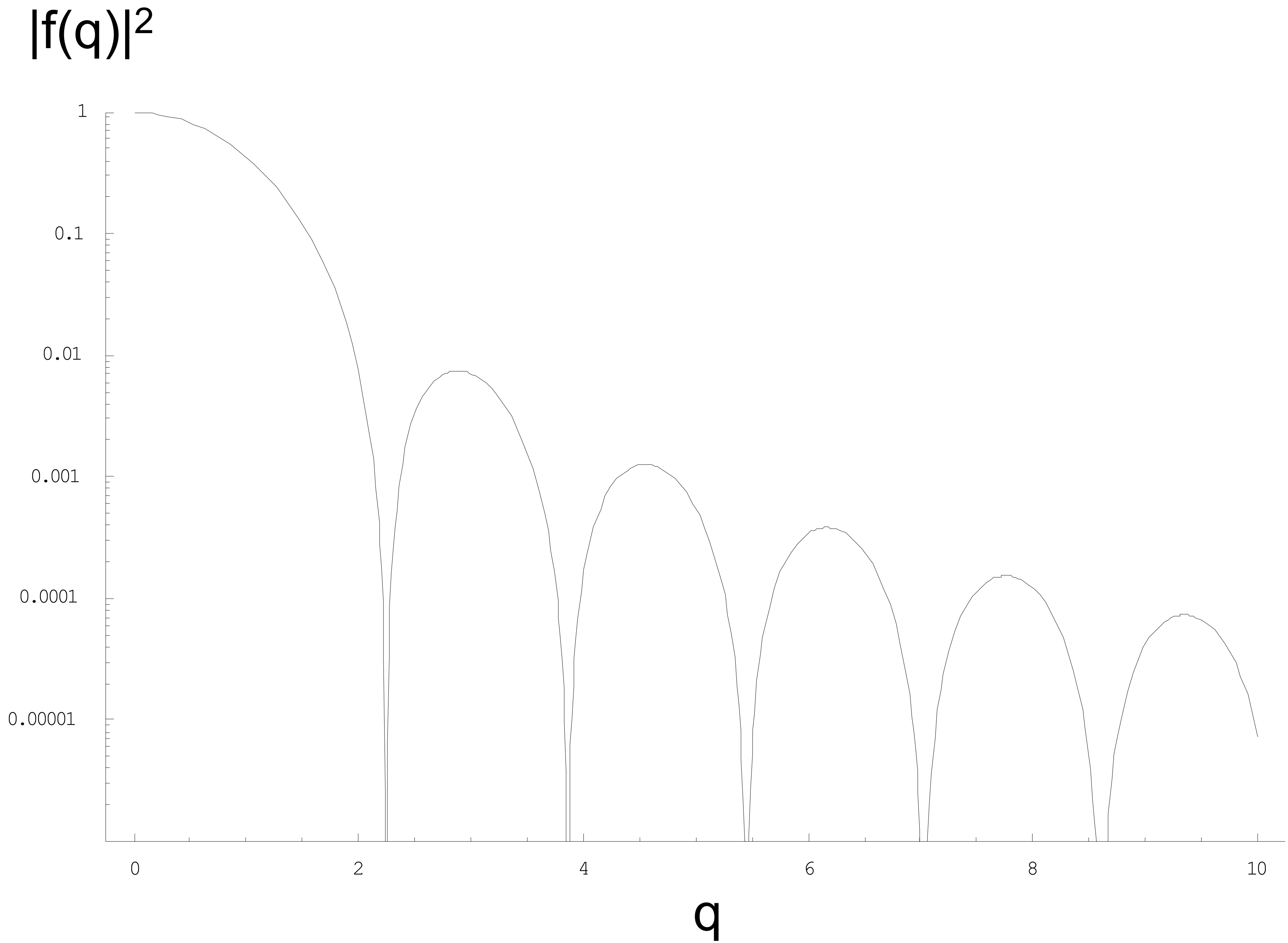
$$r = dn$$

$$A(q) = f(q)\sum_{n=1}^{N} e^{iqdn} = f(q)\frac{1-e^{iqdN}}{1-e^{iqd}}$$

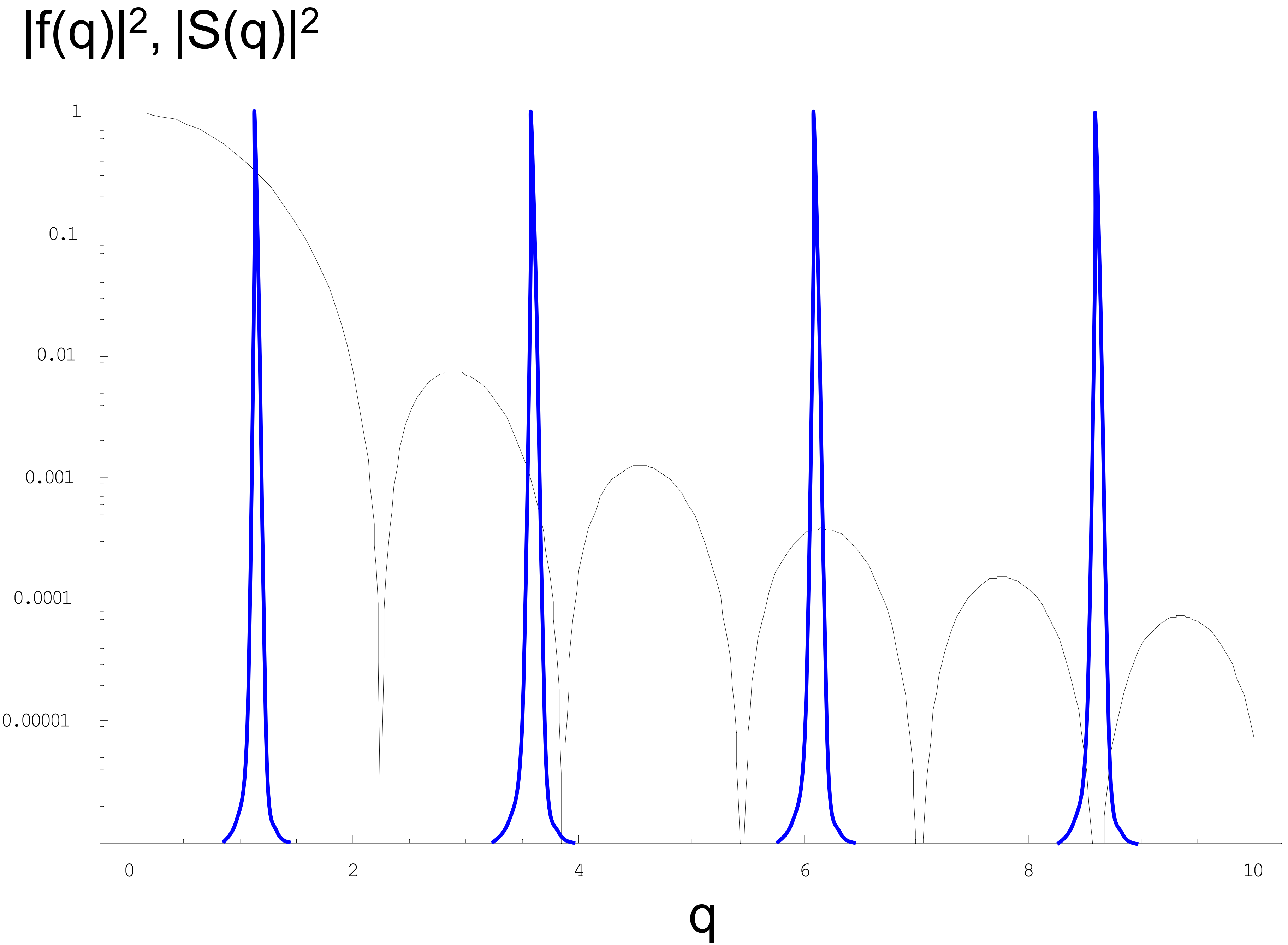
$$I(q) \propto |A(q)|^2 = f^2(q)\frac{\sin^2(Nqd/2)}{\sin^2(qd/2)}$$



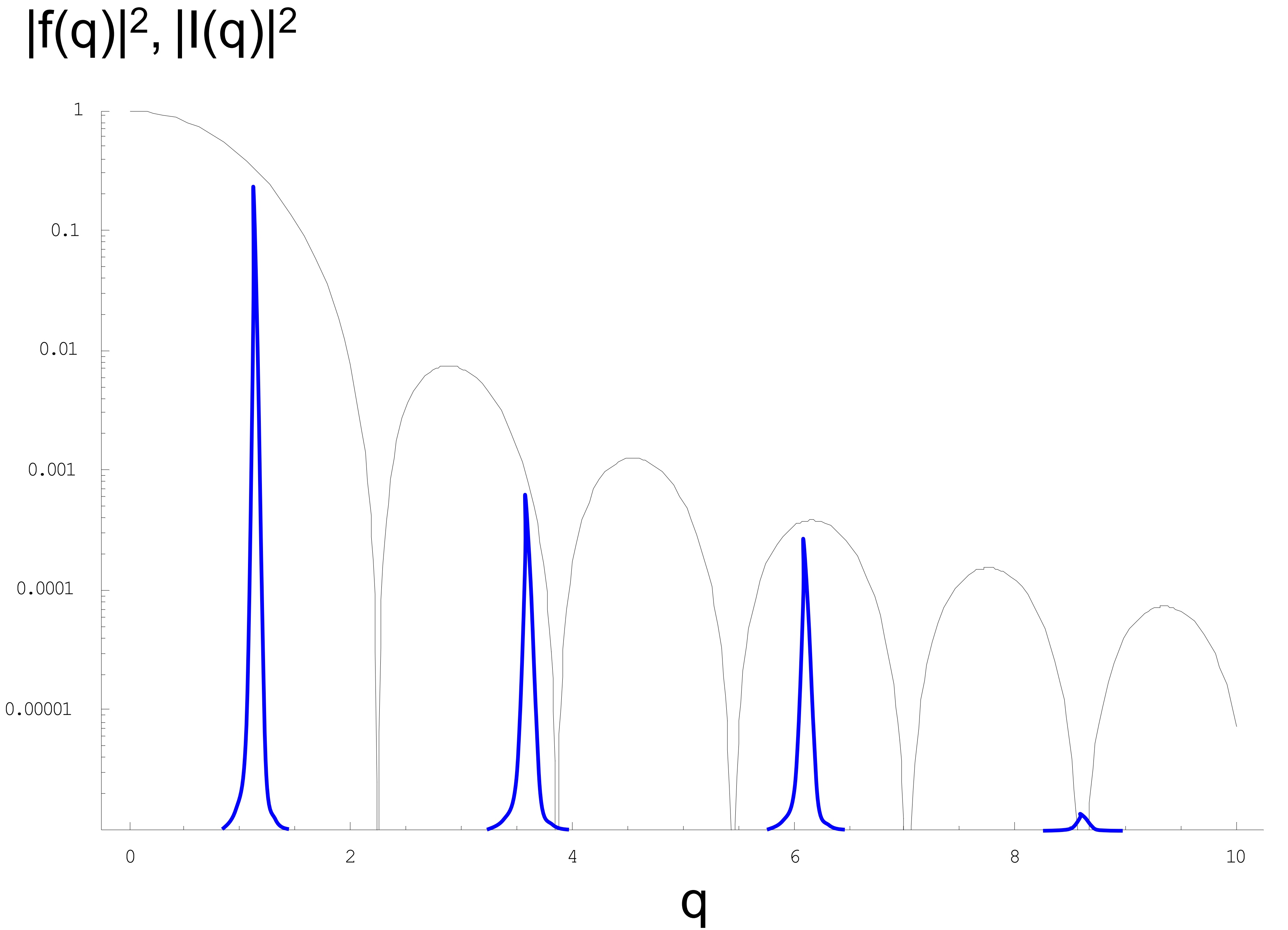
$$f(q) = \frac{3[\sin(qR) - qr\cos(qR)]}{(qR)^3}$$



|f(q)|²
1
0.1
0.01
0.001
0.0001
0.00001
0
2
4
6
8
10
q



|f(q)|², |S(q)|²
1
0.1
0.01
0.001
0.0001
0.00001
0
2
4
6
8
10
q



|f(q)|^2, |I(q)|^2
1
0.1
0.01
0.001
0.0001
0.00001
0
2
4
6
8
10
q

Fun example 1: the Plane

Fun example 1: the Plane

The delta function:

$$1(x) \equiv 1$$

$$\int 1(x) e^{-ikx} dk = \delta(x)$$

Fourier transform of delta function:

$$\int \delta(x) e^{-ikx} dk = 1$$

How do you write down the density of a plane?

Fun example 1: the Plane

$$1(x)1(y)\delta(z)$$

Fun example 1: the Plane

$1(x)1(y)\delta(z)$

$\delta(q_x)\delta(q_y)1(q_z)$

Fun example 2: the Plane with a profile

Fourier transform of a gaussian distribution:

$$\int e^{-x^2/2\sigma^2} e^{-ikx} dk = e^{-k^2\sigma^2/2}$$

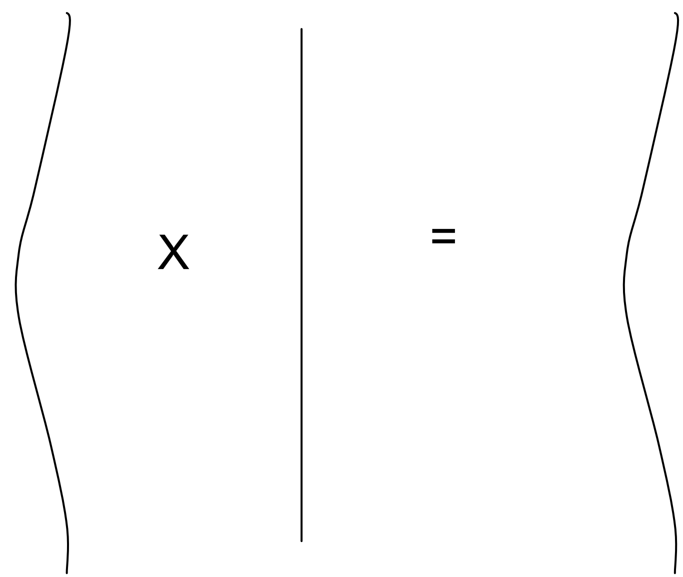
Fun example 2: the Plane with a profile

$$1(x)1(y)(\delta \otimes \mathrm{G})(z)$$

Fun example 2: the Plane with a profile

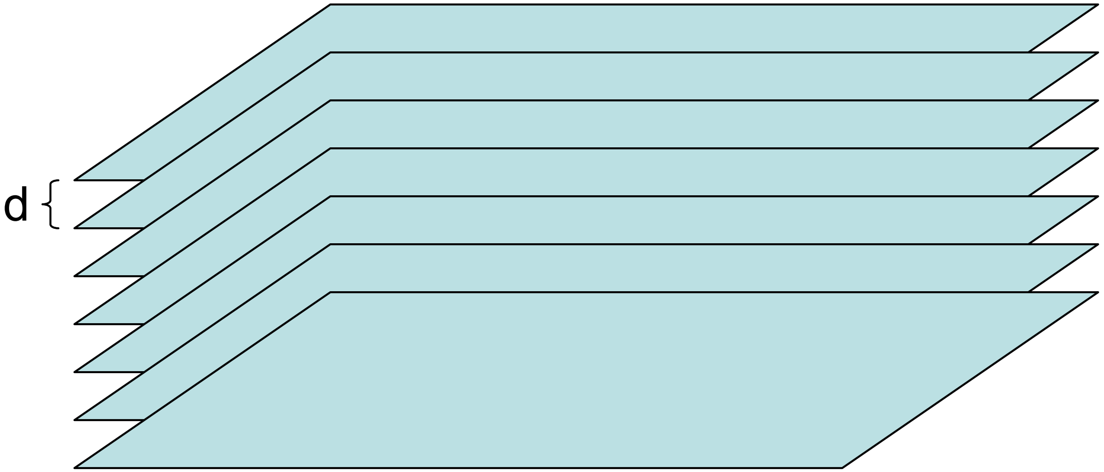
$$1(x)1(y)(\delta \otimes G)(z)$$

$$\delta(q_x)\delta(q_y)1(q_z)G'(q_z)$$



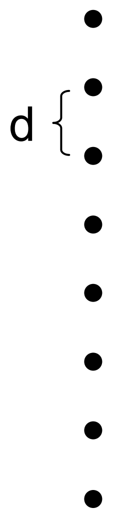
Fun example 3: a stack of planes

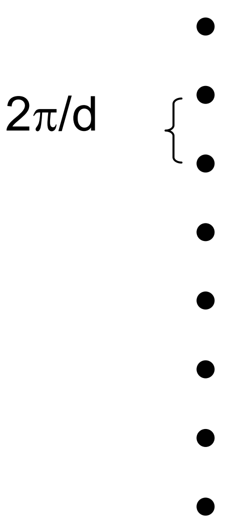
$$1(x)1(y)\delta(z) \otimes \sum_{n} \delta(z - nd)$$



Fun example 3: a stack of planes

$$\sum_n \delta(z - nd)$$

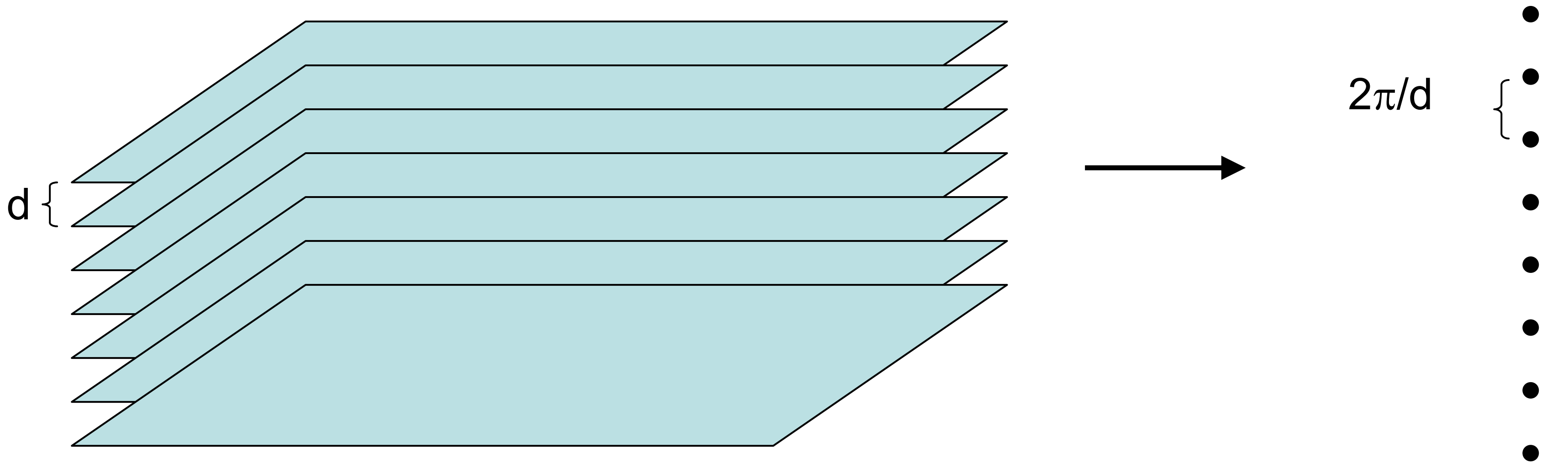




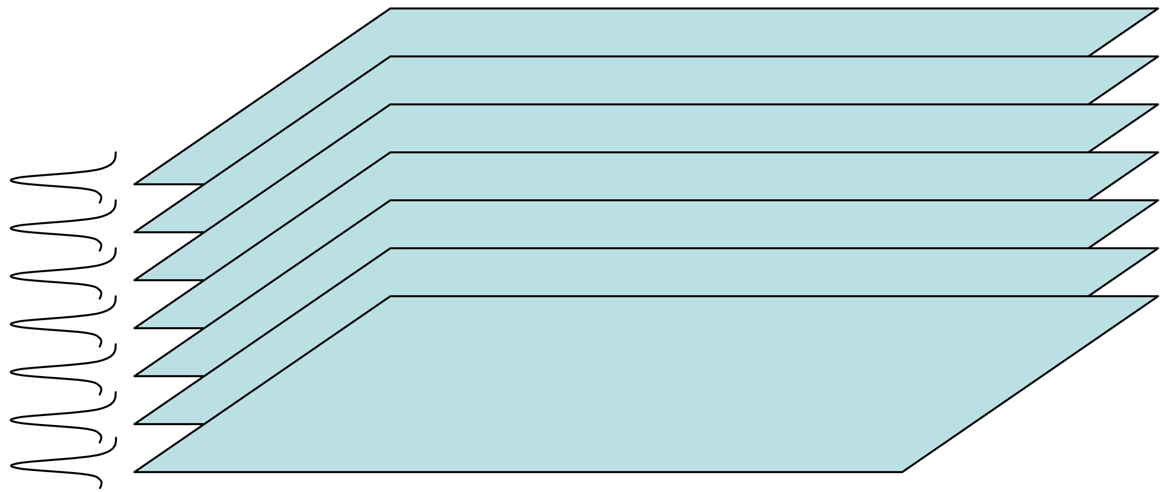
$$I(q) \propto \frac{\sin^2(Nqd/2)}{\sin^2(qd/2)}$$

Fun example 3: a stack of planes

$$\delta(q_x)\delta(q_y)\sum_n \delta(q_z - \tfrac{2\pi n}{d})$$

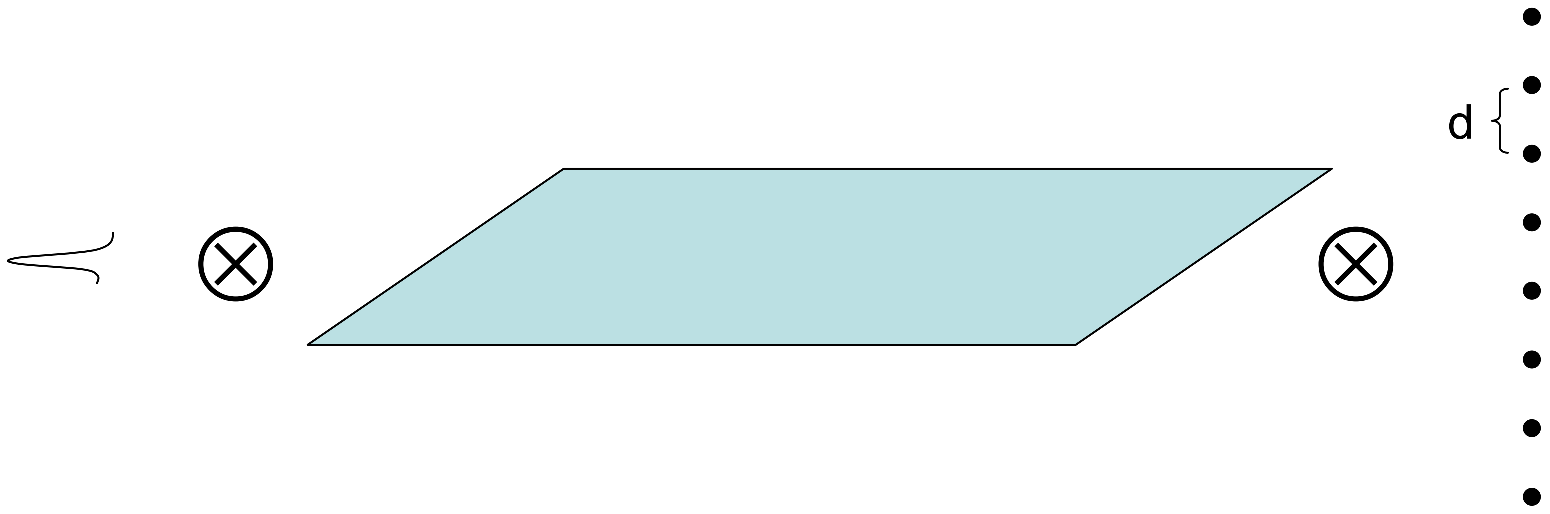


Fun example 4: a stack of gaussian planes

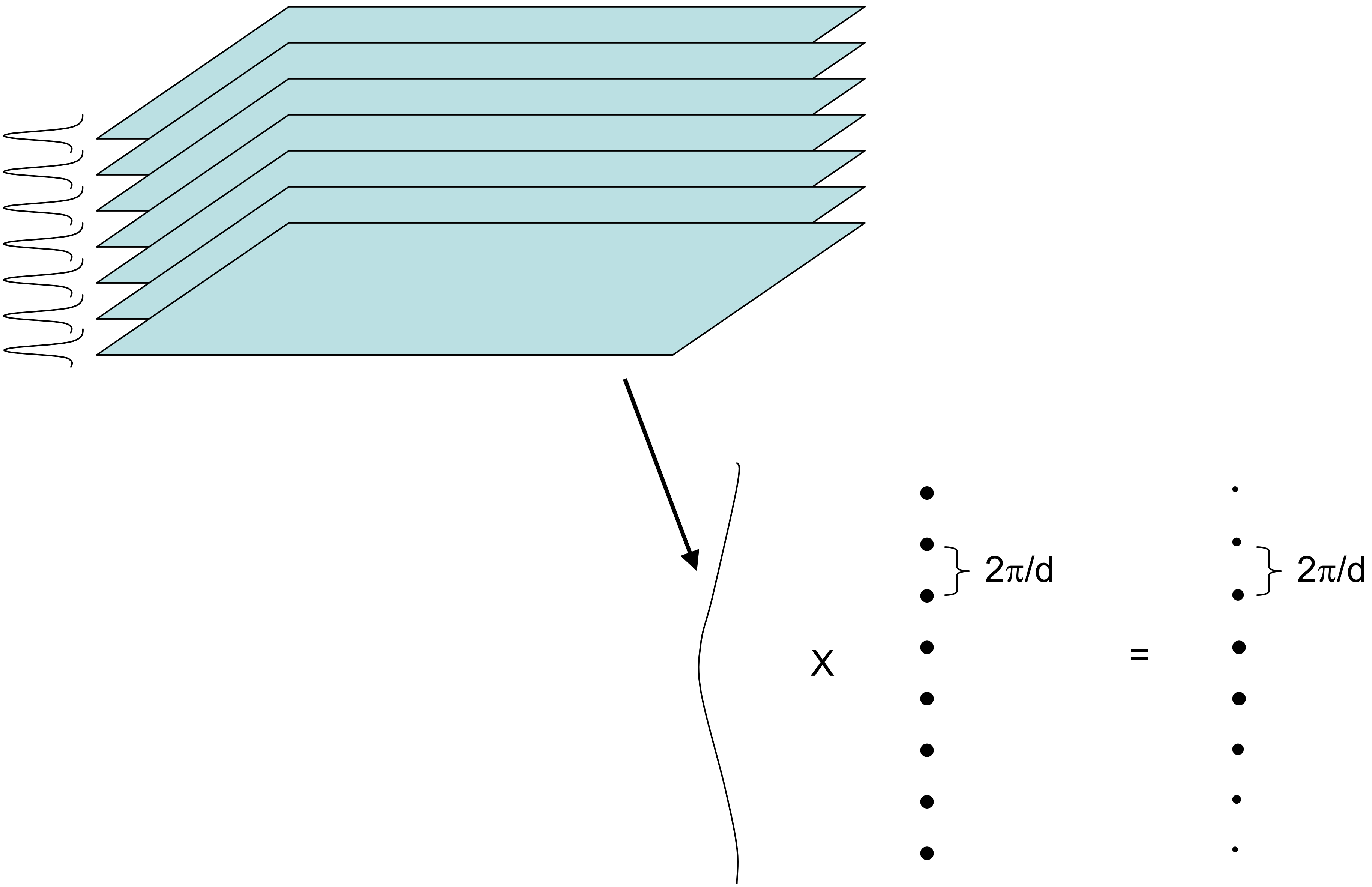


Fun example 4: a stack of gaussian planes

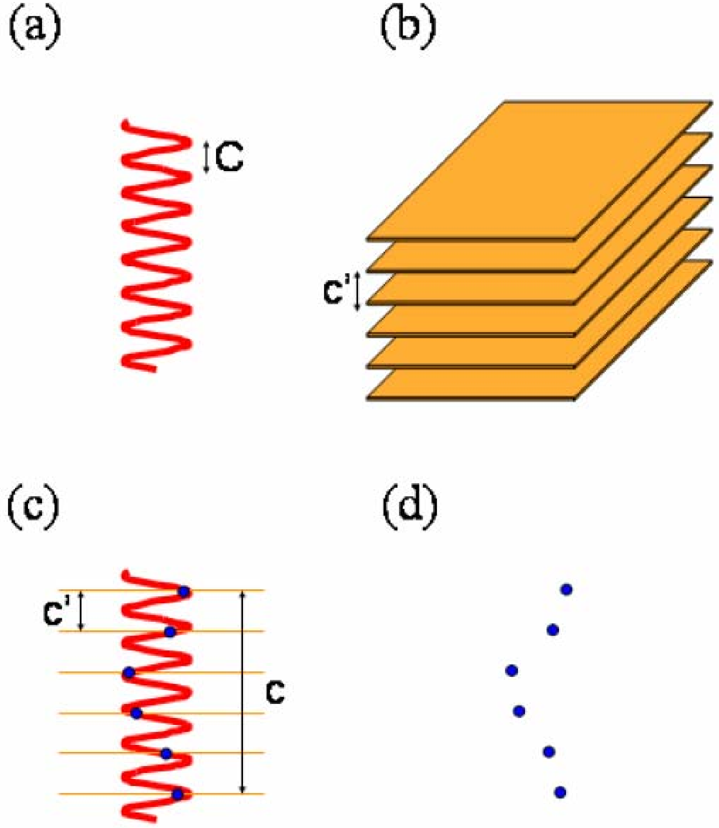
$$1(x)1(y)\delta(z)\otimes G(z)\otimes\sum_n \delta(z-nd)$$



Fun example 4: a stack of gaussian planes



No fun example 1: a helix



a. Continuous helix
b. Series of planes
c. Product of a and b
d. The discontinuous helix

$$\rho_c(r,\psi,z) = \delta(r-r_0)\delta(\psi - \tfrac{2\pi z}{C})$$

$$\rho_p(r,\psi,z) = 1(r,\psi)\sum_l \delta(z - lc')$$

$$\rho_d(r,\psi,z) = \rho_c(r,\psi,z)\rho_p(r,\psi,z)$$

No fun example 1: a helix

How to take an FT in cylindrical coordinates

$$A(\mathbf{q}) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \, \rho(\mathbf{r}) e^{i(q_x x + q_y y + q_z z)}$$

$$x = r\cos\psi, \quad y = r\sin\psi, \quad z = z$$

$$q_x = q_r \cos\Psi, \quad q_y = q_r \sin\Psi, \quad q_z = q_z$$

$$\cos(\psi - \Psi) = \cos\psi\cos\Psi + \sin\psi\sin\Psi,$$

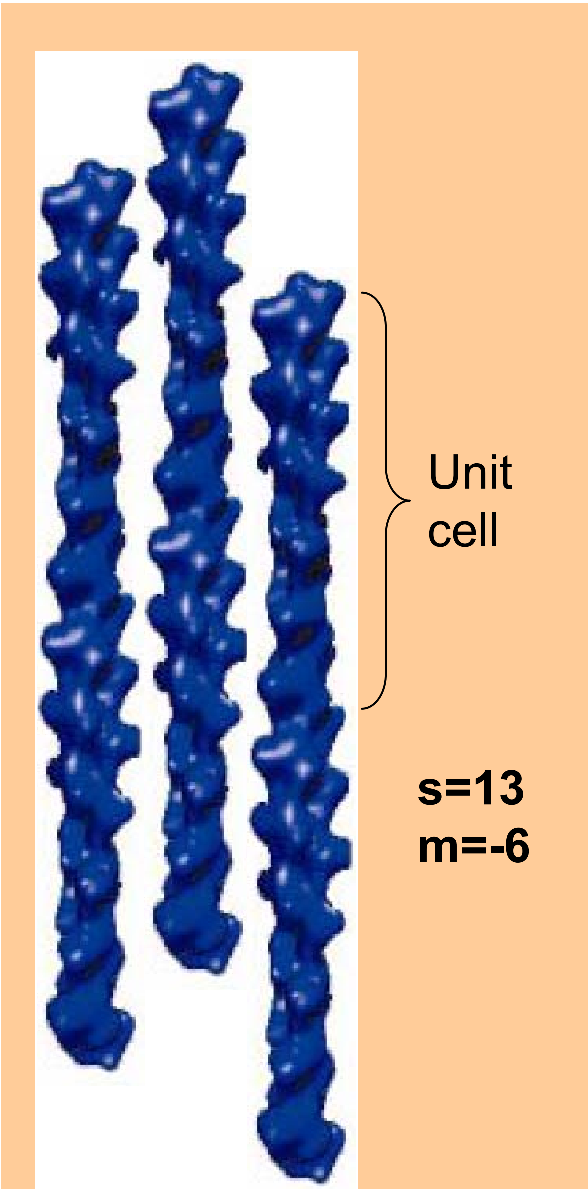
$$A(\mathbf{q}) = \int_{-\infty}^{\infty} dz \int_{0}^{2\pi} d\psi \int_{0}^{\infty} r dr \, \rho(\mathbf{r}) e^{i(rq_r \cos(\psi - \Psi) + zq_z)}$$

"Bessel's 1st integral" →

$$\int_0^{2\pi} e^{ix\cos\varphi + in\varphi} d\varphi = 2\pi i^n J_n(x)$$

$$I_l(q_r) = \left| \sum_n \sum_j f_j J_n(q_r r_j) i^n e^{-i\left(n\psi_j - \frac{2\pi l}{c} z_j\right)} \right|^2$$

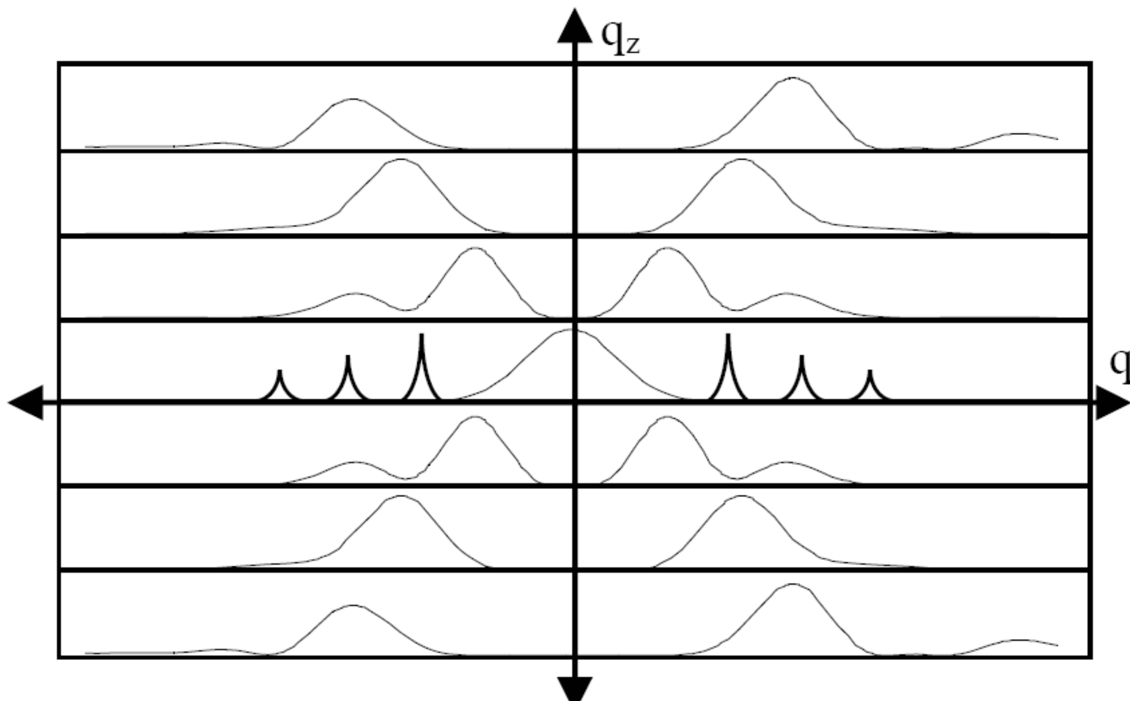
example: F-actin



$$I_l(q_r) = \left| \sum_n \sum_j f_j J_n(q_r r_j) i^n e^{-i\left(n\psi_j - \frac{2\pi l}{c} z_j\right)} \right|^2$$

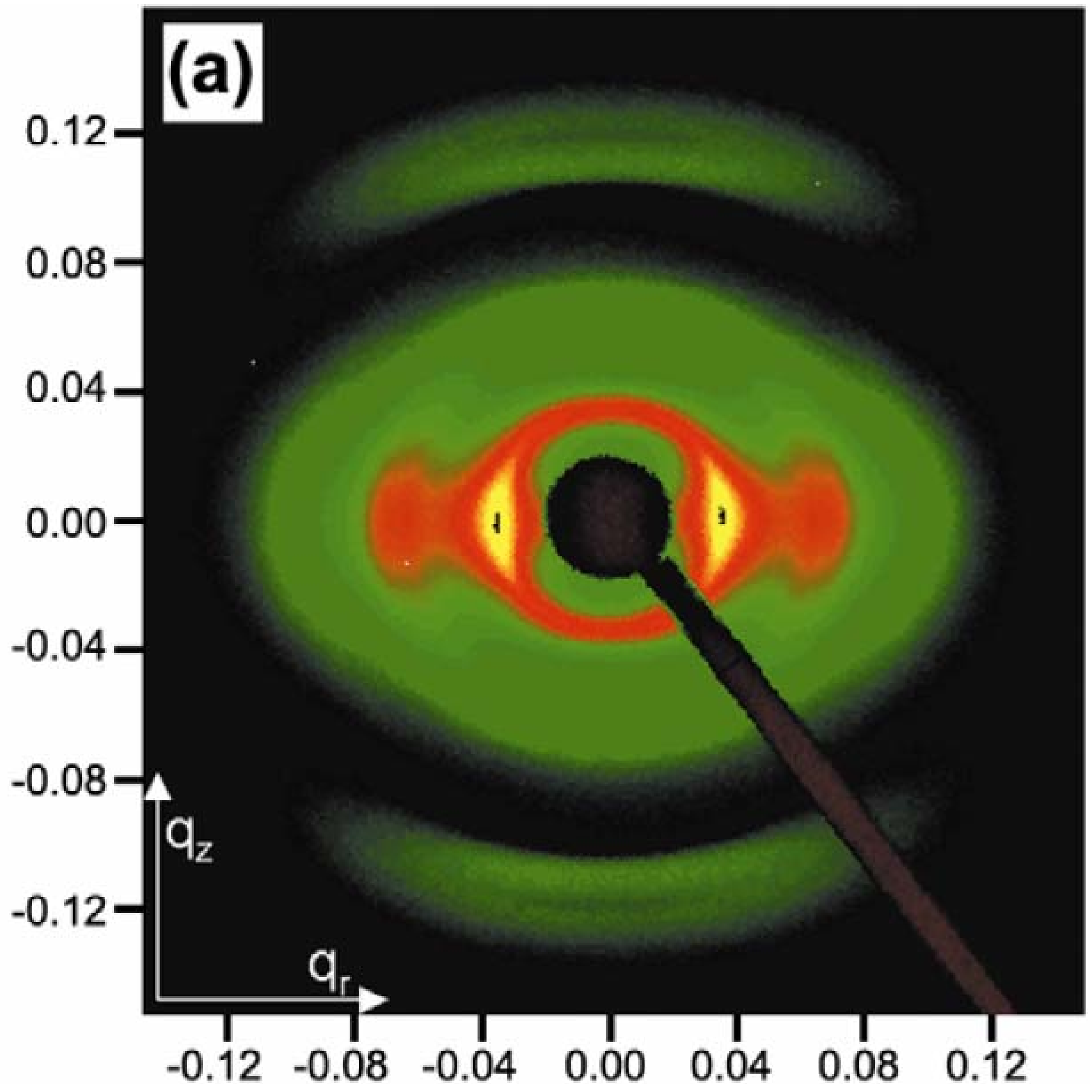
Selection rule: $l = sn + pm$

s= turns per unit cell
m=monomers per unit cell



ex: F-actin / what the diffraction really looks like

Liquid crystalline hexagonal collumnar f-actin lattice.

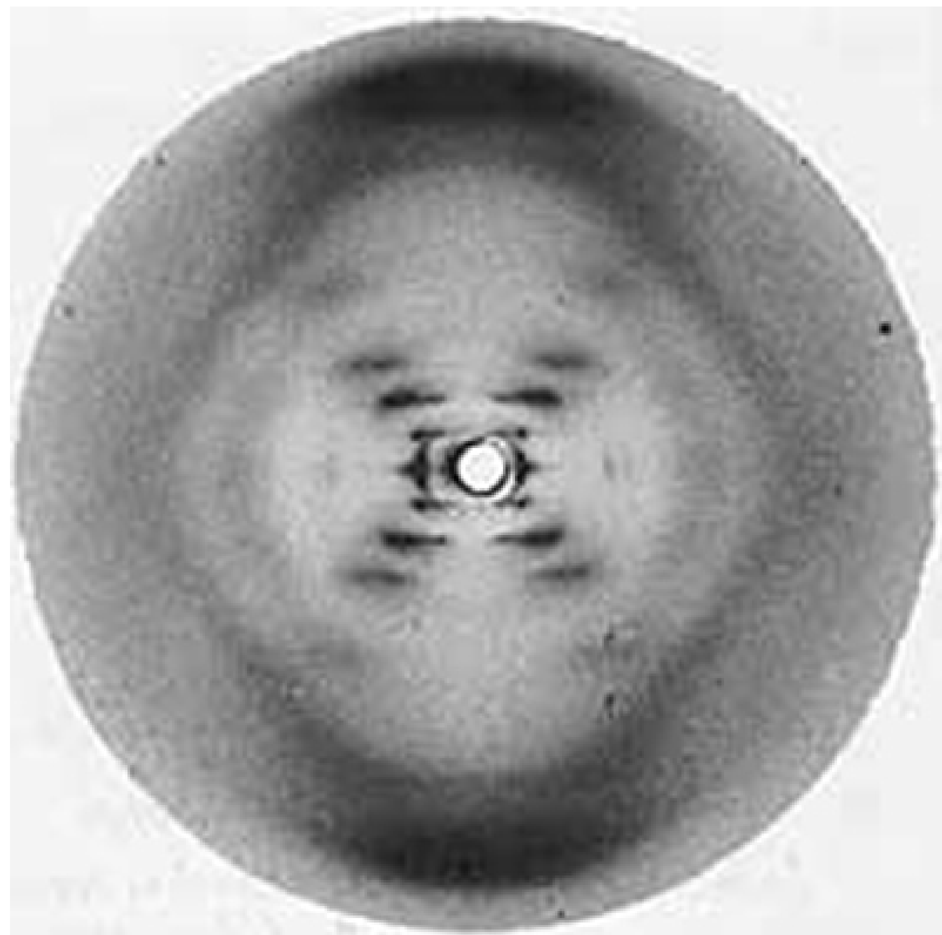


($Å^{-1}$)

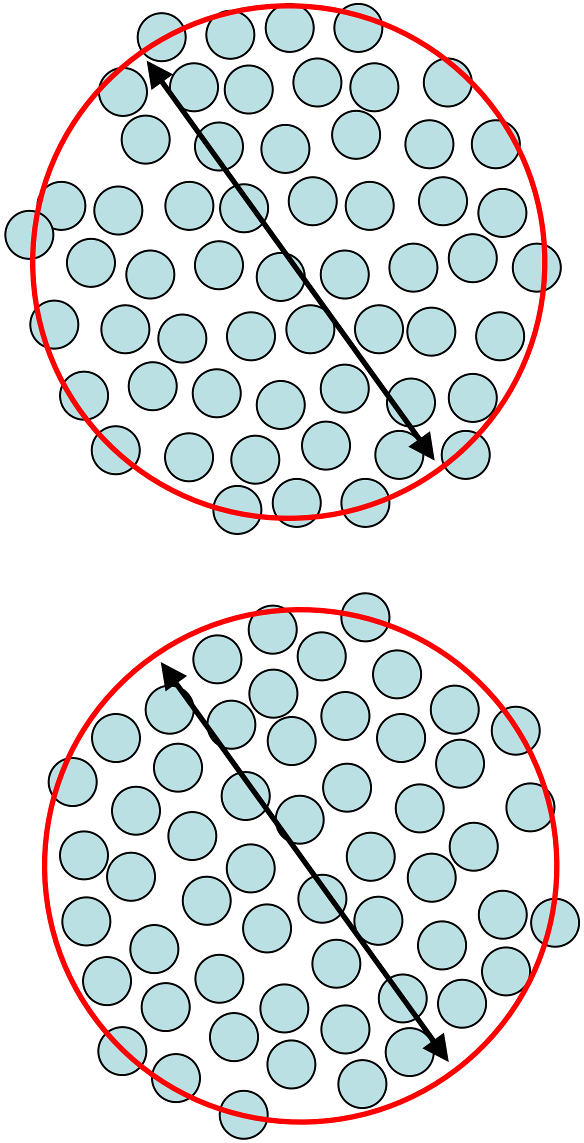
($Å^{-1}$)

ex: DNA / better looking than that actin crap

Rosalind Franklin's data.



Scattered intensity is FT of density correlation fun.



$$I(\mathbf{q}) = \left|A(\mathbf{q})\right|^2 = \int d\mathbf{R}' \int d\mathbf{R}\, \rho(\mathbf{R})\rho(\mathbf{R}')e^{-i\mathbf{q}.(\mathbf{R}-\mathbf{R}')}$$

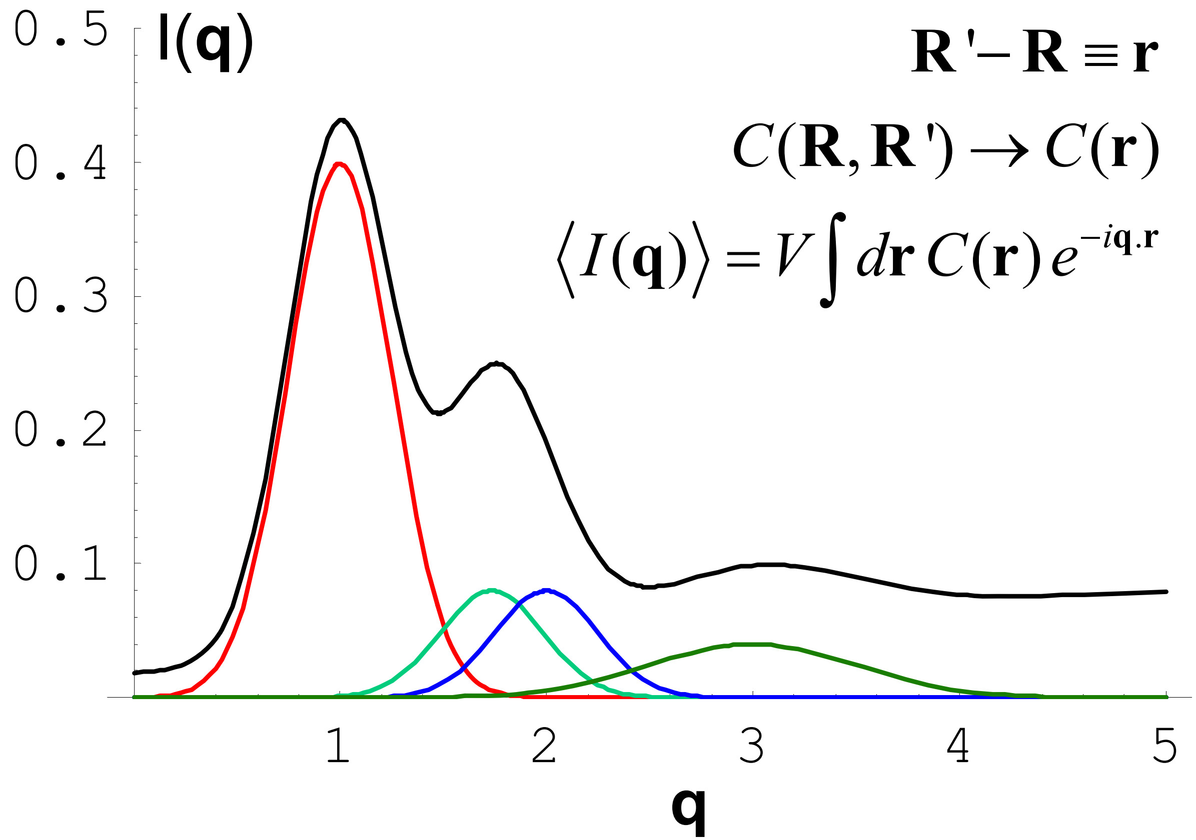
$$\left\langle I(\mathbf{q})\right\rangle = \int d\mathbf{R}' \int d\mathbf{R} \left\langle \rho(\mathbf{R})\rho(\mathbf{R}')\right\rangle e^{-i\mathbf{q}.(\mathbf{R}-\mathbf{R}')}$$

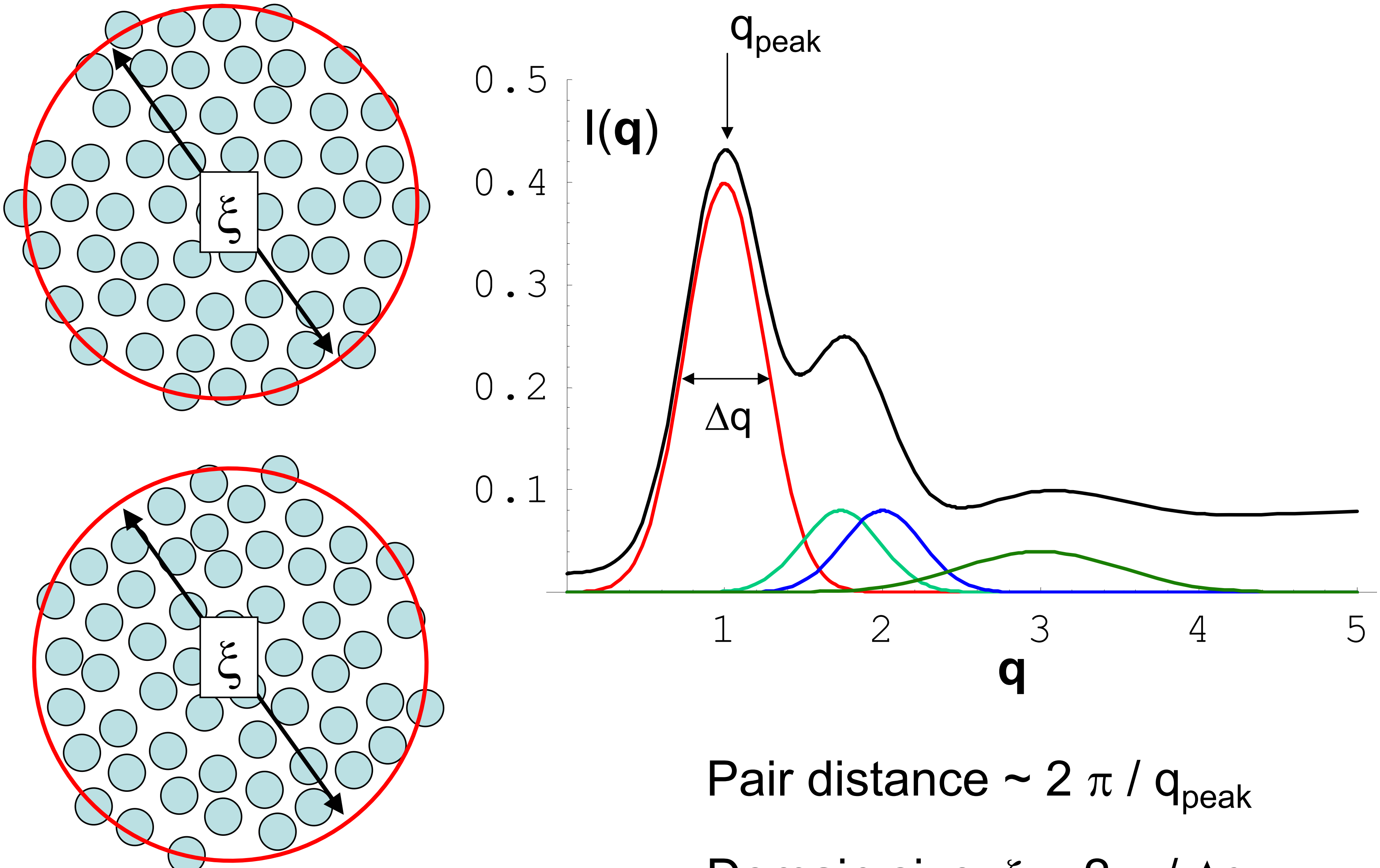
$$C(\mathbf{R},\mathbf{R}') = \left\langle \rho(\mathbf{R})\rho(\mathbf{R}')\right\rangle$$

$$\mathbf{R}' - \mathbf{R} \equiv \mathbf{r}$$

$$C(\mathbf{R},\mathbf{R}') \rightarrow C(\mathbf{r})$$

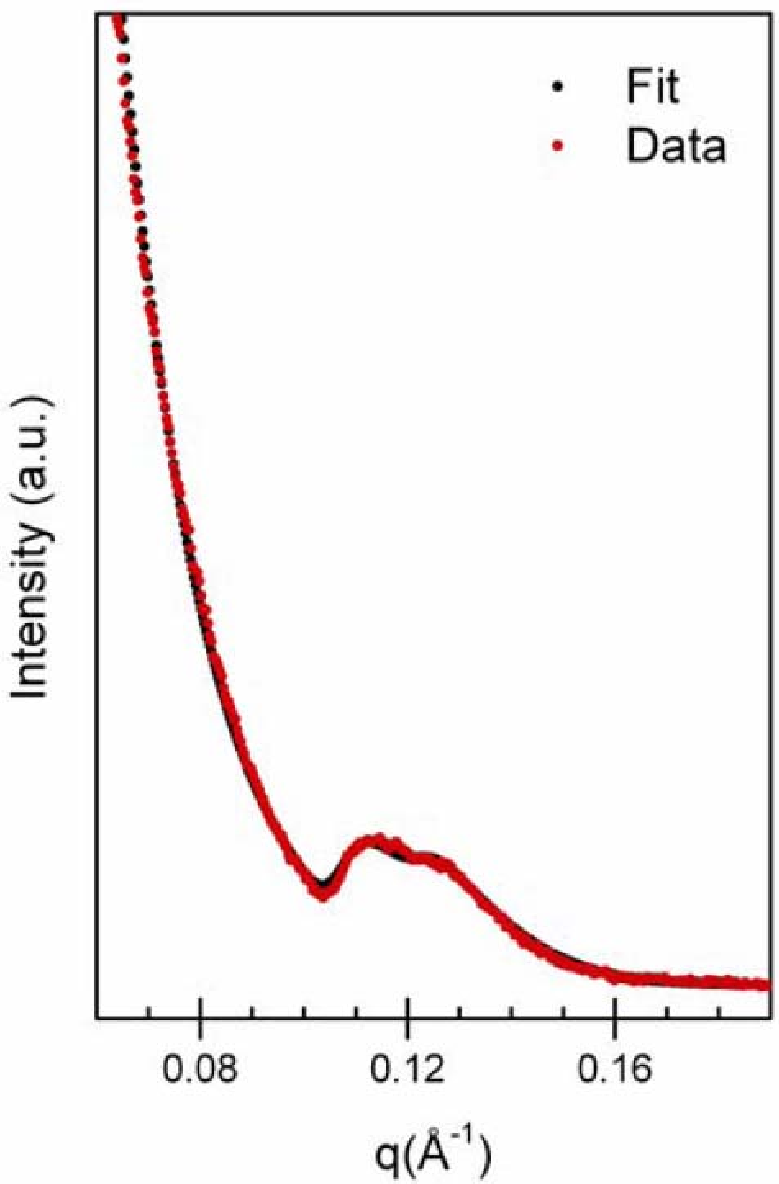
$$\left\langle I(\mathbf{q})\right\rangle = V\int d\mathbf{r}\, C(\mathbf{r})\, e^{-i\mathbf{q}.\mathbf{r}}$$

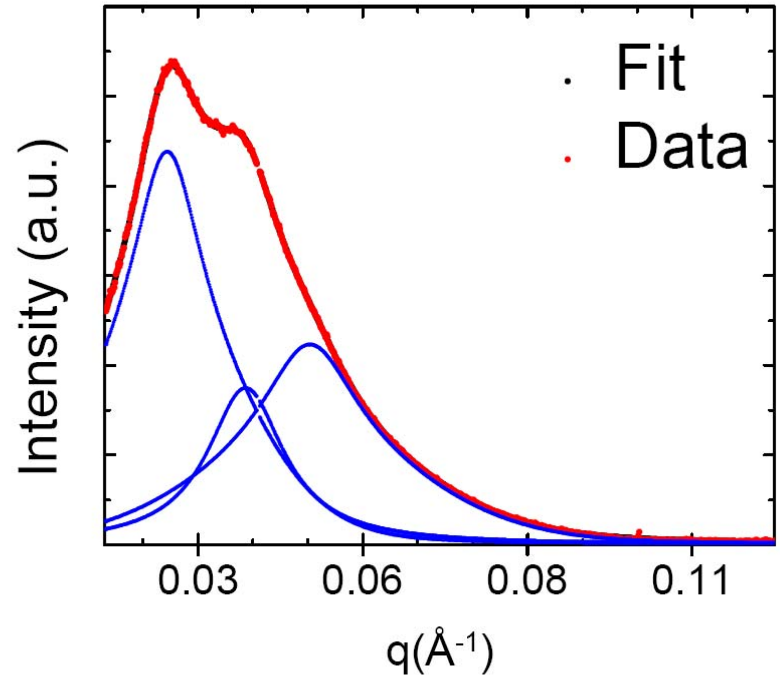


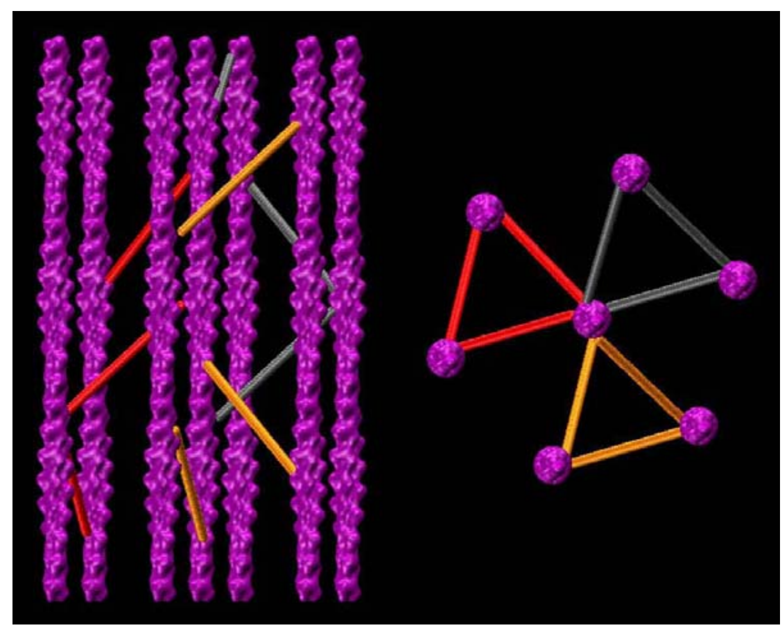


Pair distance ~ $2\pi / q_{peak}$

Domain size, $\xi \sim 2\pi / \Delta q$

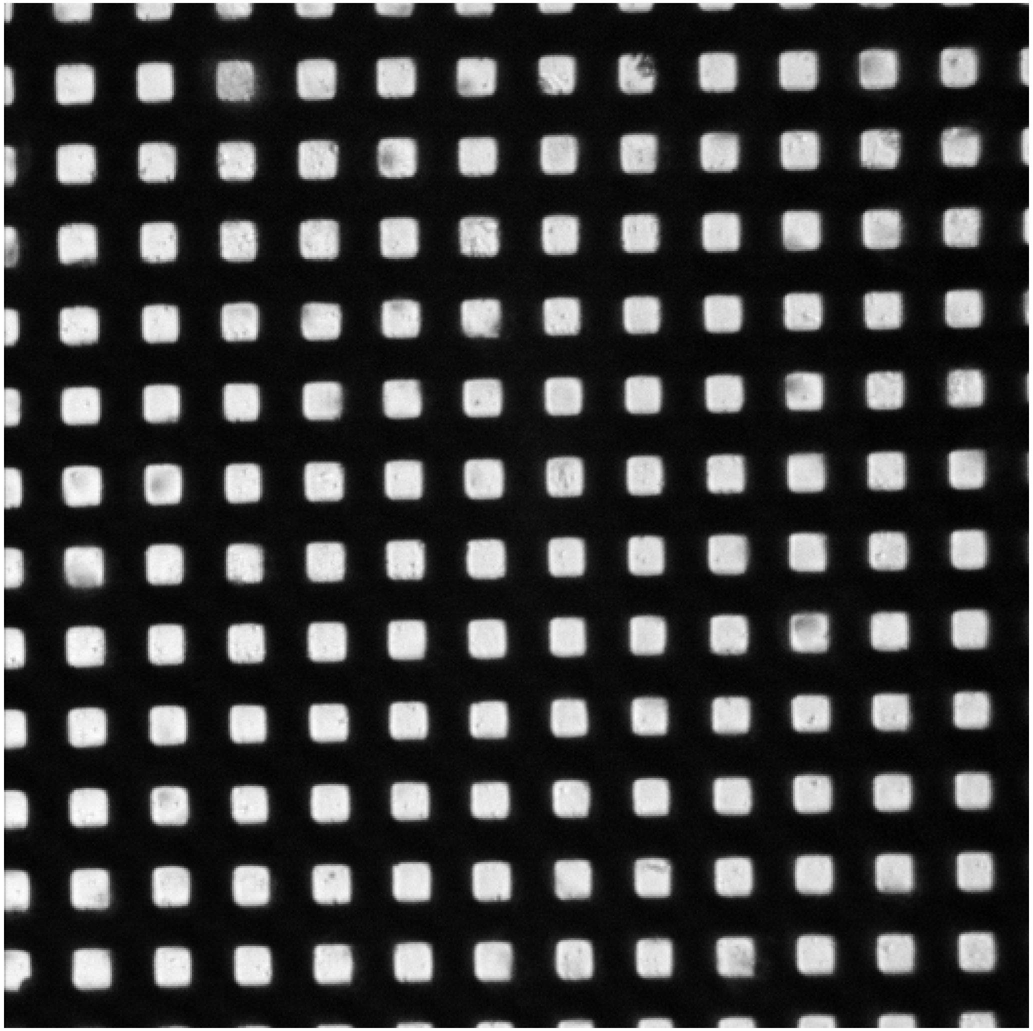

Fit
Data
Intensity (a.u.)
0.08
0.12
0.16
q(Å^{-1})

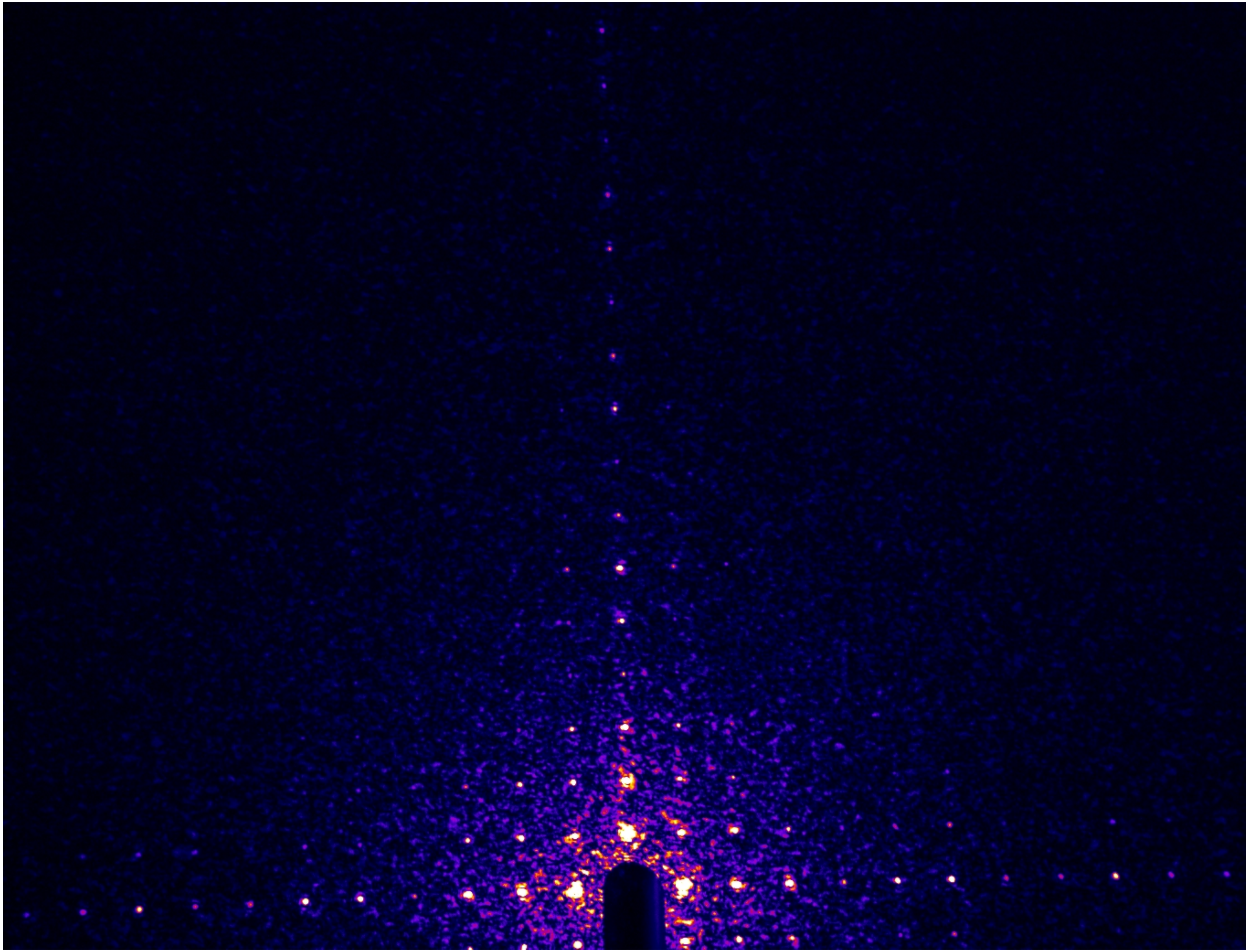

Fit
Data
Intensity (a.u.)
0.03
0.06
0.08
0.11
q(Å^{-1})

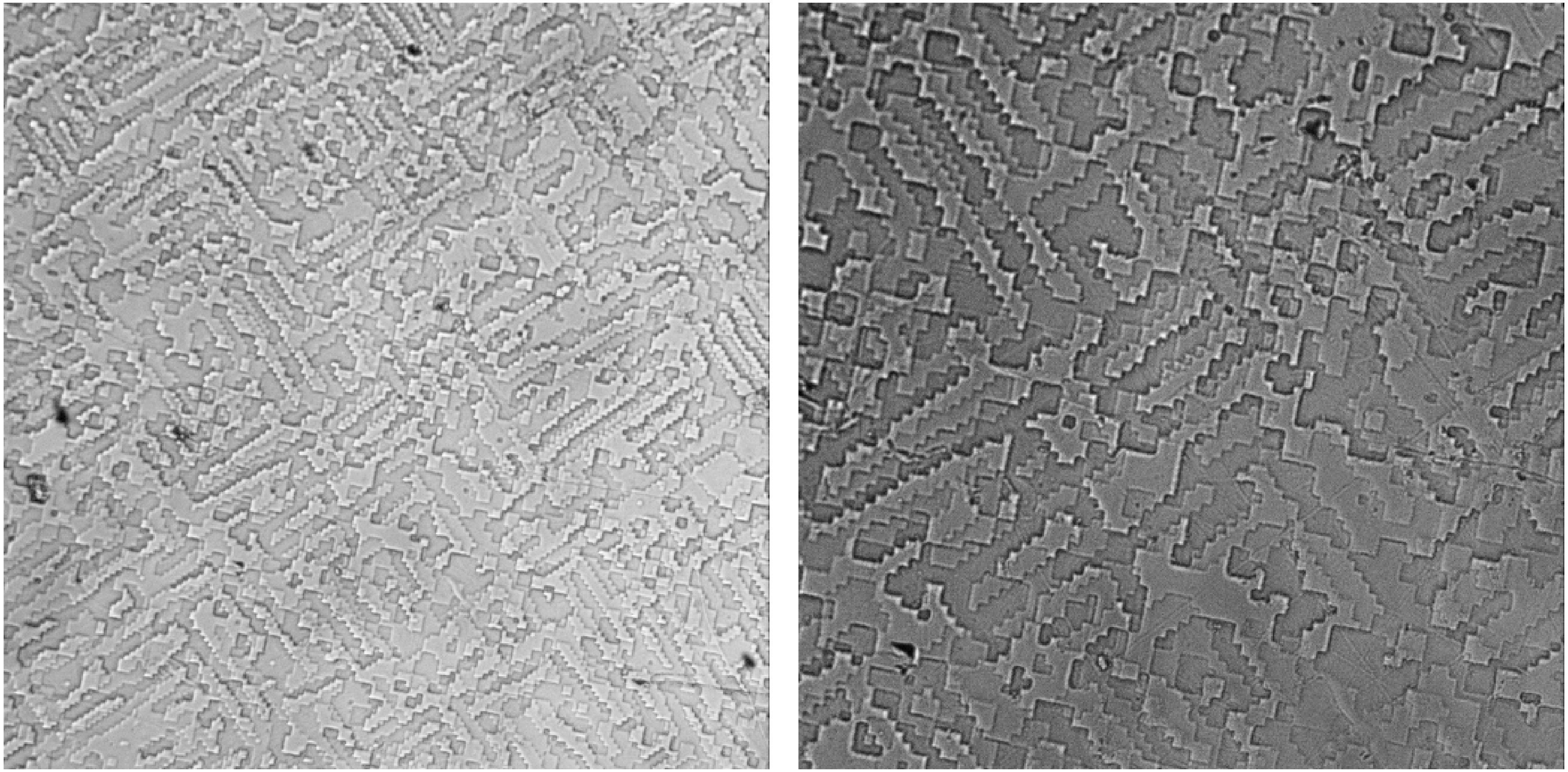


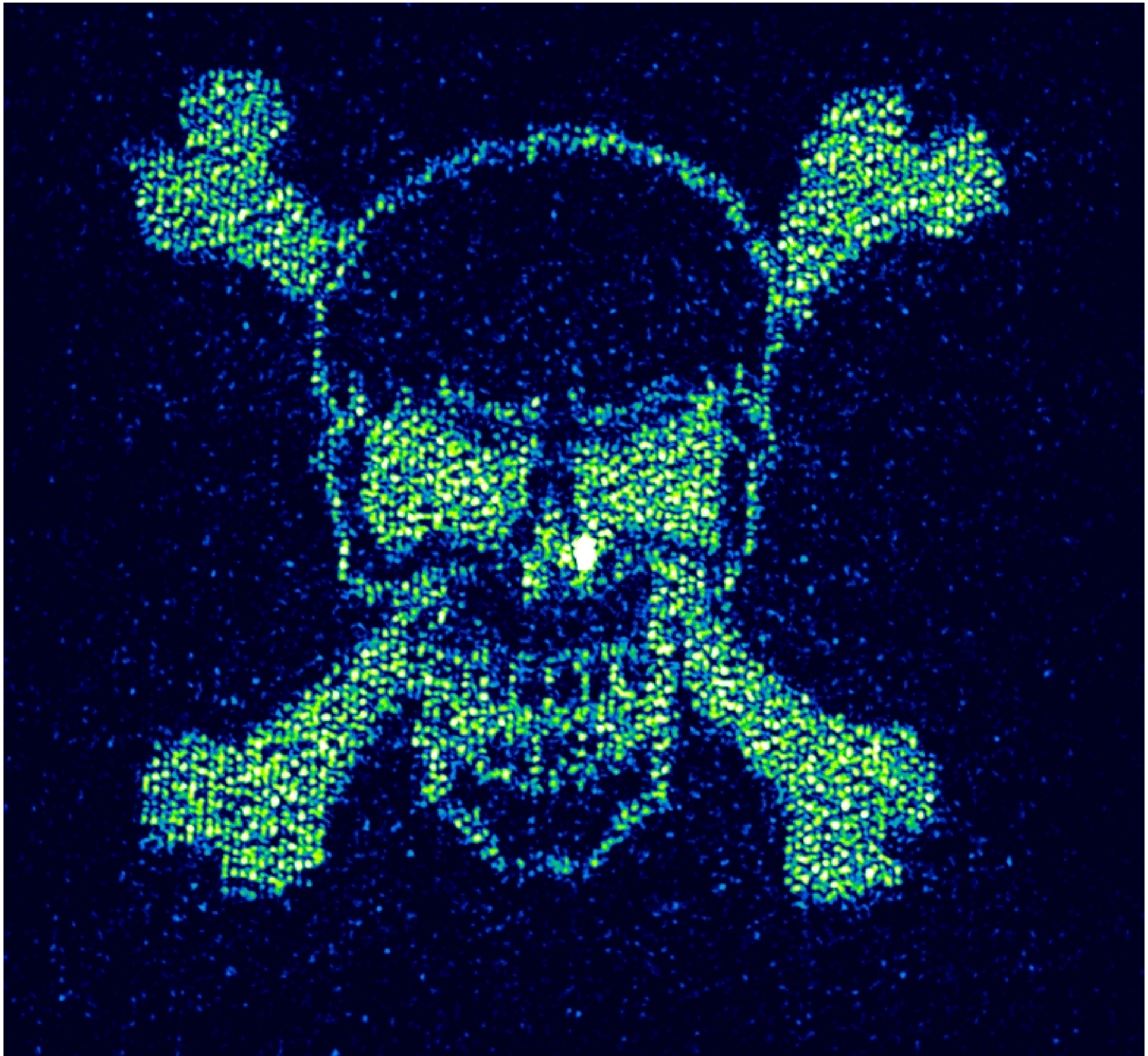
Now that we're experts…

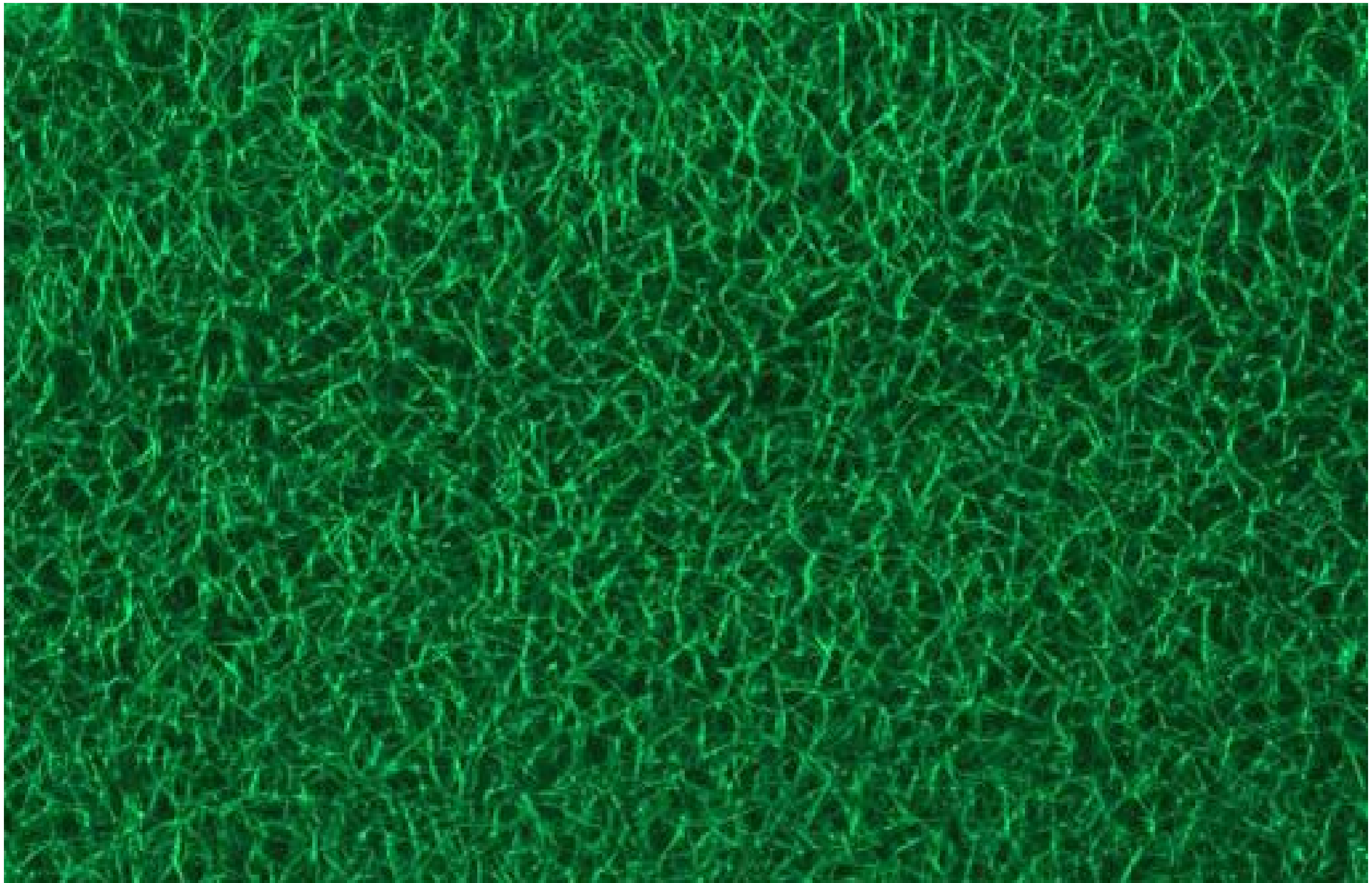
Fun with light scattering

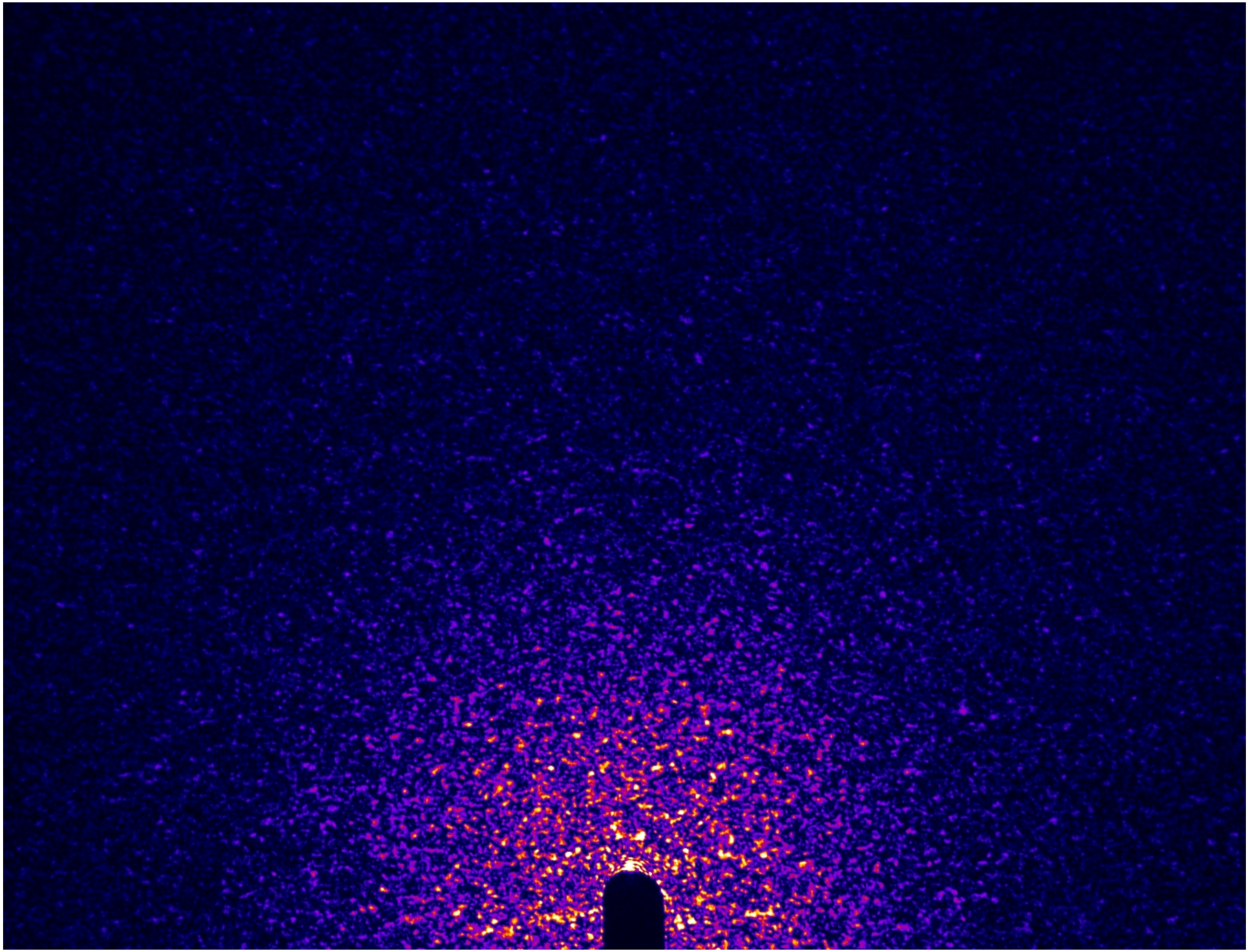








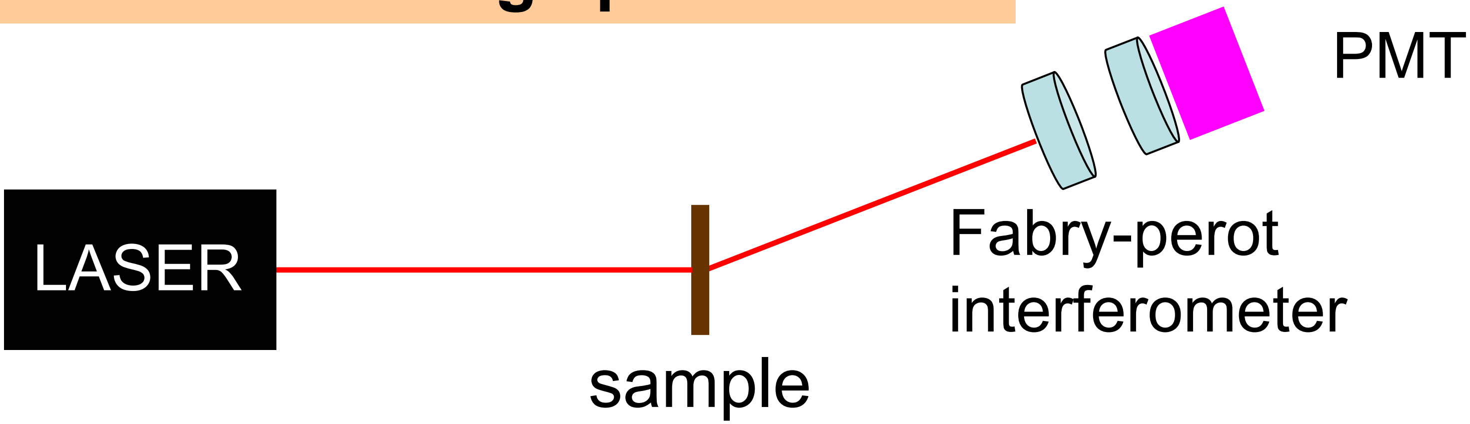




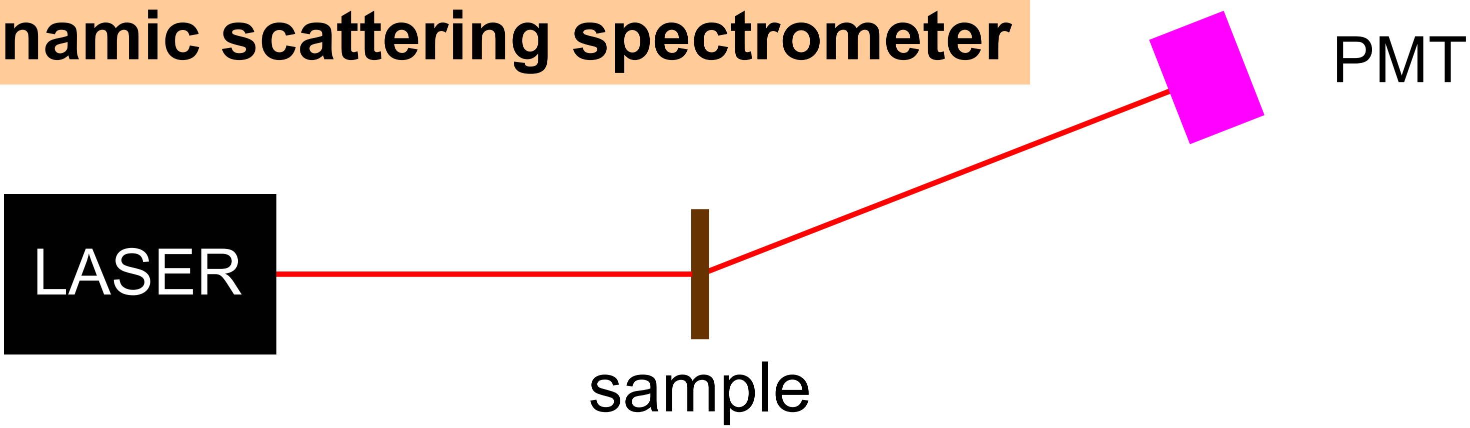
Dynamics….

IXS/DLS/Spectroscopy

Inelastic scattering spectrometer



Dynamic scattering spectrometer



Both versions are done with x-rays too… IXS and XPCS.

They all measure some form of the **dynamic structure factor**

-- S(q,ω) can be derived from basic inelastic scattering theory.
-- Way to hard to even talk about…

An easier way to get a grasp: FT of correlation function.

$$S(\mathbf{q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, e^{i\omega t} \int dr\, e^{-i\mathbf{q}\cdot\mathbf{r}} G(\mathbf{r},t)$$

$$G(\mathbf{r},t) = \frac{1}{N}\sum_{l,l'}\int \left\langle \delta(\mathbf{r}'-\mathbf{R}_{l'}(0))\delta(\mathbf{r}-\mathbf{R}_{l}(t))\right\rangle d\mathbf{r}'$$

Excitations seen in S(q,ω) yield dispersion relations;
directly measure thermodynamic quantities.

Hydrodynamic equations of **mass**, **momentum**, **energy** **conservation** yield dispersion relations.

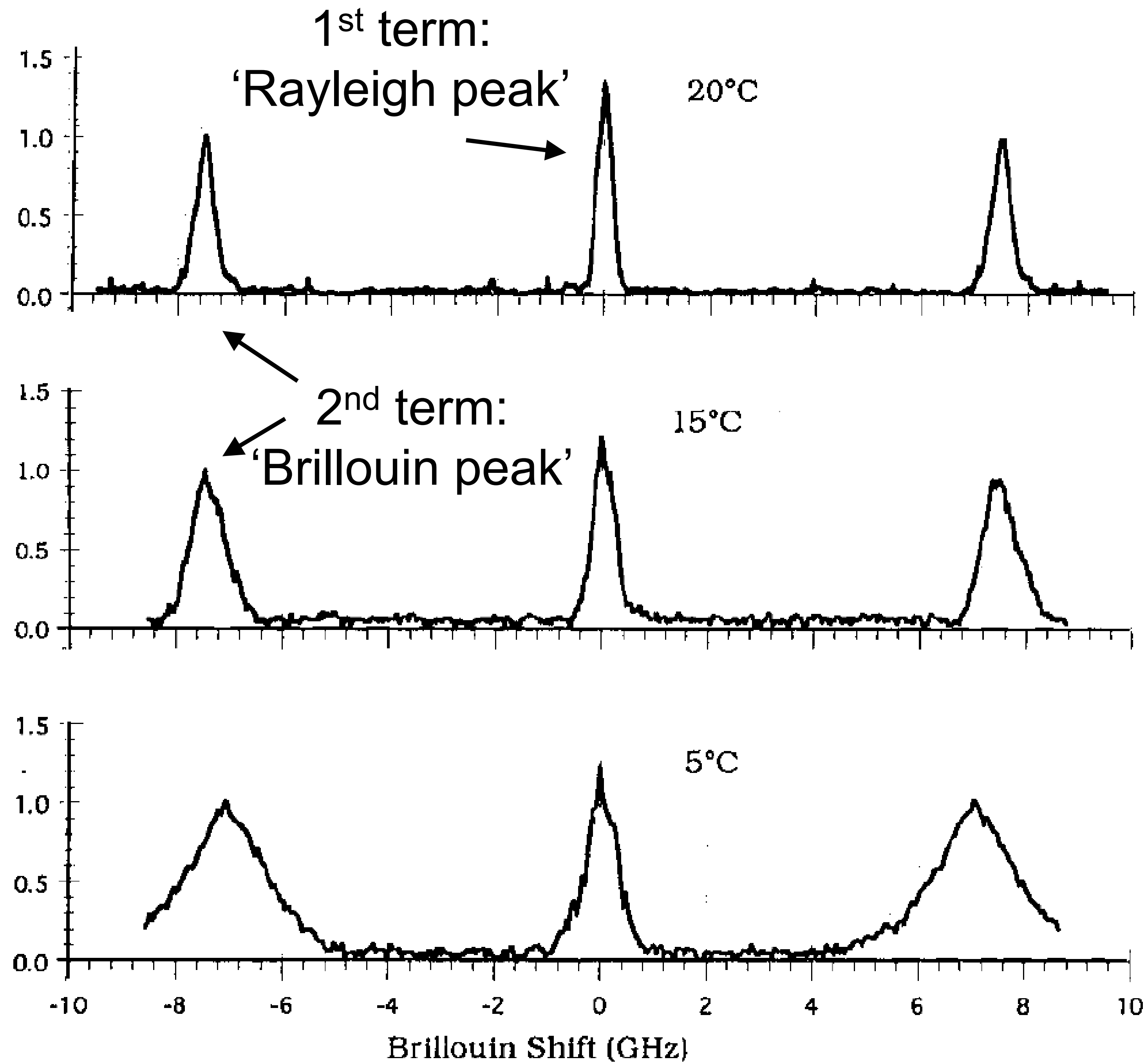
S(q,ω) is directly constructed from linearized hydrodynamic equations:

$$\frac{S(q,\omega)}{S(q)} = \frac{\gamma-1}{\gamma}\frac{2\chi q^2}{\omega^2+(\chi q^2)^2} + \frac{1}{\gamma}\left[\frac{\Gamma q^2}{(\omega+cq)^2+(\Gamma q^2)^2} + \frac{\Gamma q^2}{(\omega-cq)^2+(\Gamma q^2)^2}\right]$$

$$+\frac{1}{\gamma}[\Gamma+(\gamma-1)\chi]\frac{q}{c}\left[\frac{\omega+cq}{(\omega+cq)^2+(\Gamma q^2)^2} - \frac{\omega-cq}{(\omega-cq)^2+(\Gamma q^2)^2}\right]$$

Three terms…

Shown: S(q,ω) Single q, ω scans, 3 Temps



3rd term: Super weak

1st term, Rayleigh peak: diffusion. Exactly the same as DLS experiment

$$\frac{\gamma - 1}{\gamma} \frac{2\chi q^2}{\omega^2 + (\chi q^2)^2}$$

$\gamma = C_p/C_v$,
C_p = const. press. specific heat, C_v = constant vol. specific heat,
Thermal diffusivity, χ (length^2 sec^{-1}).

How is it exactly the same as a DLS experiment?

Simple, single exponential decay measured by DLS:

$$g^{1}(q,\tau) = g_0 e^{-\chi q^2 \tau}$$

$$\mathbb{F}[g^{1}(q,\tau)] = \frac{g_0}{\pi} \frac{\chi q^2}{\omega^2 + (\chi q^2)^2}$$

Spectroscopic measurement and dynamic measurement are Fourier pairs

Why do dynamic rather than spectroscopic measurements?

timescale of colloidal diffusion / required energy resolution.

Diffusion timescale for 1 μm particle:

$$q = \frac{2\pi}{30\mu m}, \ \tau = \frac{6\pi\eta r}{\kappa T q^2} \sim 1.5\,\mathrm{sec}$$

hbar*ω = hbar*2*π/1.5 sec^{-1} = **2.8×10^{-15} eV**

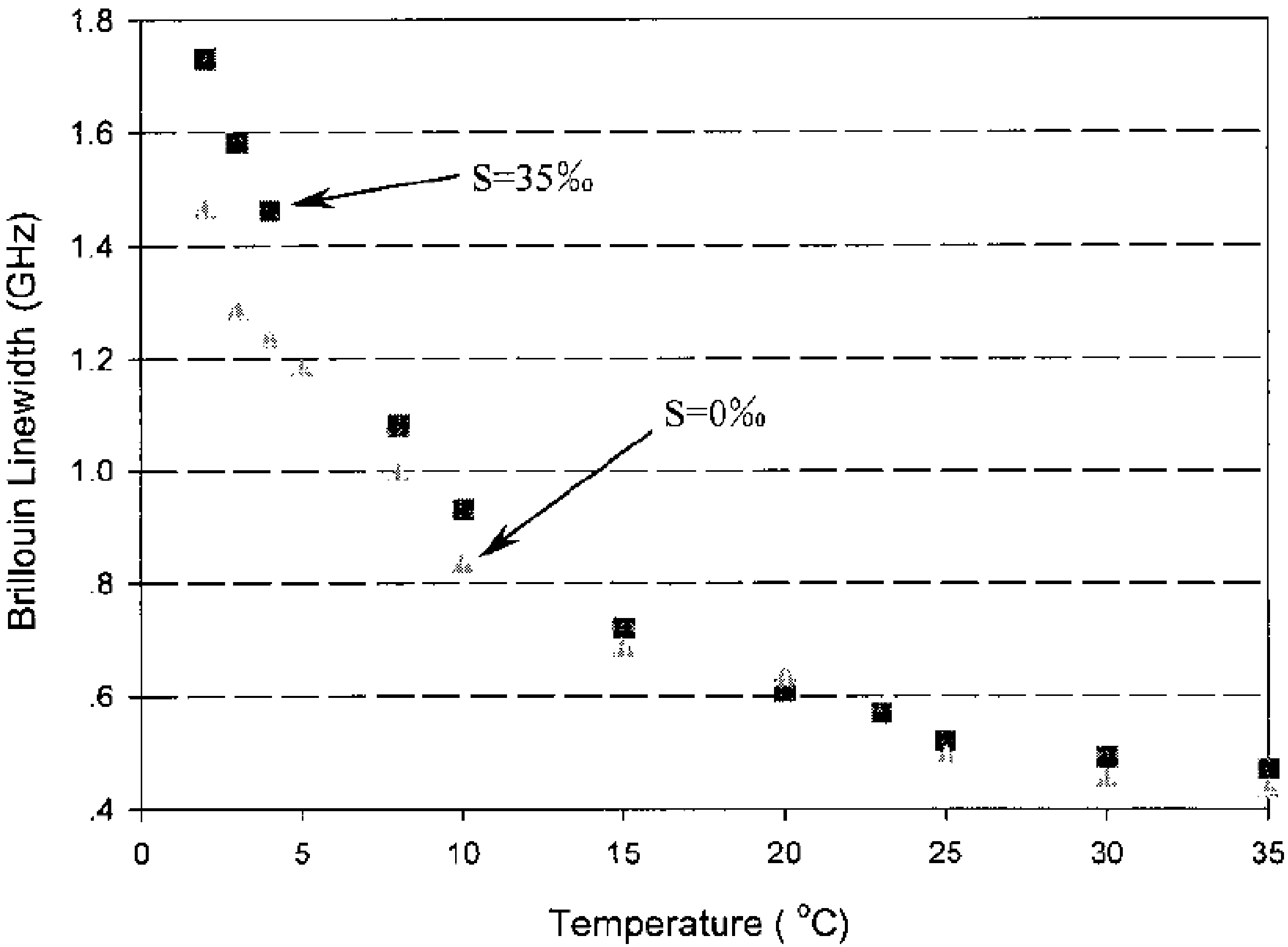
Good energy resolution for inelastic light scattering: ν~1Ghz

hbar*ω = **4.1×10^{-6} eV**

:. Colloidal density fluctuations are too low in energy to measure spectroscopically

Can you do DLS on molecular liquids with a fast camera?

Energy scale of diffusive density flucts. / required time res.



GHz is way out of camera range.

But:

τ depends on q!

$$\tau = \frac{6\pi\eta r}{\kappa T q^2}$$

$$\tau_1 q_1^{\ 2} = \tau_2 q_2^{\ 2}$$

$$\nu_1 d_1^{\ 2} = \nu_2 d_2^{\ 2}$$

$$\nu_2 = 10^9 \left(\frac{1.53}{300}\right)^2$$

$$\nu_2 = 26\,\text{kHz! Wow!}$$

Hydrodynamic equations of **mass**, **momentum**, **energy conservation** yield dispersion relations.

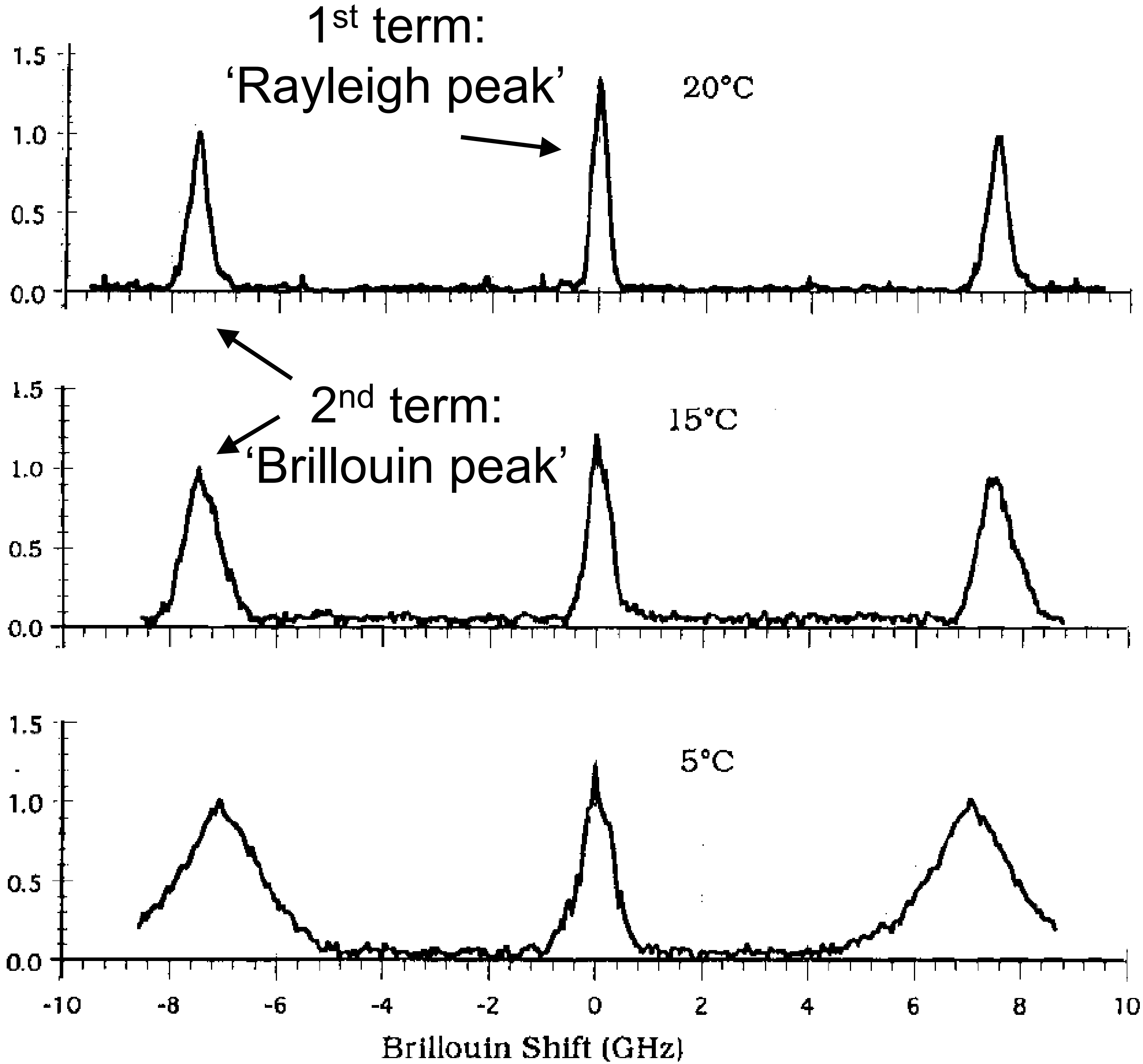
S(q,ω) is directly constructed from linearized hydrodynamic equations:

$$\frac{S(q,\omega)}{S(q)} = \frac{\gamma-1}{\gamma}\frac{2\chi q^2}{\omega^2+(\chi q^2)^2} + \frac{1}{\gamma}\left[\frac{\Gamma q^2}{(\omega+cq)^2+(\Gamma q^2)^2} + \frac{\Gamma q^2}{(\omega-cq)^2+(\Gamma q^2)^2}\right]$$

$$+\frac{1}{\gamma}[\Gamma+(\gamma-1)\chi]\frac{q}{c}\left[\frac{\omega+cq}{(\omega+cq)^2+(\Gamma q^2)^2} - \frac{\omega-cq}{(\omega-cq)^2+(\Gamma q^2)^2}\right]$$

Three terms…

Shown: $S(q,\omega)$ Single q, ω scans, 3 Temps



3rd term: Super weak

2^{nd} term, Brillouin peak: propagation, acoustic mode

$$\frac{1}{\gamma}\left[\frac{\Gamma q^2}{(\omega+cq)^2+(\Gamma q^2)^2}+\frac{\Gamma q^2}{(\omega-cq)^2+(\Gamma q^2)^2}\right]$$

$$\Gamma=\frac{1}{2}[\nu_l+(\gamma-1)\chi]$$

$\gamma = C_p/C_v$,

C_p = const. press. specific heat, C_v = constant vol. specific heat,

ν_l = longitudinal viscosity, $\nu_l = (4\eta/3+\eta_B)\rho_o^{-1}$

Thermal diffusivity, χ (length^2 sec^{-1}),

c = speed of sound.

Rheology from S(q,w)?

$$\Gamma(\omega) = \frac{1}{2}\{v_l(\omega) + [\gamma(\omega) - 1]\chi(\omega)\}$$

$$E \equiv \text{modulus}$$

$$E(\omega) = c(\omega)^2 \rho$$

Let's try it.

Thanks!