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Reconstructing particle shape from small-angle scattering

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The scattering experiment

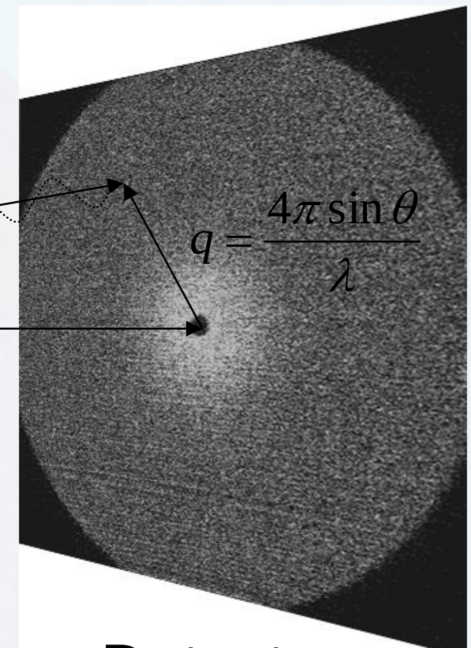
λ

Sample

Incident beam

$|\mathbf{k}_i| = 2\pi/\lambda$

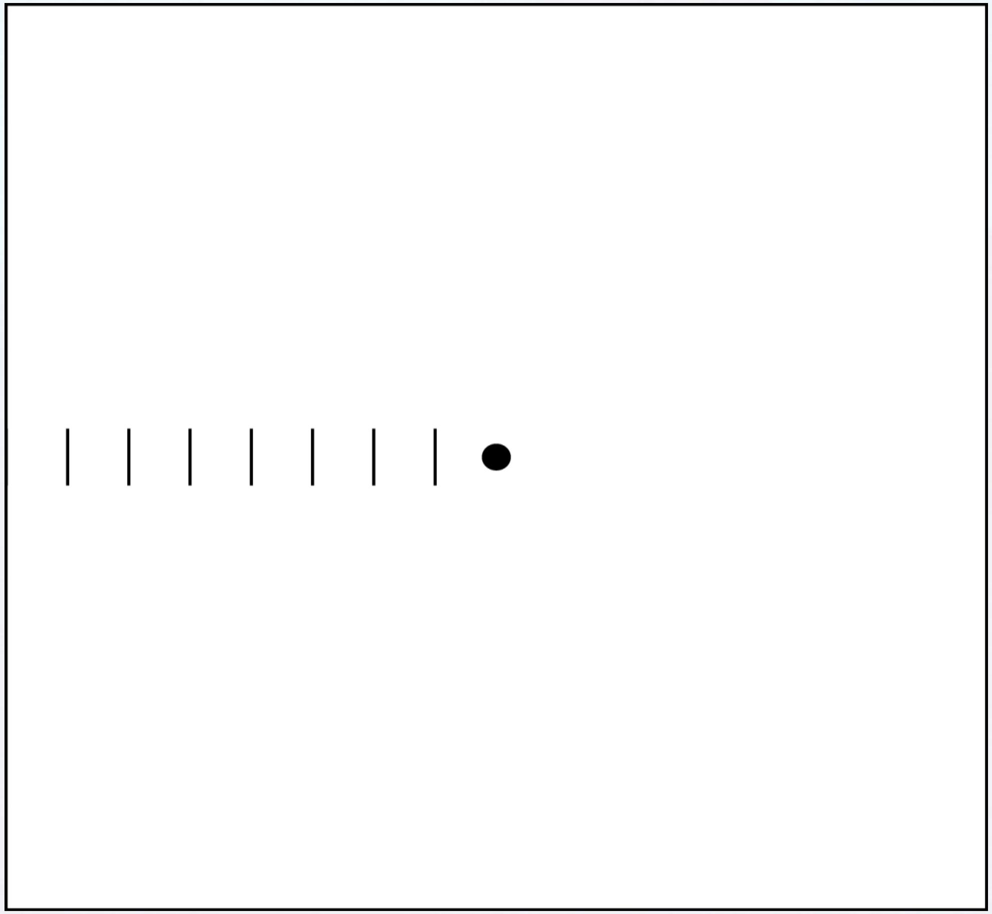
2θ



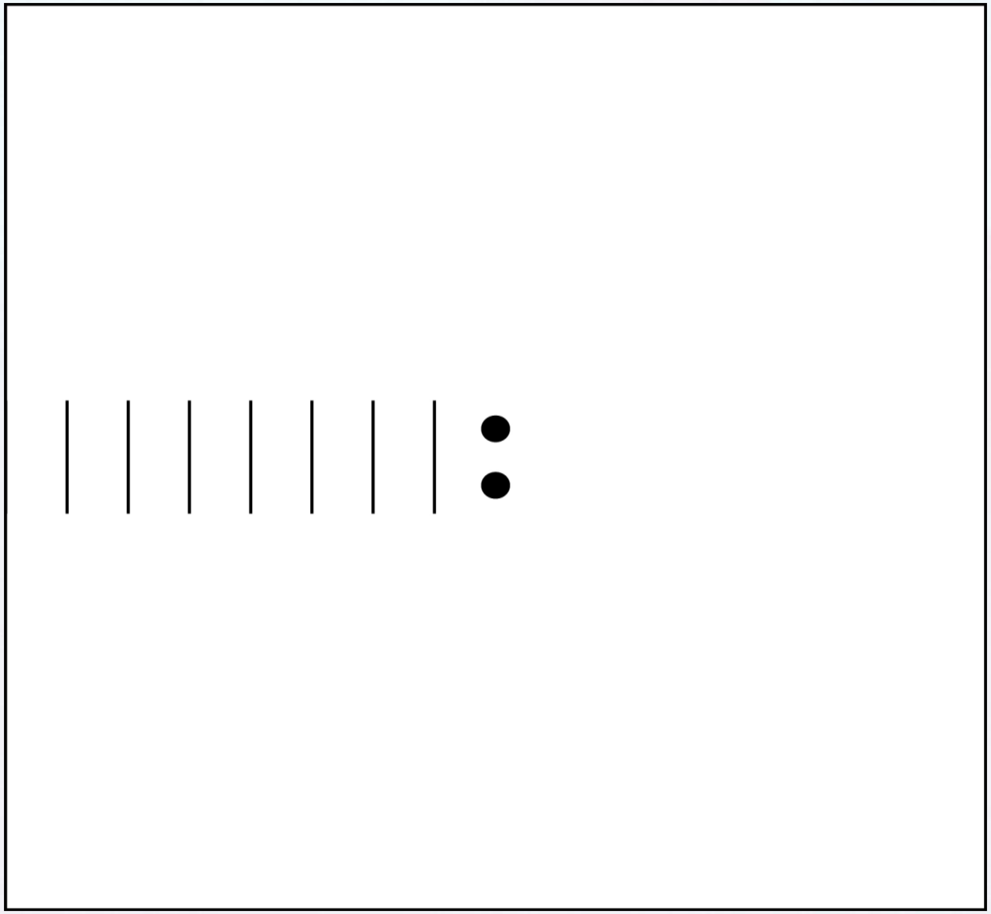
$$q = \frac{4\pi \sin\theta}{\lambda}$$

Detector

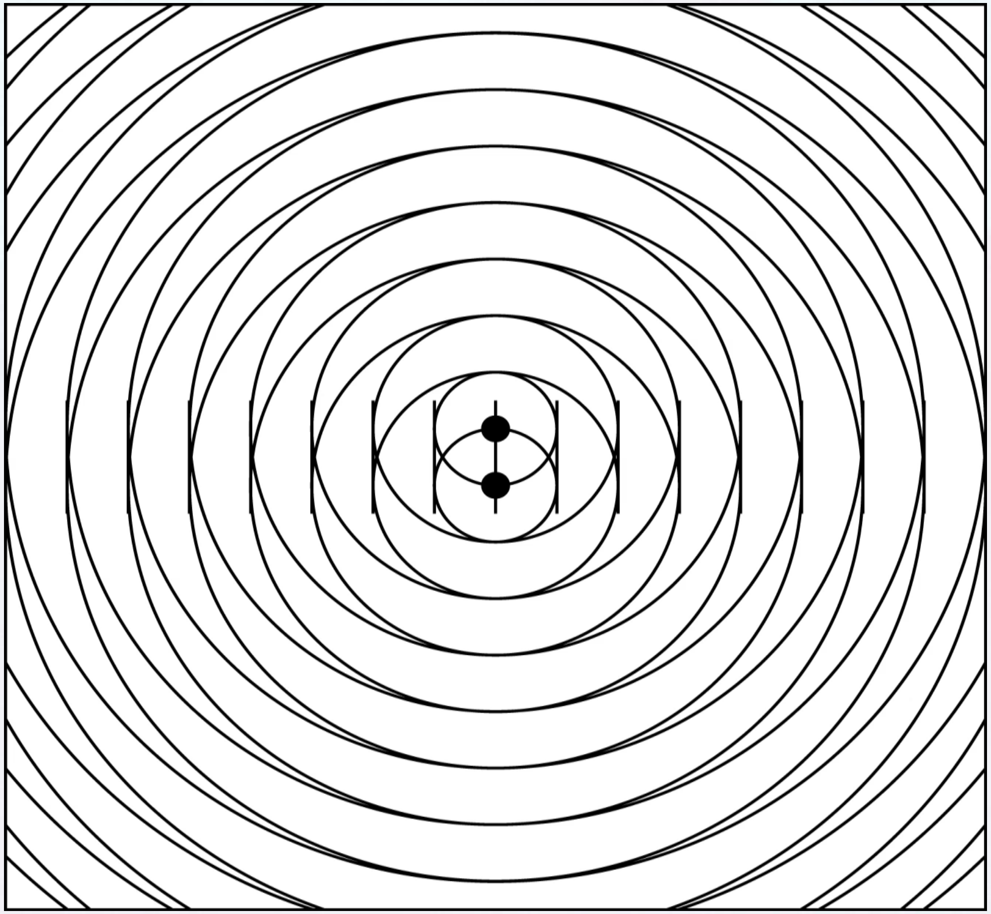
Scattering from a single atom



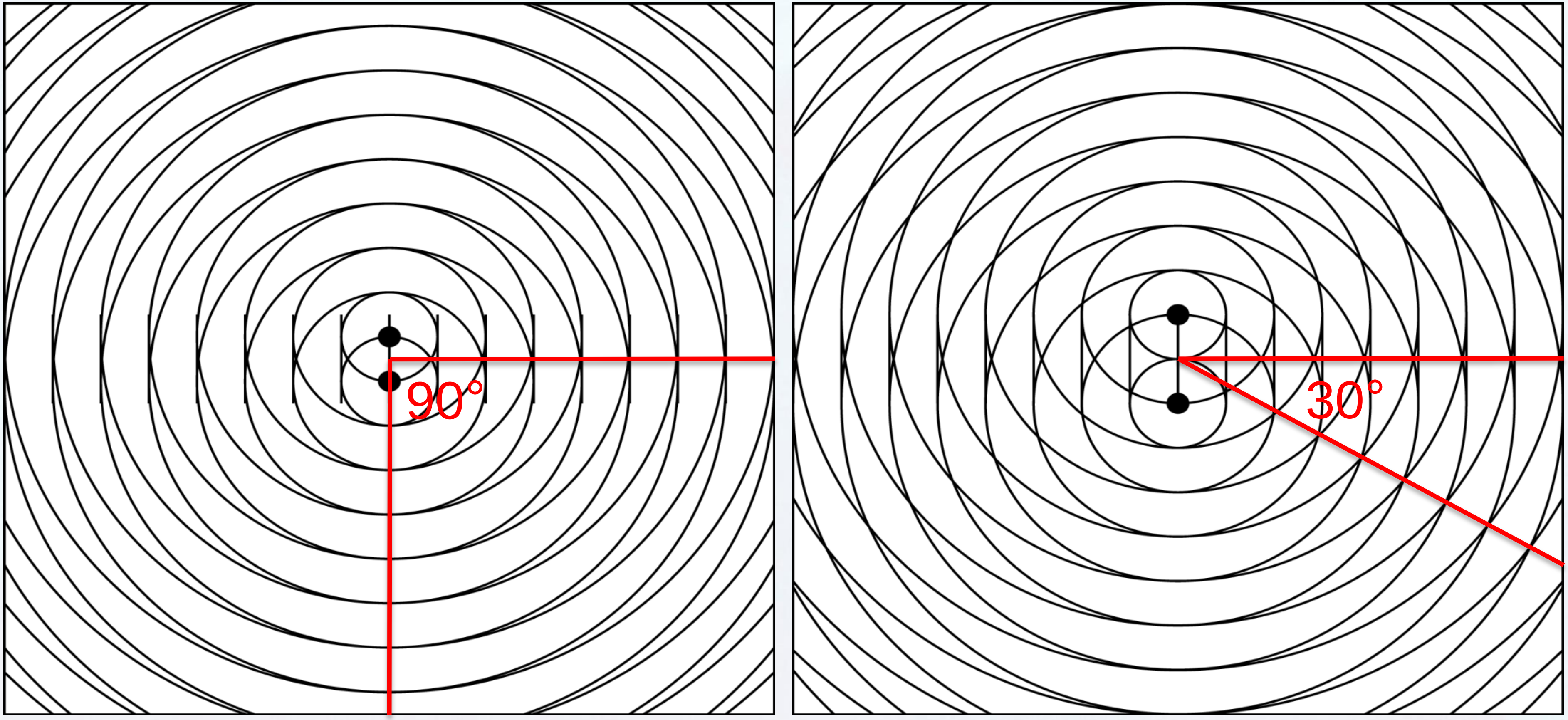
Interference pattern from two atoms



Interference pattern dependence on distance



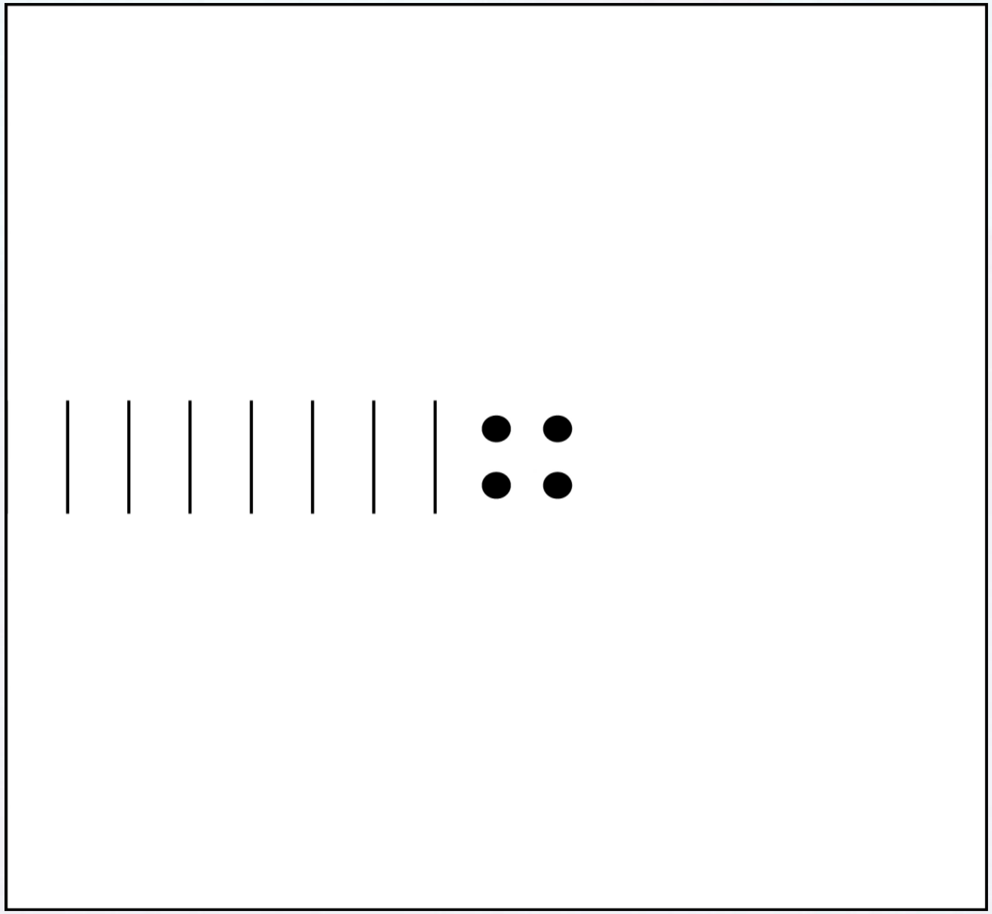
Interference pattern dependence on distance



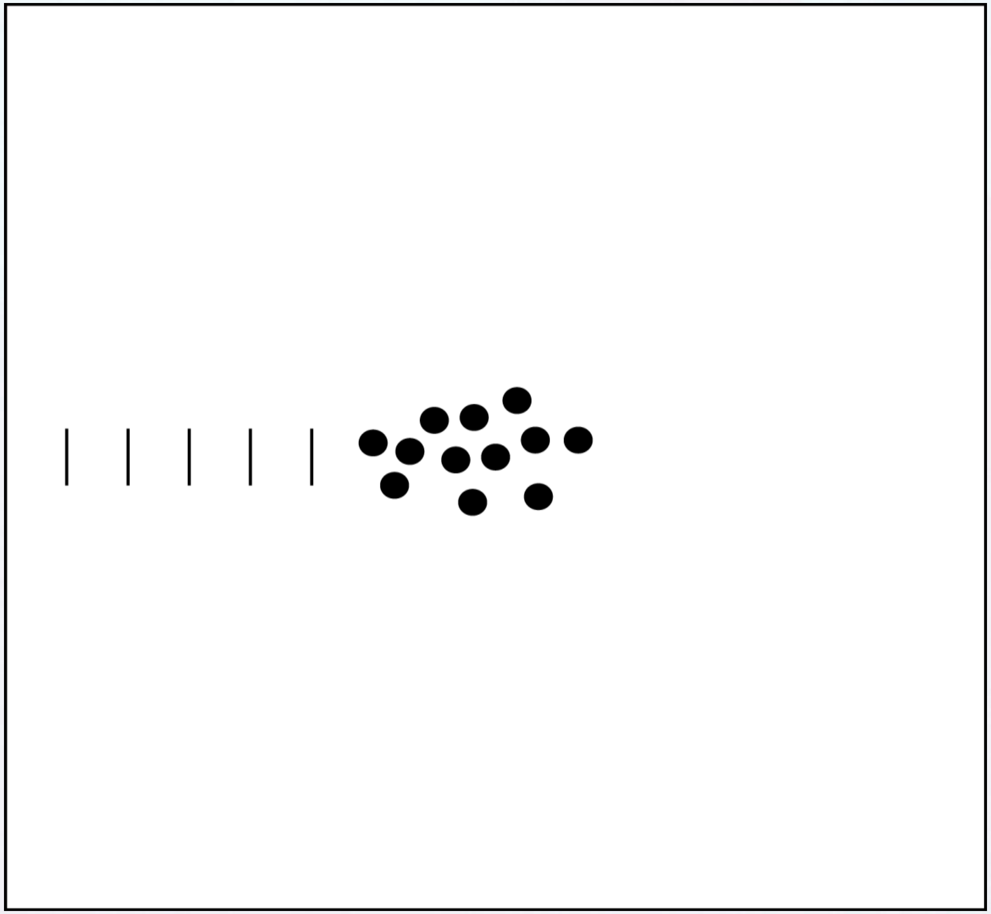
Distance is inversely related to the sine of the scattering angle

sin(90°) = 1.0 sin(30°) = 0.5

Interference pattern for a regular array



Interference pattern for an irregular array



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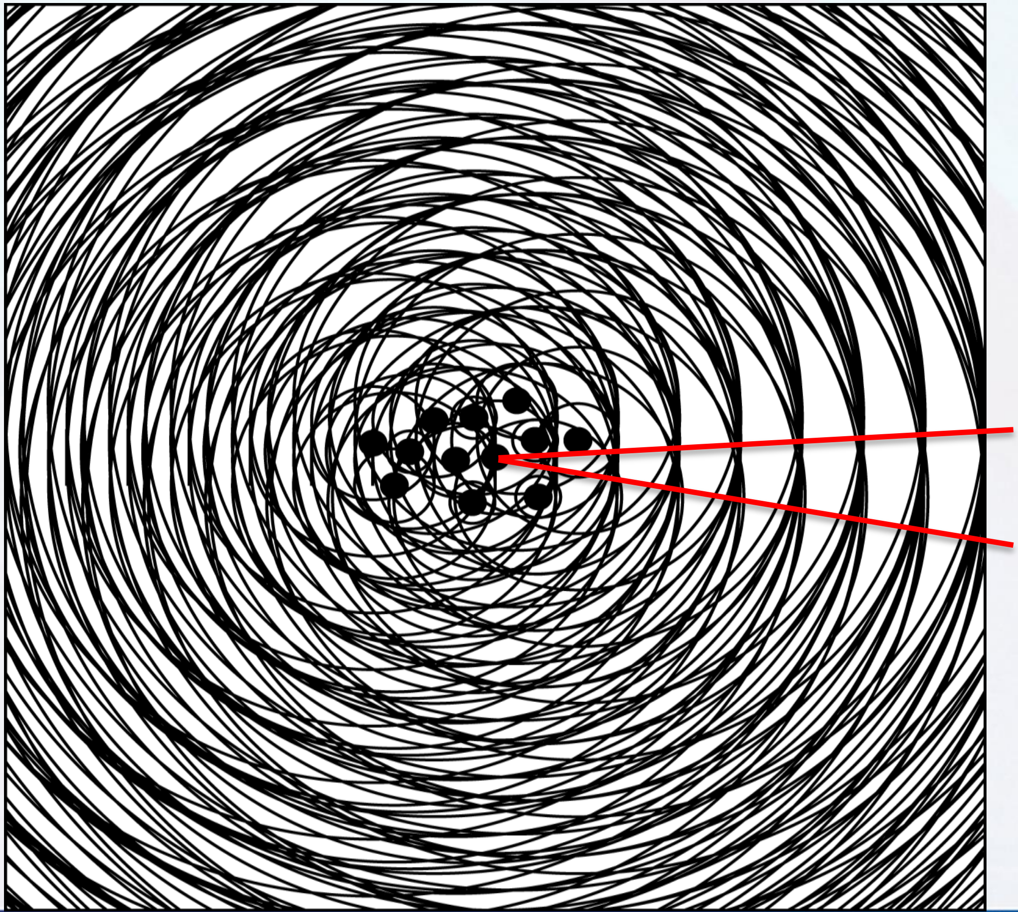
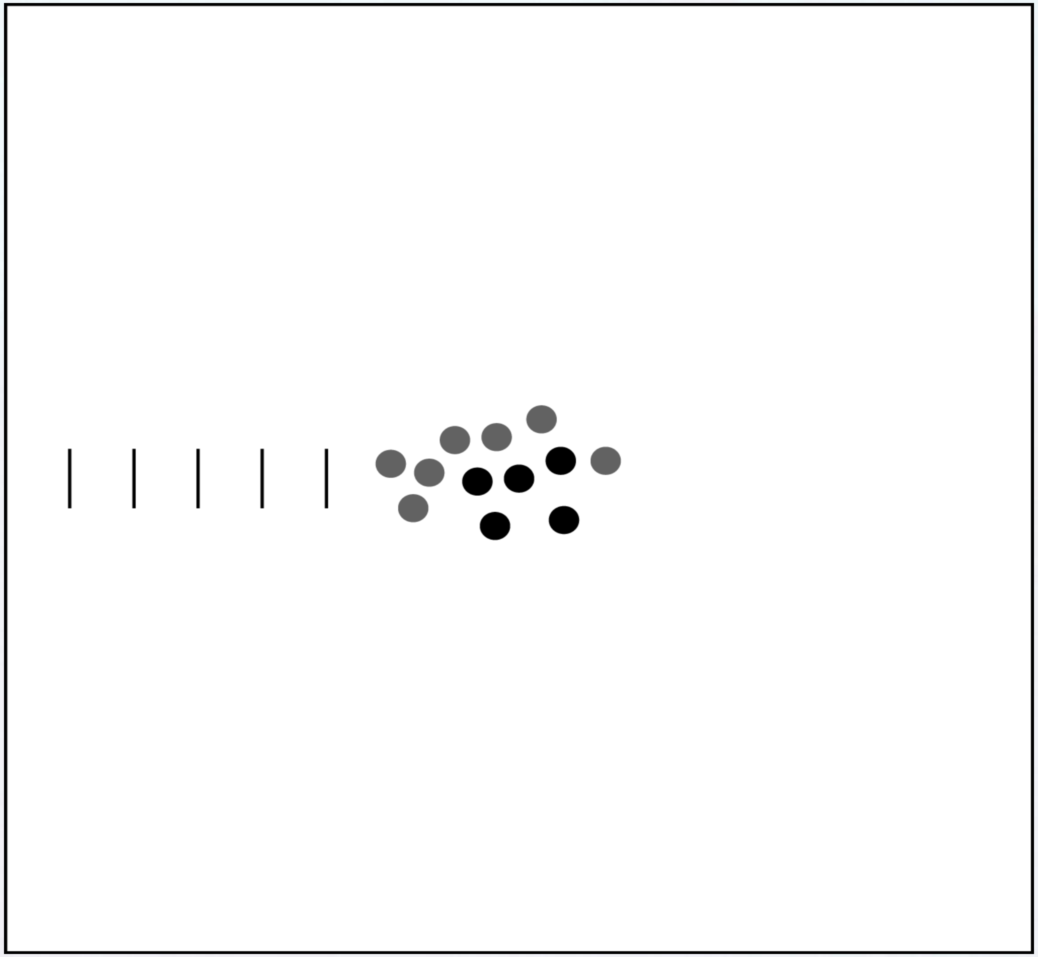
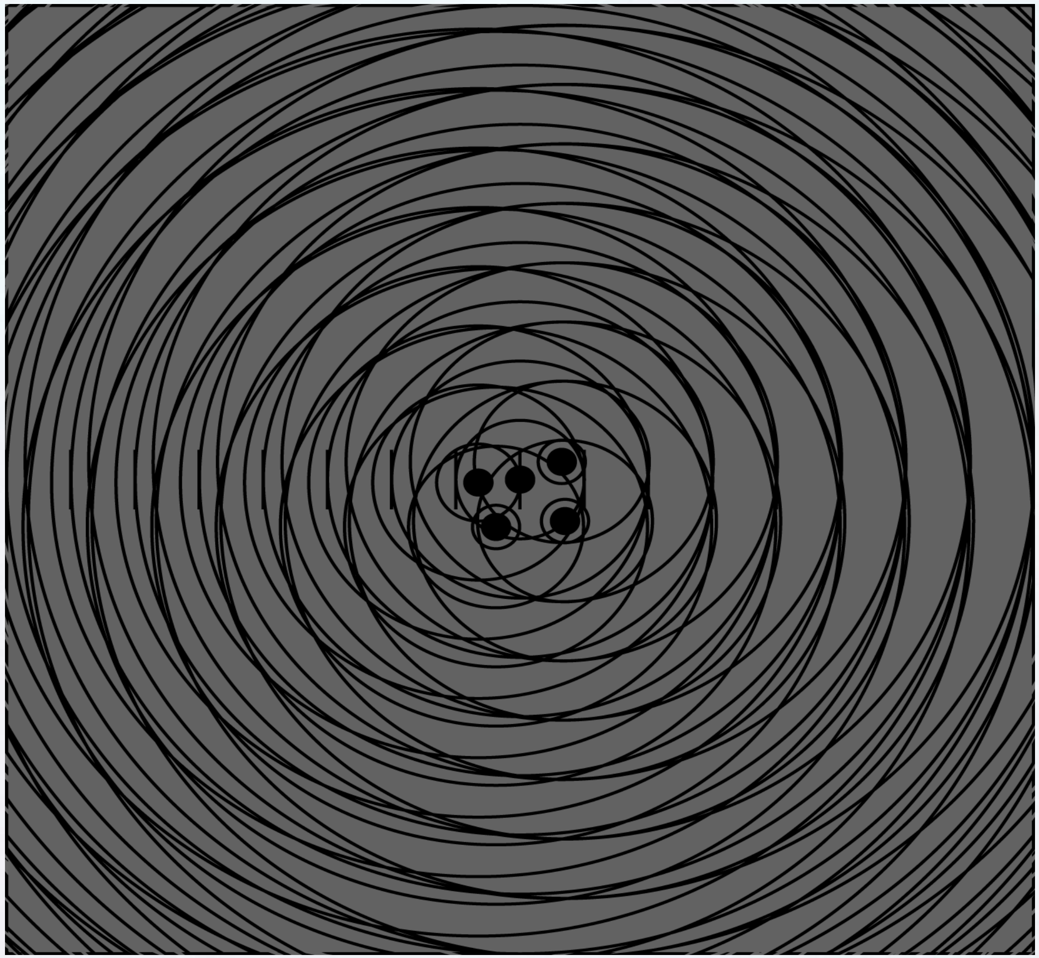
The small-angle scattering signal



Contrast in small-angle scattering



Contrast in small-angle scattering



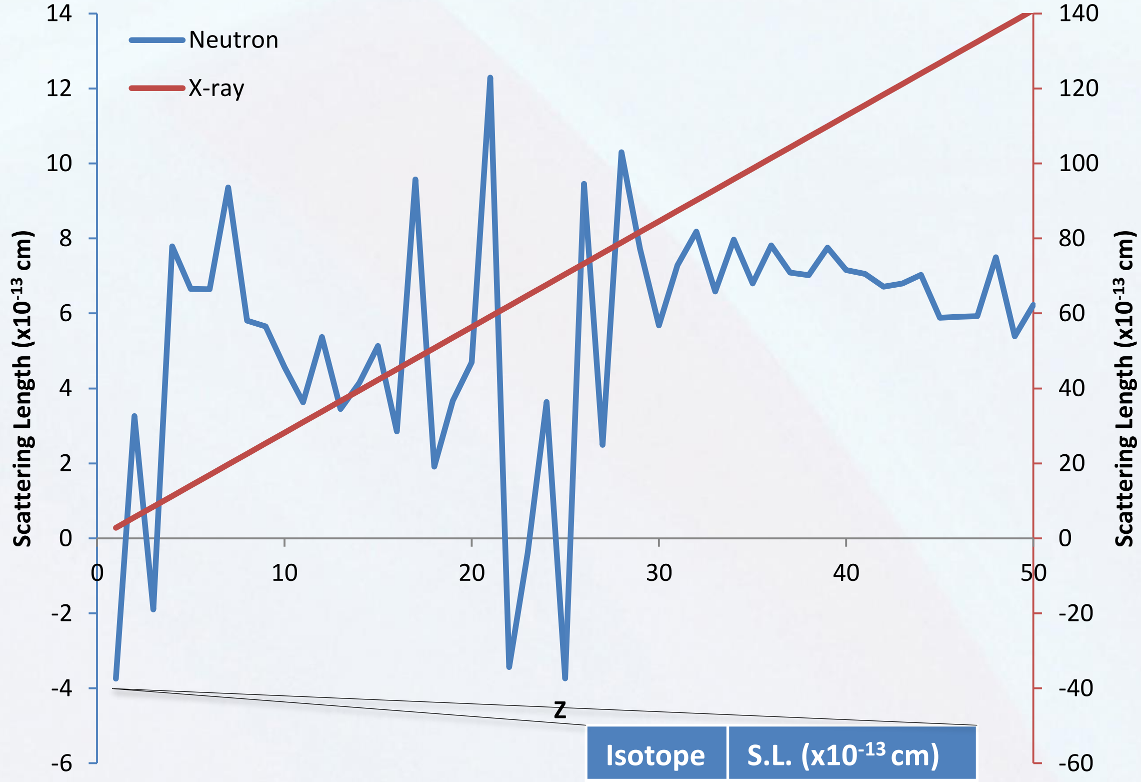
Contrast in small-angle scattering

- Contrast of a volume element V_i is:

$$\Delta\rho(\mathbf{r}) = \frac{b_i}{V_i} - \rho_{solvent}$$

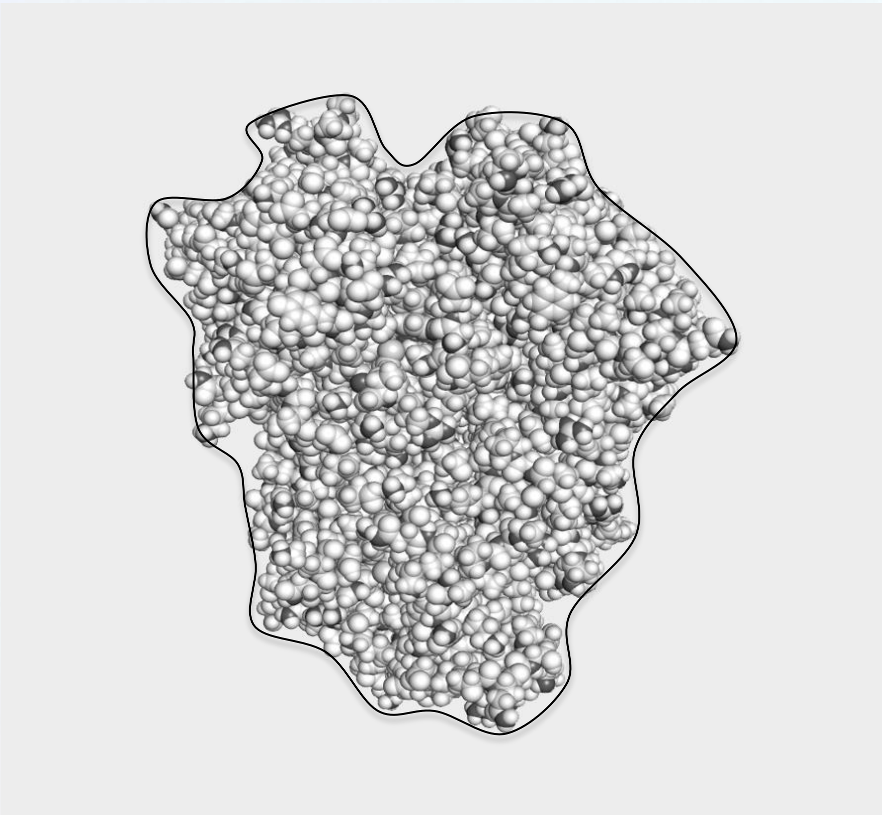
- At low resolution:

$$\Delta\overline{\rho} = \frac{\sum_i b_i}{\sum_i V_i} - \rho_{solvent}$$

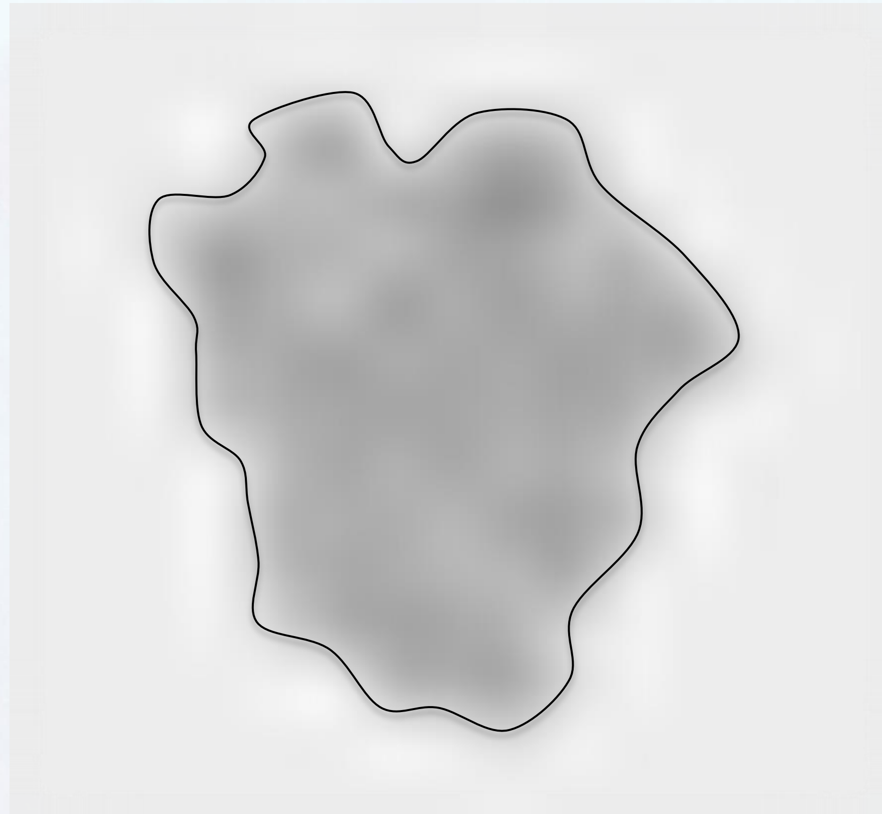


Isotope	S.L. ($\times10^{-13}$ cm)
^{1}H	-3.74
^{2}H (D)	6.67
^{3}H	4.79

What is a low-resolution structure?



High-resolution image



Smeared image ~10Å/pixel

What is a form factor?

- $A(\mathbf{q})$ for an object of uniform scattering density is given by:

$$A(\mathbf{q}) = \int_V \Delta\rho(\mathbf{r}) \cdot e^{i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r}$$

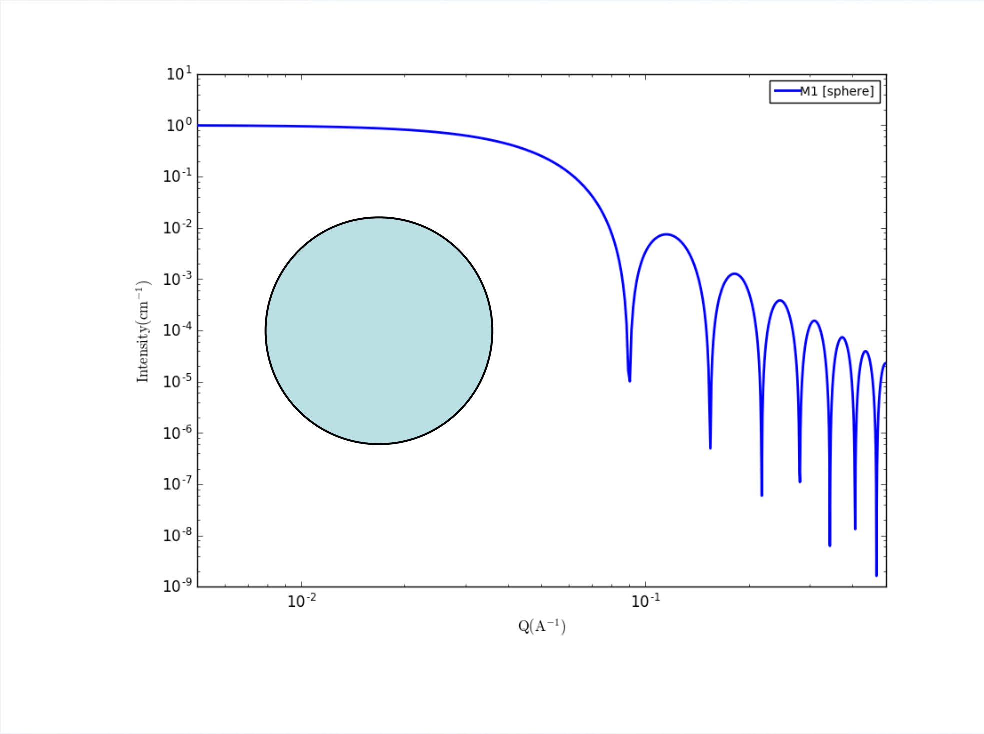
- The form factor (which will be referred to a $P(q)$ herein) is related to the scattering amplitude $A(\mathbf{q})$ by the following:

$$P(q) = \frac{\left\langle A(\mathbf{q}) \cdot A^*(\mathbf{q}) \right\rangle_\Omega}{\left(\Delta\overline{\rho}V\right)^2}$$

Form factor of a uniform sphere

$$A_s(q) = \frac{3\Delta\rho_s V_s\left[\sin(qR_s) - qR_s\cos(qR_s)\right]}{(qR_s)^3}$$

$$P_s(q) = \left(\frac{3\left[\sin(qR_s) - qR_s\cos(qR_s)\right]}{(qR_s)^3}\right)^2$$



Relationship between *I*(*q*) and *P*(*q*)

- For a single object in solution:

$$I(q) = \left\langle A(\mathbf{q}) \cdot A^*(\mathbf{q}) \right\rangle_\Omega$$
$$= \left(\Delta\overline{\rho}V\right)^2 P(q)$$

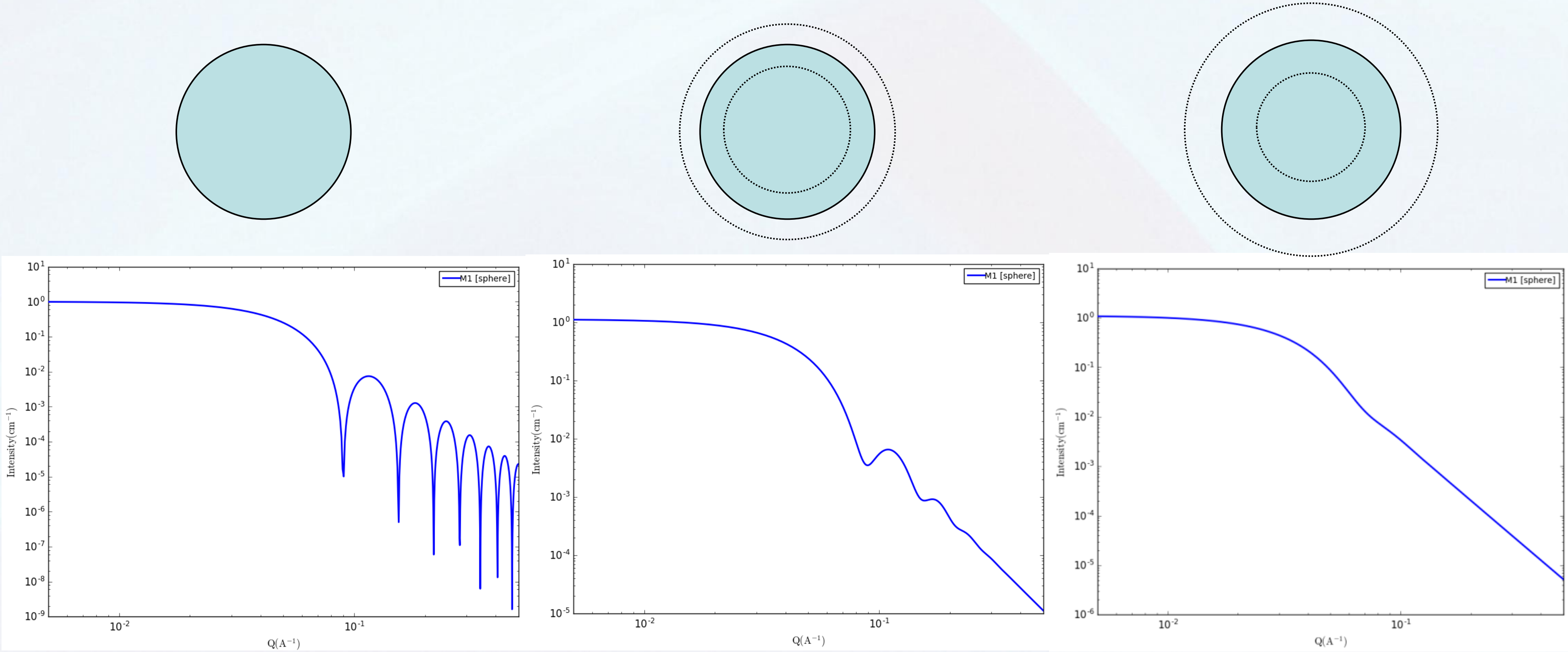
- For an ensemble of non-interacting objects:

$$I(q) = \sum_i^N \left(\Delta\overline{\rho}_i V_i\right)^2 P_i(q)$$

- If all objects are identical:

$$I(q) = N\left(\Delta\overline{\rho}V\right)^2 P(q)$$

The effect of polydispersity



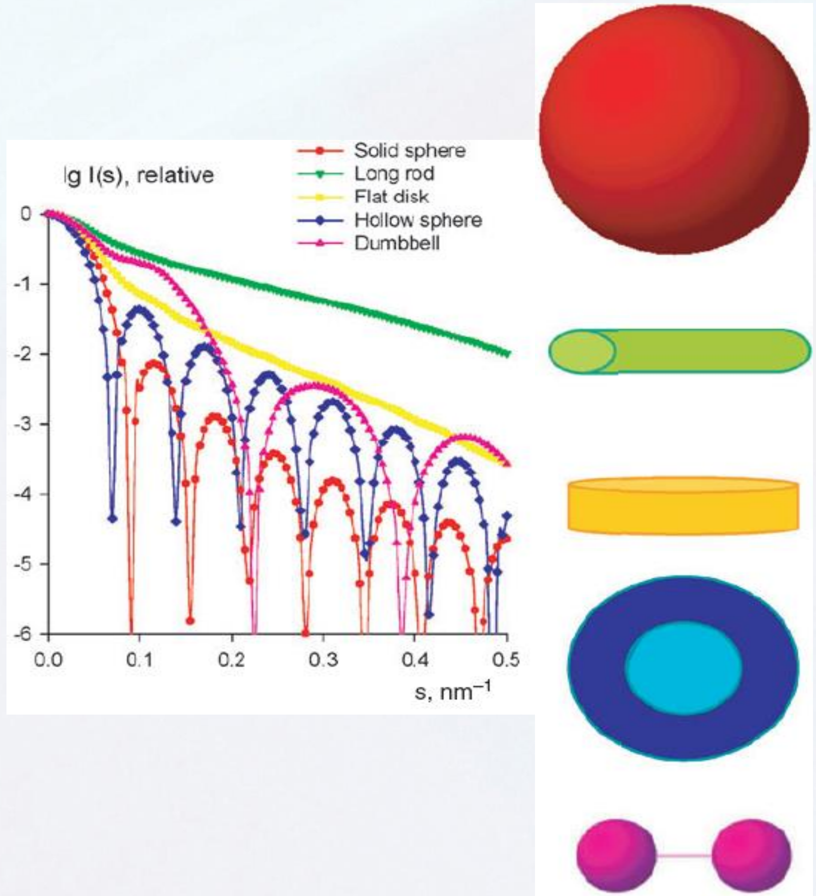
Requirements for shape reconstruction

- The intensity profile must be a good approximation of the form factor for the object.

$$I(q) \propto P(q)$$

  - Pure homogenous solutions / monodisperse (identical particles)
  - Approximate dilute conditions (no attractive or repulsive interactions between particles)

Form factors for a variety of shapes



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D.I. Svergun, M.H.J. Koch, *Reports on Progress in Physics* (2003), 66, 1735-1782

The pair-distance distribution function (PDDF)

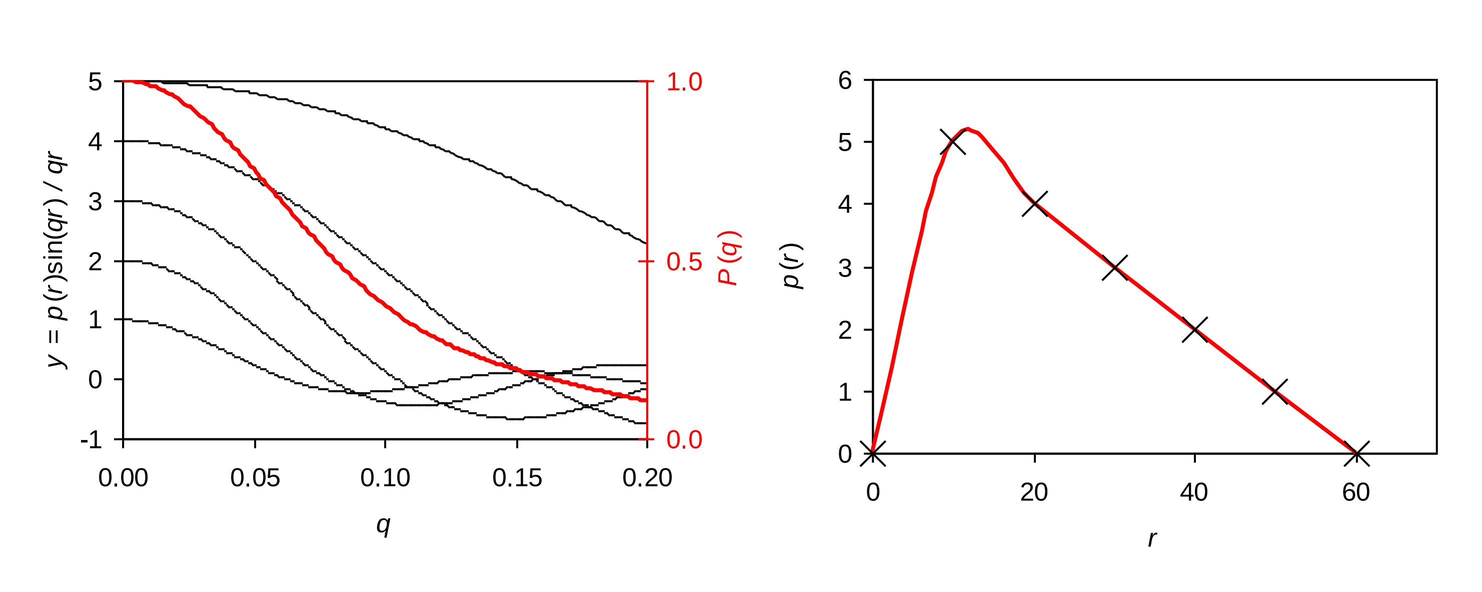
- Is a histogram of interatomic distances, and is related to *I*(*q*) via

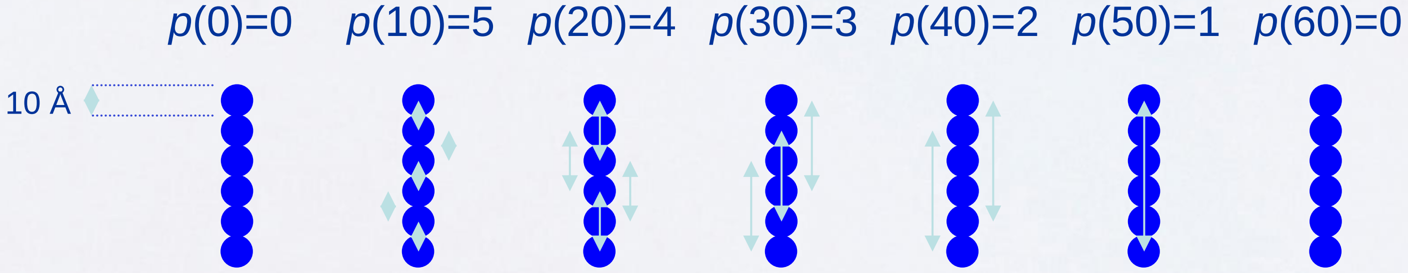
$$p(r) = \frac{r^2}{2\pi}\int_0^\infty I(q)q^2 \frac{\sin qr}{qr} dq$$

- Also, the I(q) can be calculated from the p(r) via

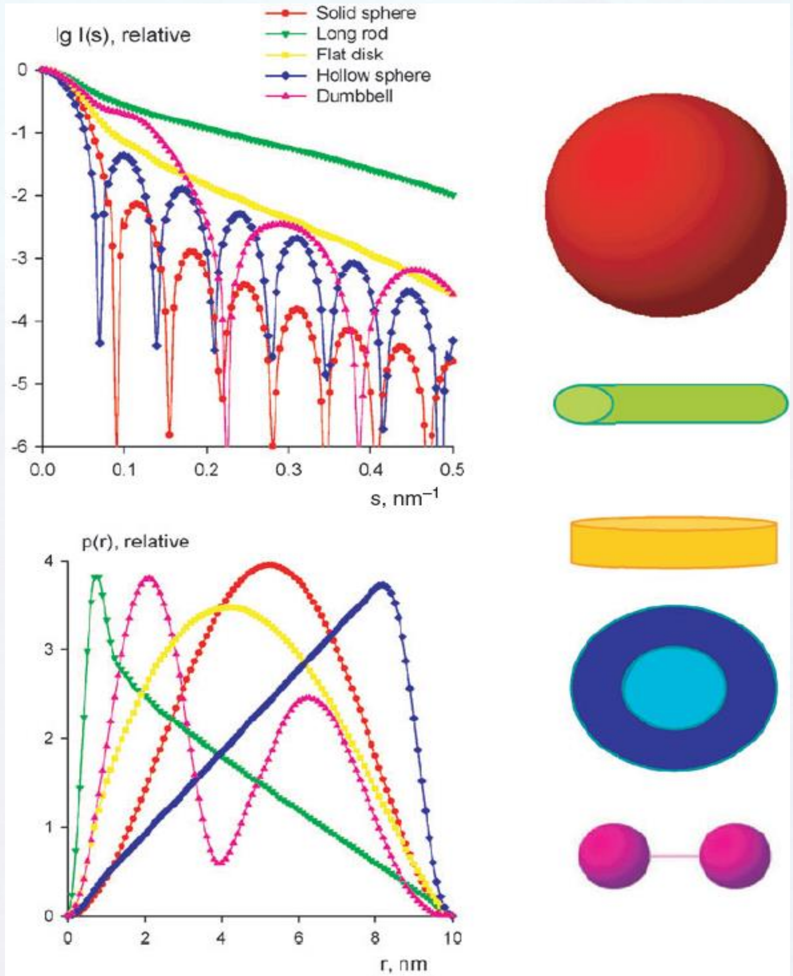
$$I(q) = 4\pi \int_0^{D_{\max}} p(r) \frac{\sin(qr)}{qr} dr$$

What is the PDDF?





The PDDF and *P*(*q*) for a variety of shapes



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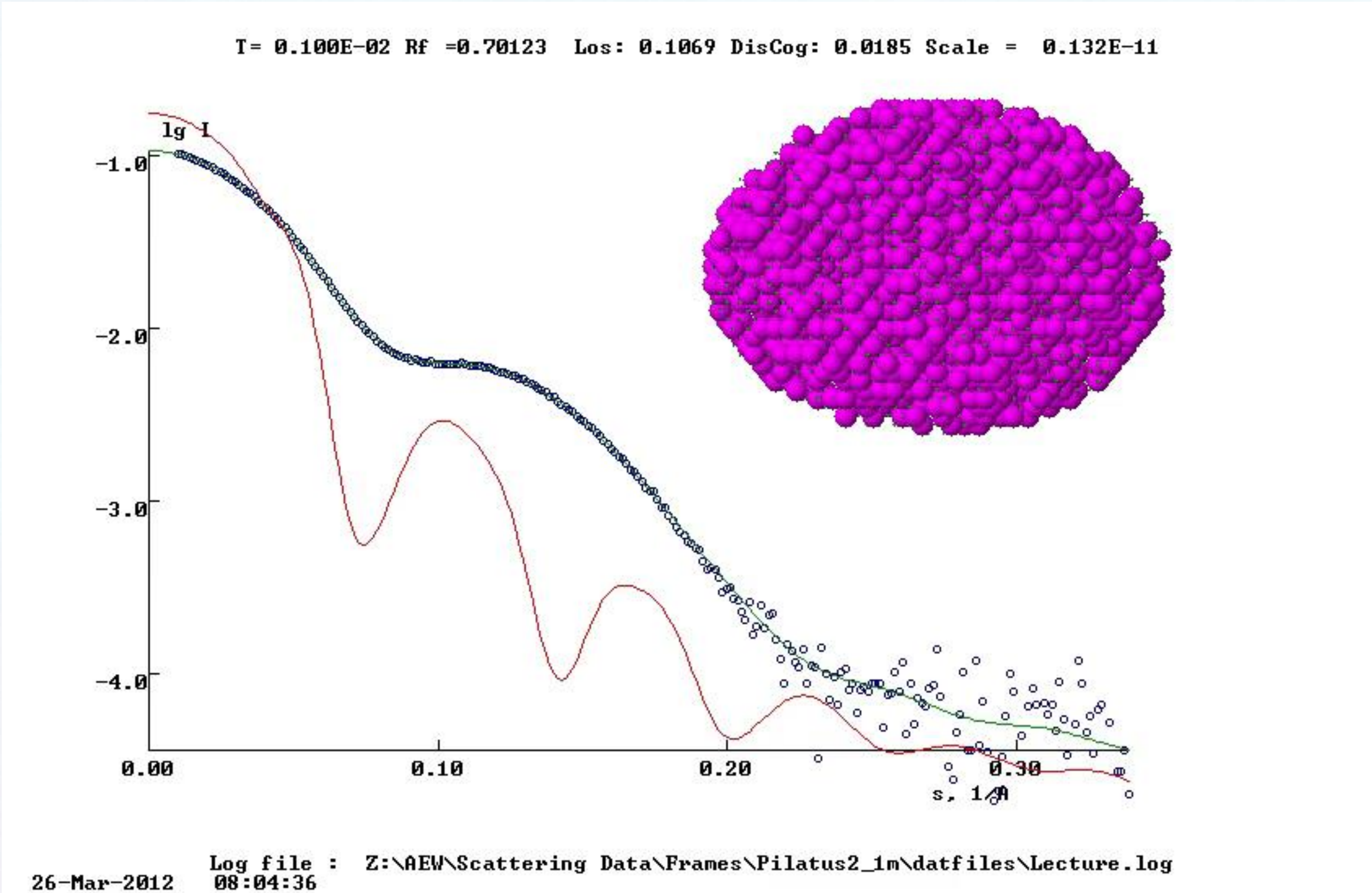
Shape restoration



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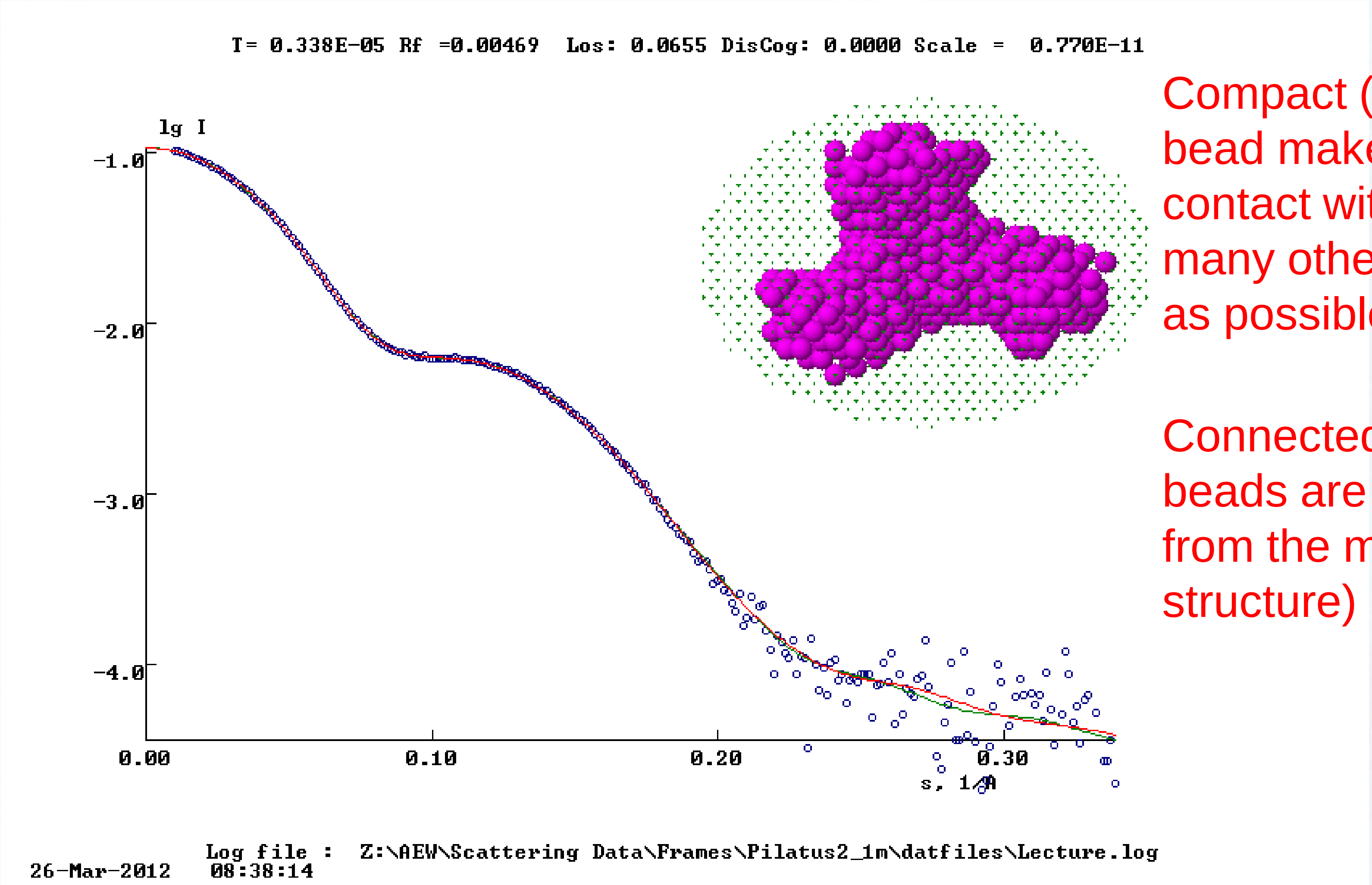
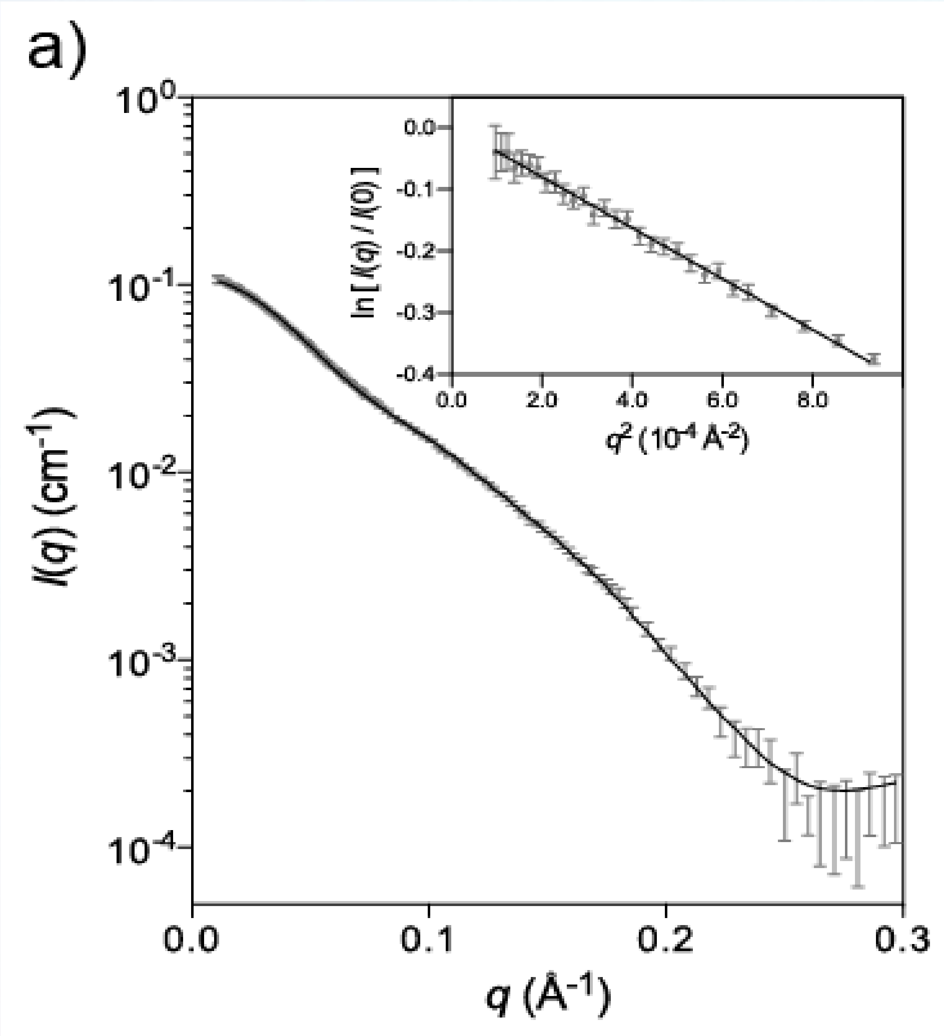
Shape restoration

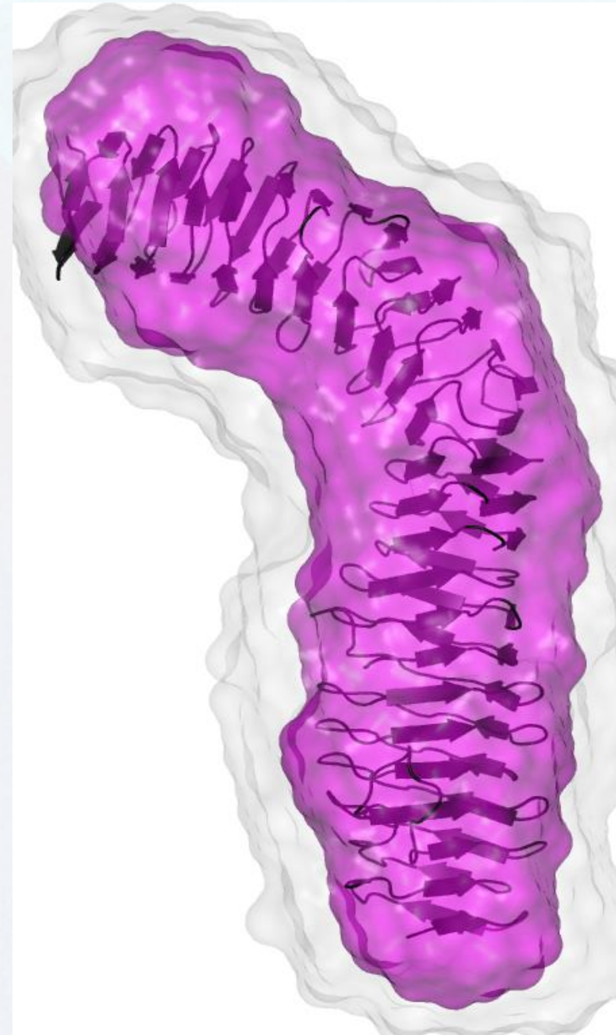


Compact (i.e. each bead makes contact with as many other beads as possible)

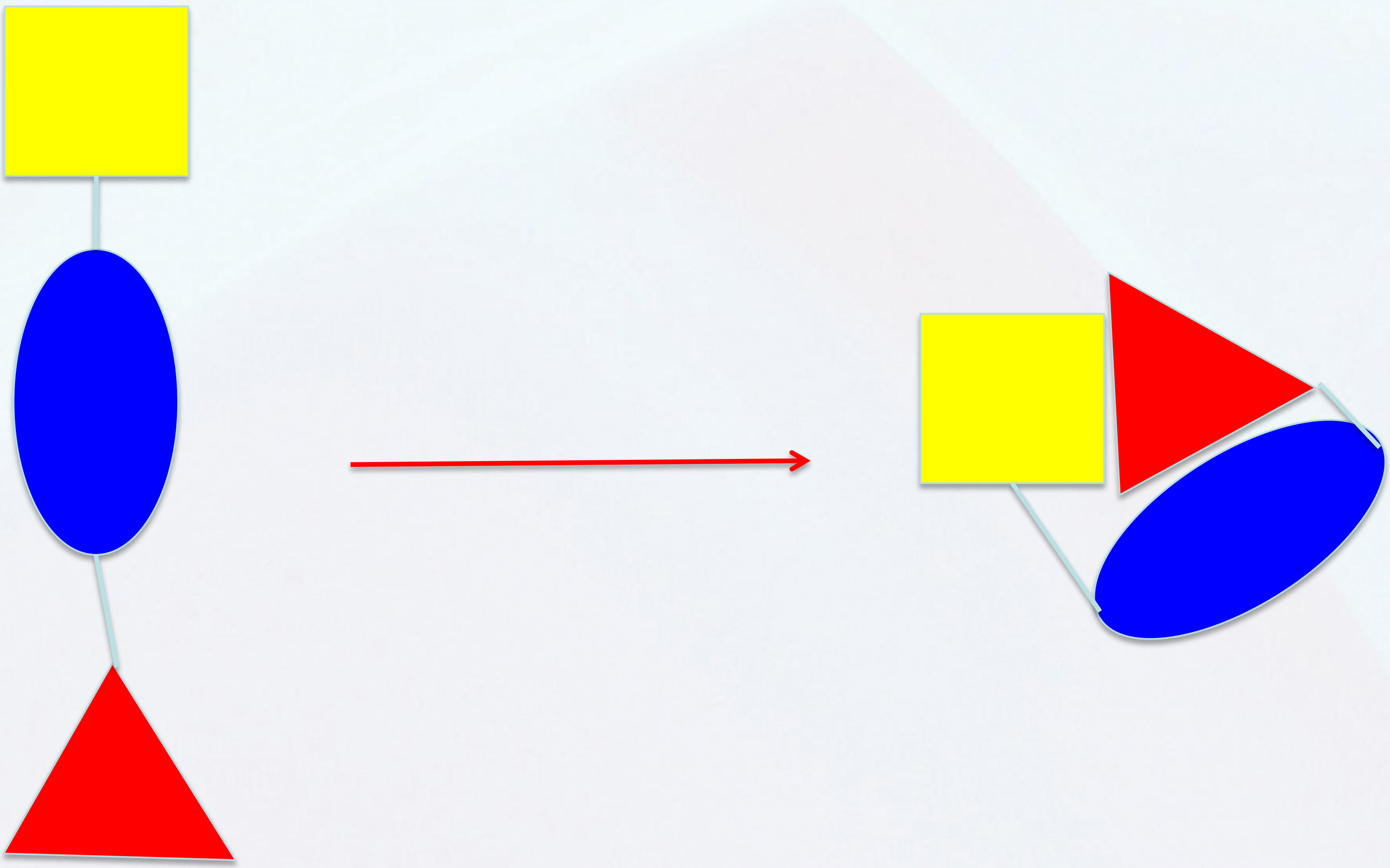
Connected (i.e. no beads are isolated from the main structure)

Shape restoration

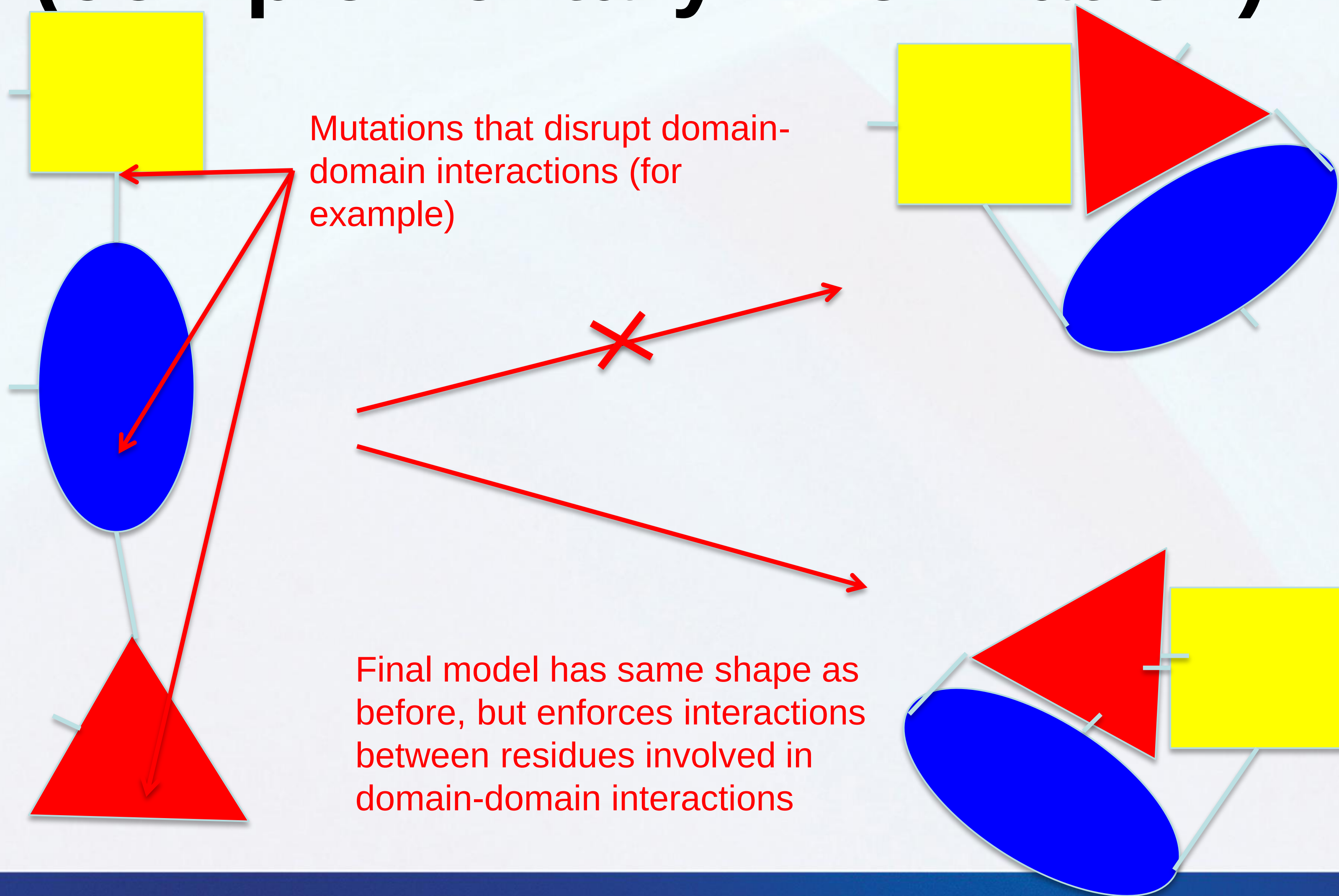




Rigid-body methods



Rigid-body methods (complementary information)



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