

Diffusion de neutrons aux petits angles: application à l'étude des macromolécules biologiques en solution.

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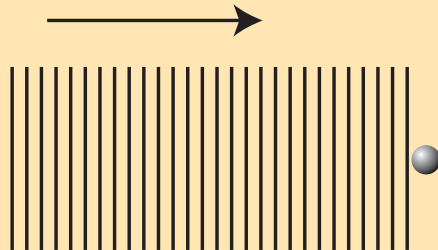
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Définitions et notations

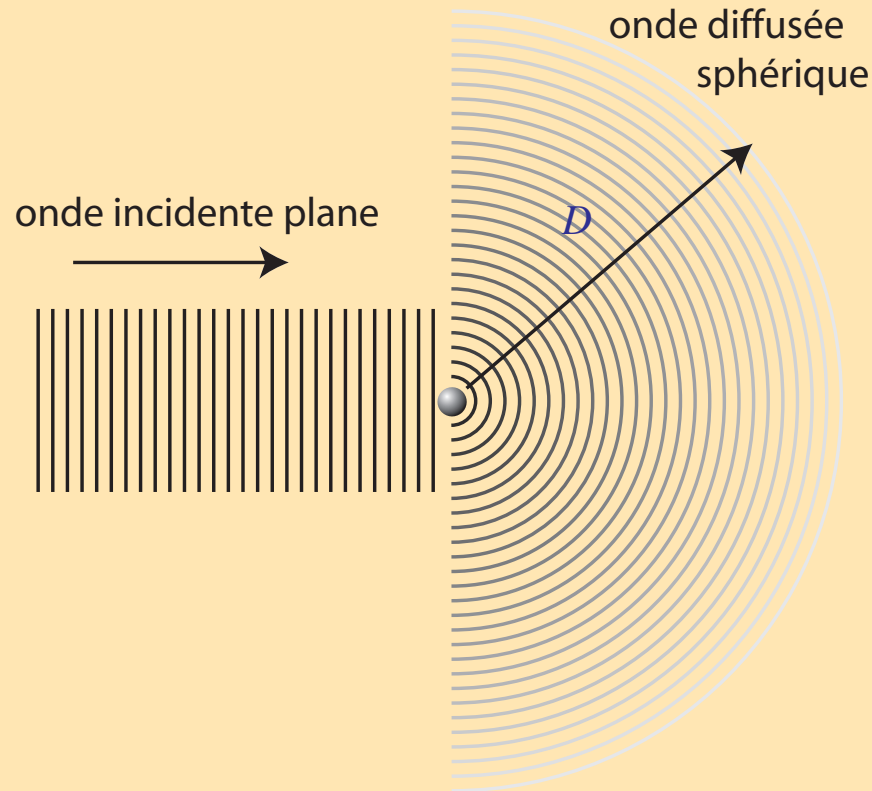
Section efficace de diffusion : $4\pi b^2$
taille de l'atome "vu" par le rayonnement.

Longueur de diffusion : b , caractérise
l'interaction atome-rayonnement.

onde incidente plane



Définitions et notations



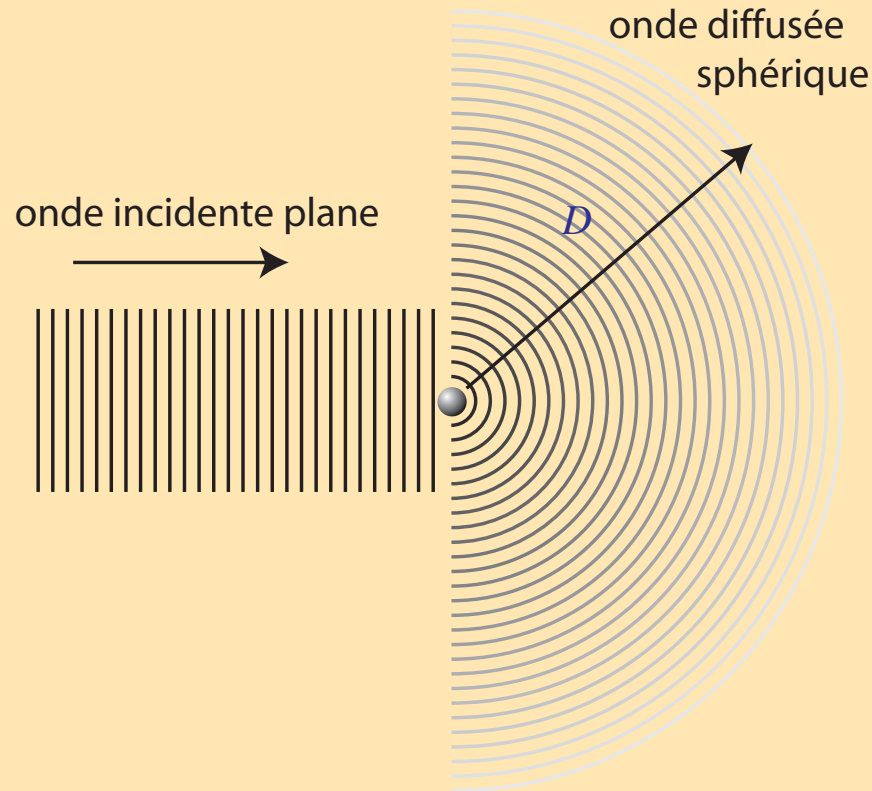
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L'onde diffusée est sphérique

$$I = \Phi \frac{4\pi b^2}{4\pi D^2} s = \Phi \left(\frac{b}{D} \right)^2 s$$

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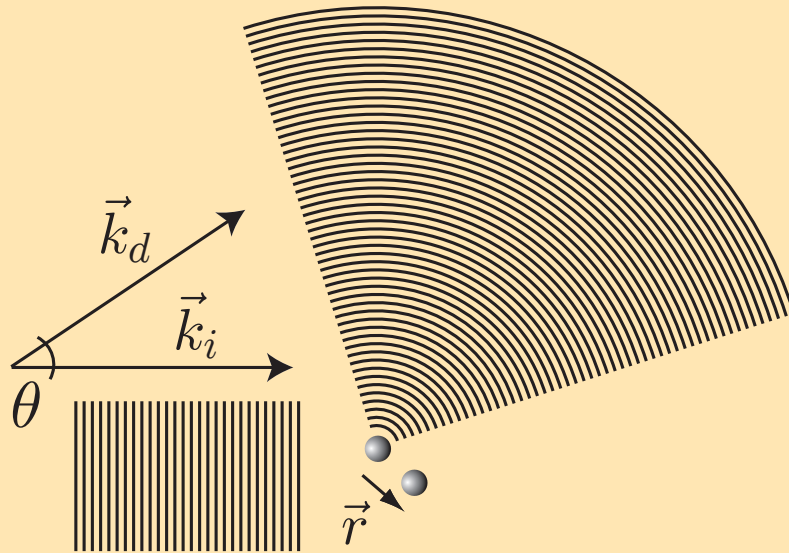
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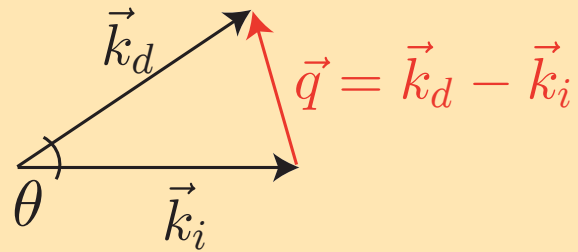
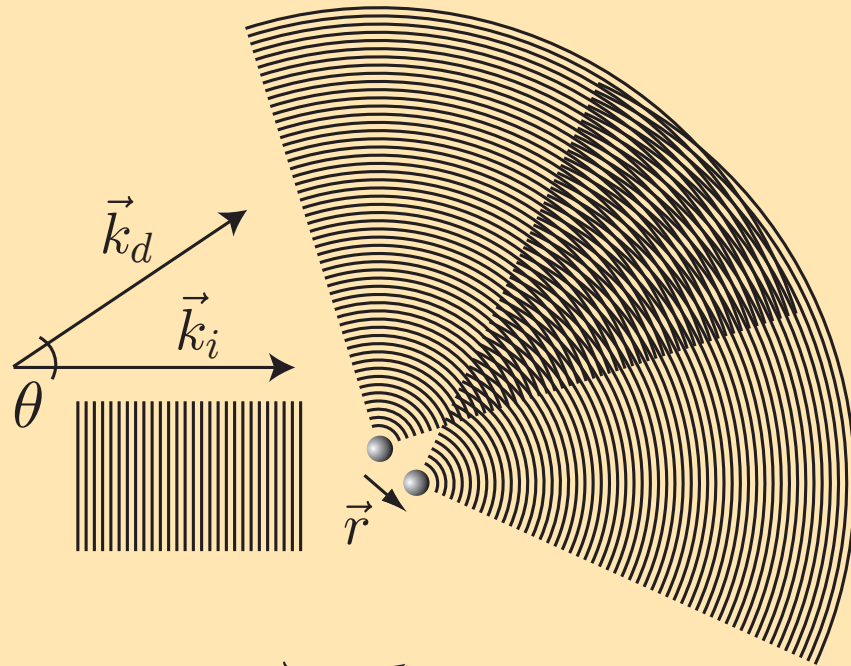
La diffusion est **élastique** : $k_i = k_d$

$$\psi = \psi_0 \frac{b}{D} e^{i(\omega t - kD)}$$

Interférences



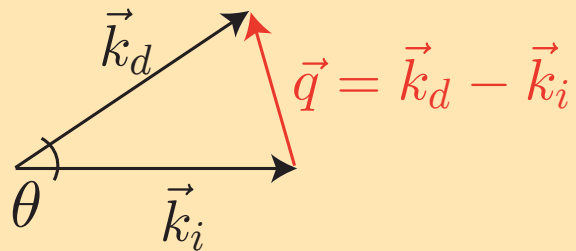
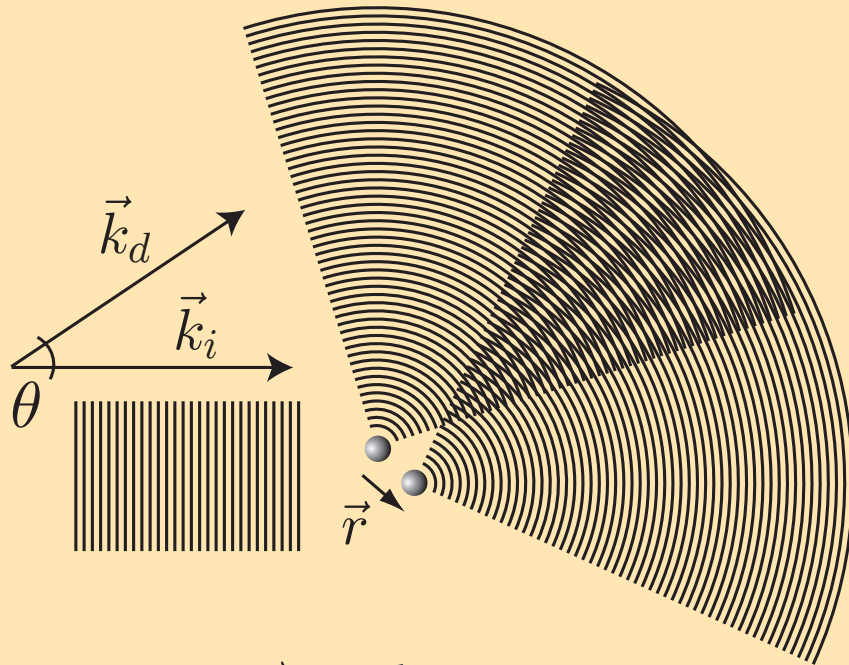
Interférences



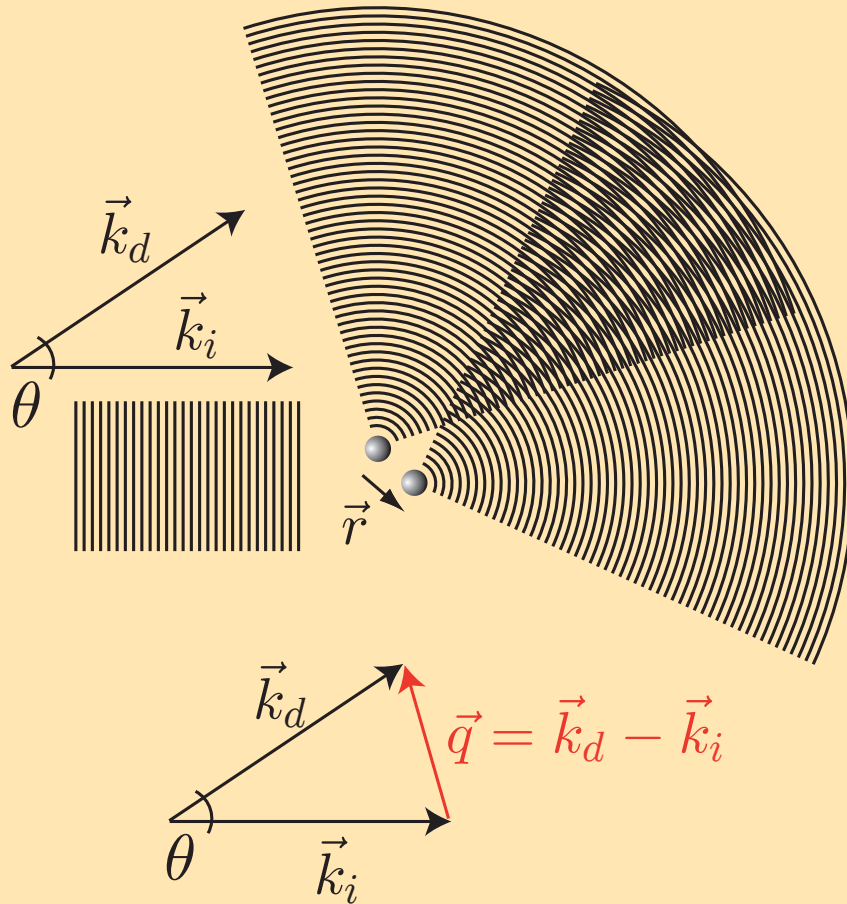
Interférences

Différence de phase :

$$\Delta\phi = \vec{r}(\vec{k}_d - \vec{k}_i)$$



Interférences



Différence de phase :

$$\Delta\phi = \vec{r}(\vec{k}_d - \vec{k}_i)$$

Vecteur de diffusion :

$$q = \frac{4\pi}{\lambda} \sin(\theta/2)$$

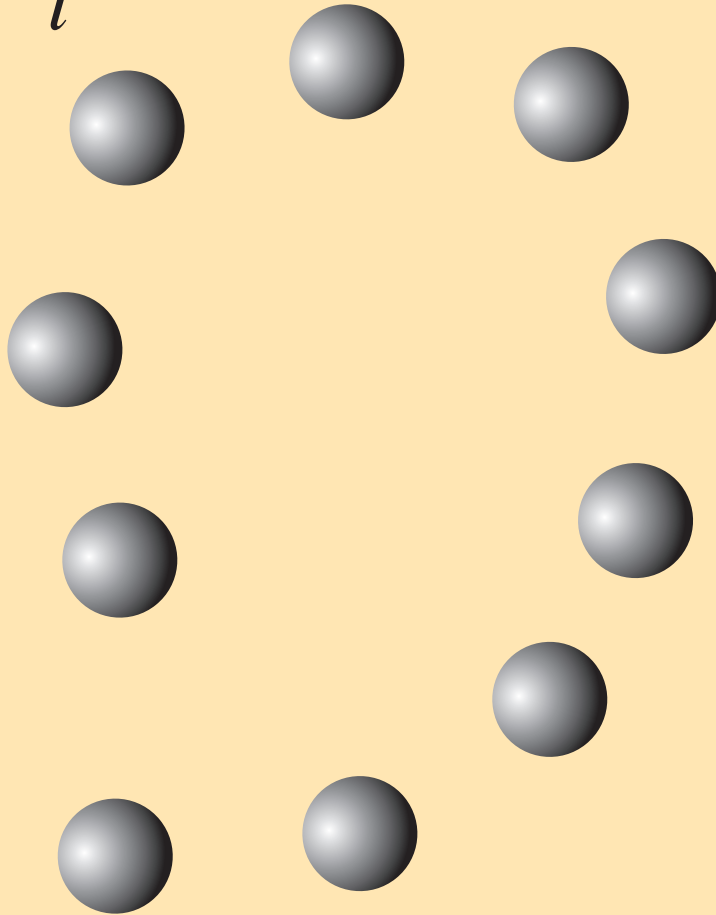
C'est l'inverse d'une longueur qui joue le rôle de l'échelle d'observation.

Si $\psi(0, x, t)$ est l'onde diffusée par une origine, l'onde diffusée par un point situé en \vec{r} est

$$\psi(r, x, t) = \psi(0, x, t) \cdot e^{i(\vec{q} \cdot \vec{r})}$$

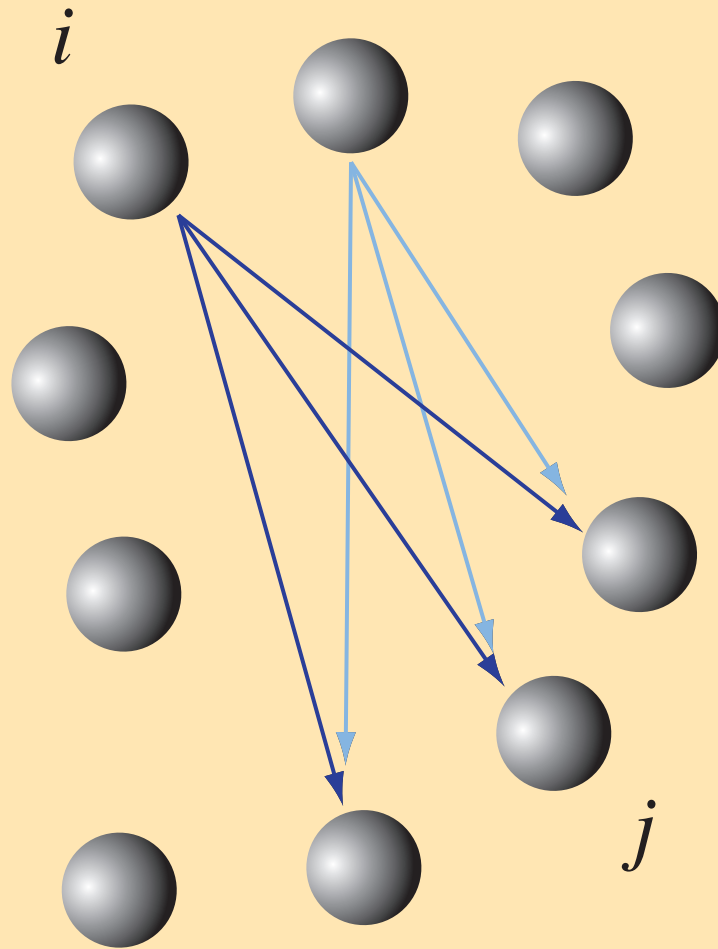
n atomes

i



$$\psi = \frac{\psi_0}{D} \times \sum_{i=1}^n b_i e^{iqr_i}$$

n atomes

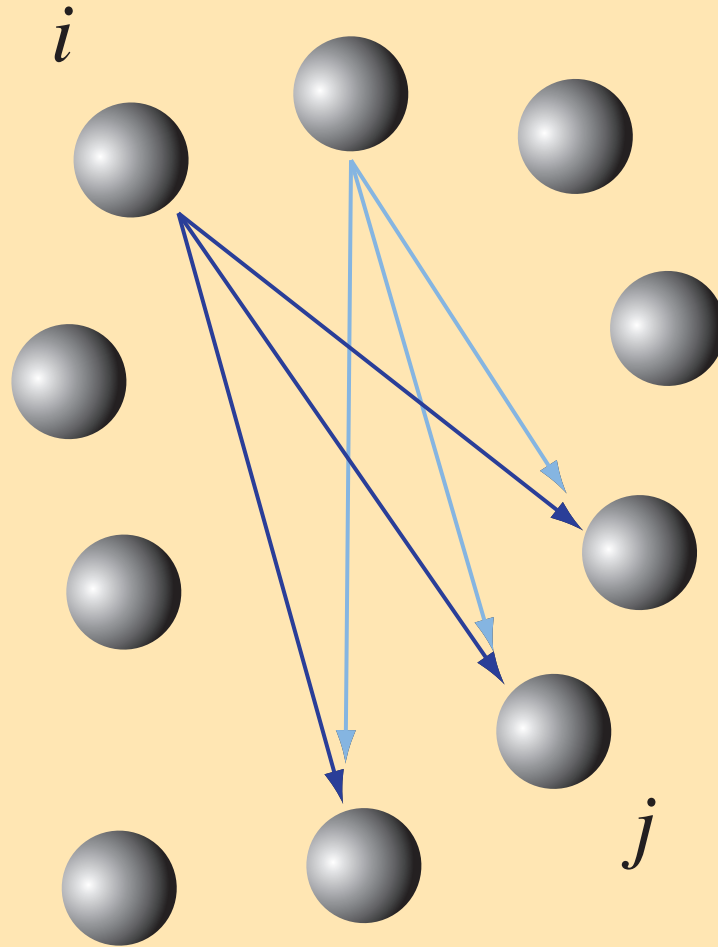


$$\psi = \frac{\psi_0}{D} \times \sum_{i=1}^n b_i e^{iqr_i}$$

Intensité diffusée : $\psi^2 = \psi\psi^*$

$$\begin{aligned} \psi^2 &= \frac{\psi_0^2}{D^2} \times \left[\sum_i^n b_i e^{iqr_i} \times \sum_j^n b_j e^{-iqr_j} \right] \\ &= \frac{\psi_0^2}{D^2} \times \sum_i^n \sum_j^n b_i b_j e^{iq(r_i - r_j)} \end{aligned}$$

n atomes



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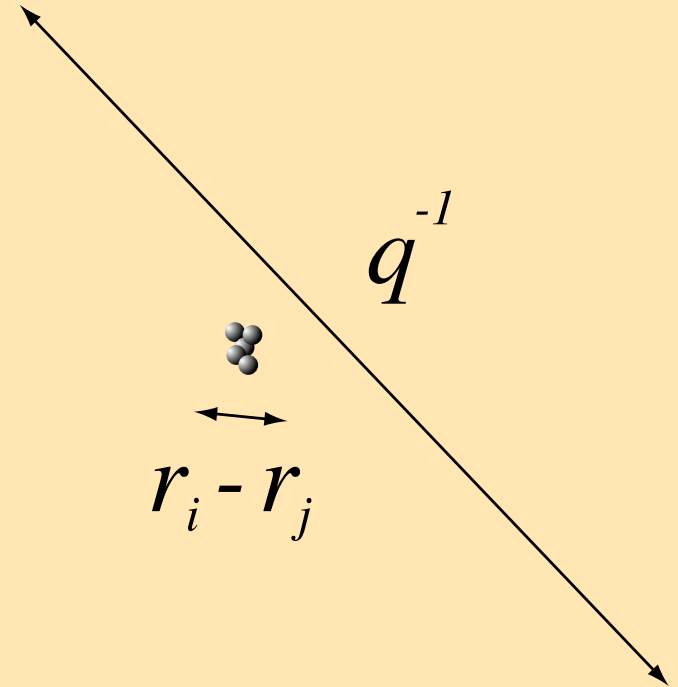
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Section efficace différentielle :

$$\mathcal{S}(q) = \sum_i^n \sum_j^n b_i b_j e^{iq(r_i - r_j)}$$

Diffuseurs élémentaires

$$\begin{aligned}
 \mathcal{S}(q) &= \sum_i^n \sum_j^n b_i b_j e^{iq(r_i - r_j)} \\
 &= \sum_i^n \sum_j^n b_i b_j \\
 &= \sum_i^n b_i \times \sum_j^n b_j
 \end{aligned}$$

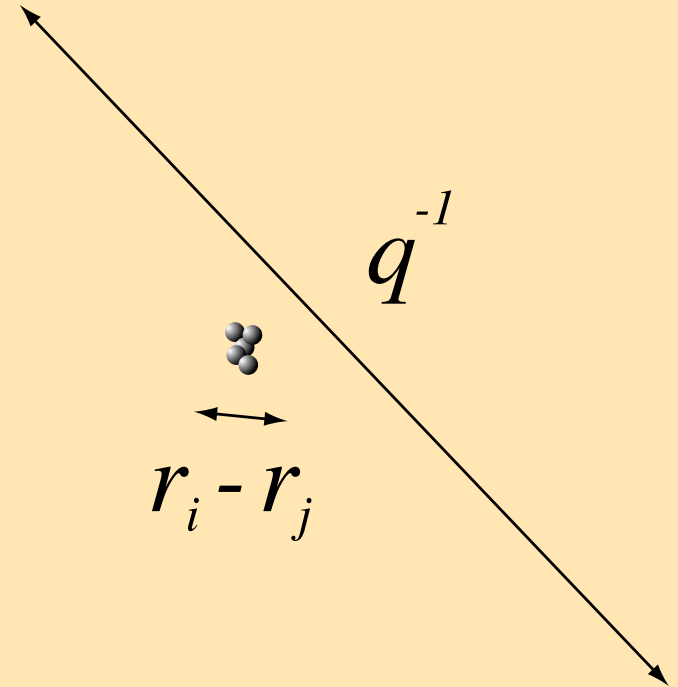


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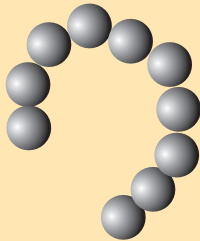
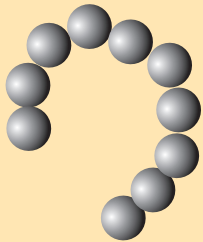
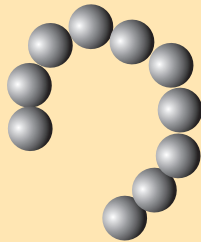
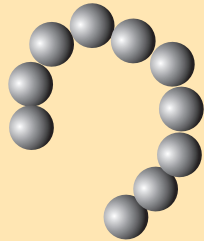
$$\sigma_{\text{dif.}\text{élem.}} = \left(\sum_i^n b_i \right)^2$$

$$\text{Ex : } C_l O_m N_n H_p \rightarrow b = \underbrace{lb_C + mb_O + nb_N + pb_H}_{\text{grandeurs tabulées}}$$



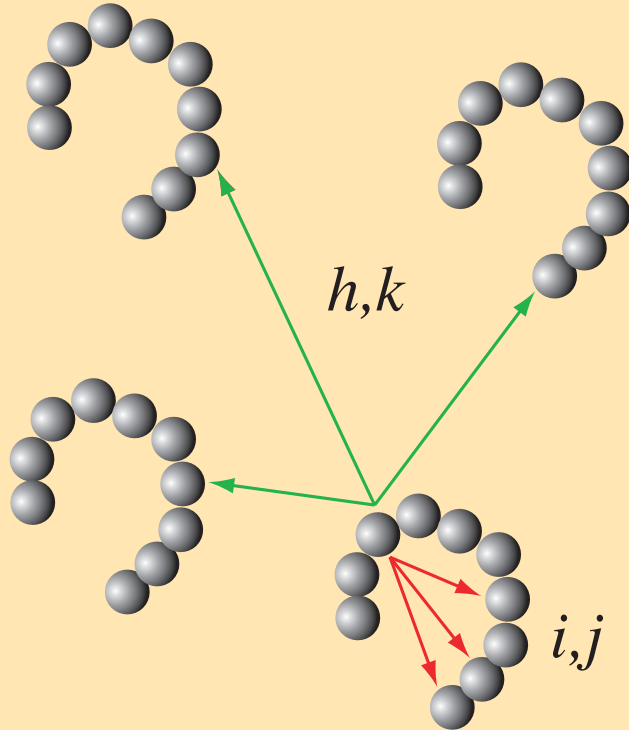
n macromolécules de N diffuseurs

$$\mathcal{S}(q) = \sum_i^{\mathcal{N}} \sum_j^{\mathcal{N}} b_i b_j e^{iq(r_i - r_j)} = b^2 \sum_h^n \sum_k^n \sum_i^N \sum_j^N e^{iq(r_{h,i} - r_{k,j})}$$



n macromolécules de N diffuseurs

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$$\mathcal{S}(q)/b^2 = nN^2 P(q) + n^2 N^2 Q(q)$$

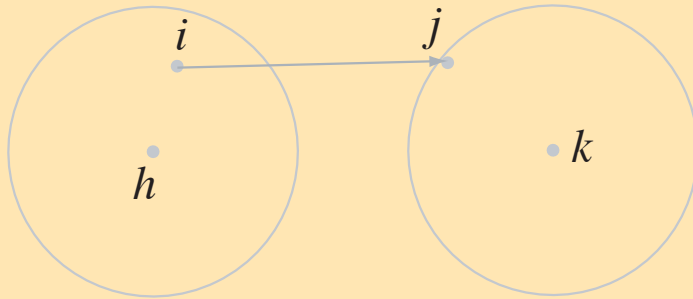
$$Q(q) = \frac{1}{N^2} \sum_{i_h}^N \sum_{j_k}^N e^{iq(r_{i_h} - r_{j_k})}$$

$$P(q) = \frac{1}{N^2} \sum_{i_h}^N \sum_{j_h}^N e^{iq(r_{i_h} - r_{j_h})}$$

facteur de forme

Molécules à symétrie sphérique

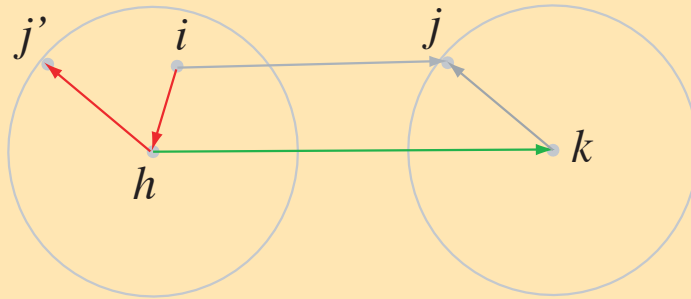
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Molécules à symétrie sphérique

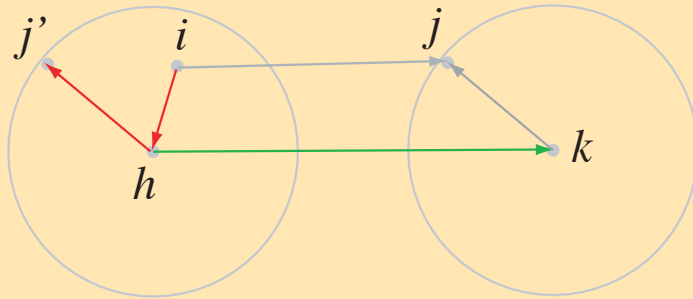
$$\vec{kj} = \vec{hj'} \rightarrow \vec{ij} = \vec{ij'} + \vec{hk}$$

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Molécules à symétrie sphérique

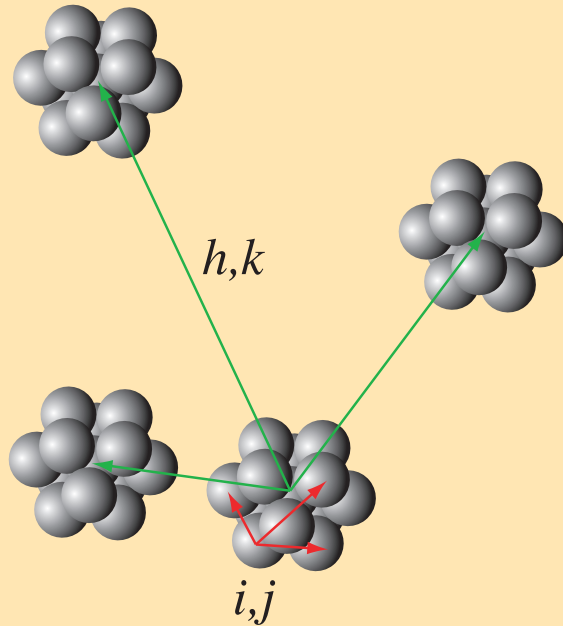
$$\vec{kj} = \vec{hj'} \rightarrow \vec{ij} = \vec{ij'} + \vec{hk}$$



$$\begin{aligned} \mathcal{S}(q)/b^2 &= nN^2P(q) + n^2N^2Q(q) \\ &= nN^2 \times P(q) \times S(q) \end{aligned}$$

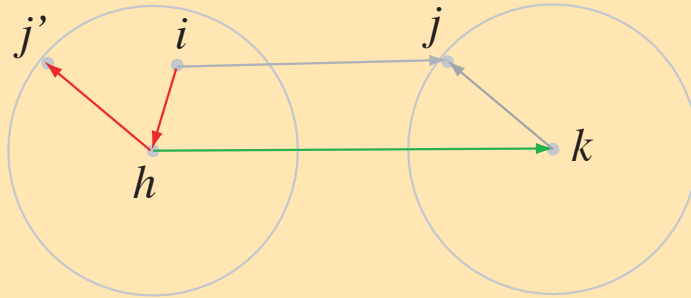
$$S(q) = \frac{1}{n} \sum_h^n \sum_k^n e^{iq\vec{hk}}$$

facteur de structure



Molécules à symétrie sphérique

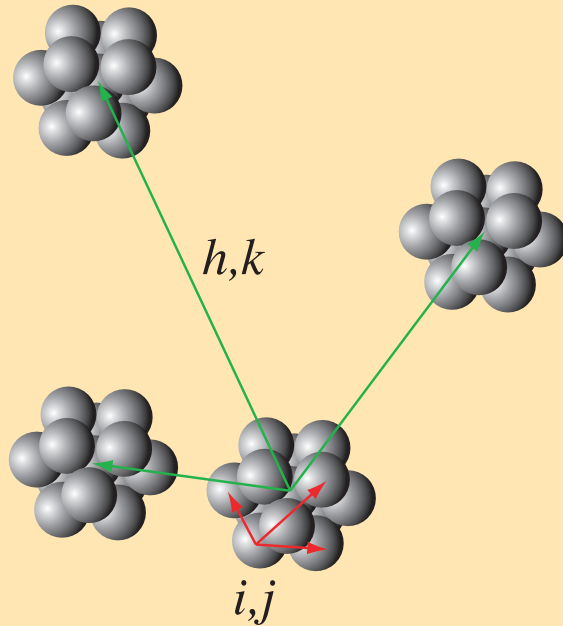
$$\vec{kj} = \vec{hj'} \rightarrow \vec{ij} = \vec{ij'} + \vec{hk}$$



$$\begin{aligned}\mathcal{S}(q)/b^2 &= nN^2P(q) + n^2N^2Q(q) \\ &= nN^2 \times \textcolor{red}{P}(q) \times \textcolor{green}{S}(q)\end{aligned}$$

$$\textcolor{green}{S}(q) = \frac{1}{n} \sum_h^n \sum_k^n e^{iq\vec{h}\vec{k}}$$

facteur de structure

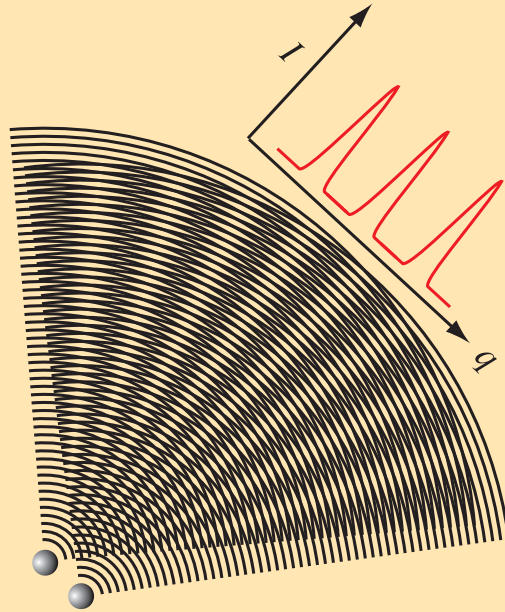


$$\begin{aligned}S(q \rightarrow \infty) &= 1 \\ \left. \frac{\mathcal{S}(q)}{b^2 \times nN^2} \right]_{qR \gg 1} &= \textcolor{red}{P}(q)\end{aligned}$$

$$P(q \rightarrow 0) = 1$$

$\mathcal{S}(q \rightarrow 0) = (bN)^2 \times n\textcolor{green}{S}(q)$
 n objets ponctuels de longueur
 de diffusion bN

Milieu homogène, diffusion et diffraction

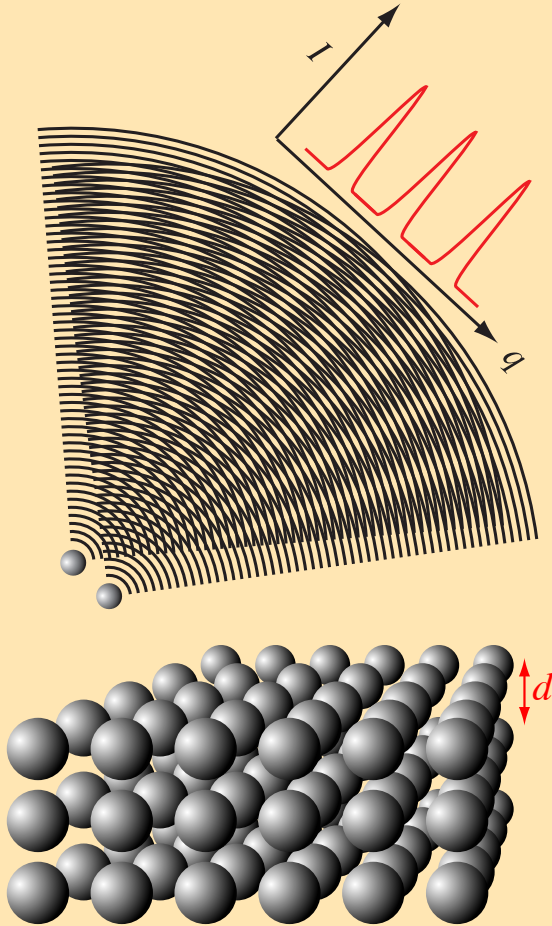


Milieu homogène, diffusion et diffraction

Milieu homogène : $\rho = b/v = Cst$

densité de longueur de diffusion

Cristal : $\vec{q}^* \cdot \vec{d}_{ij} = n2\pi$



Milieu homogène, diffusion et diffraction

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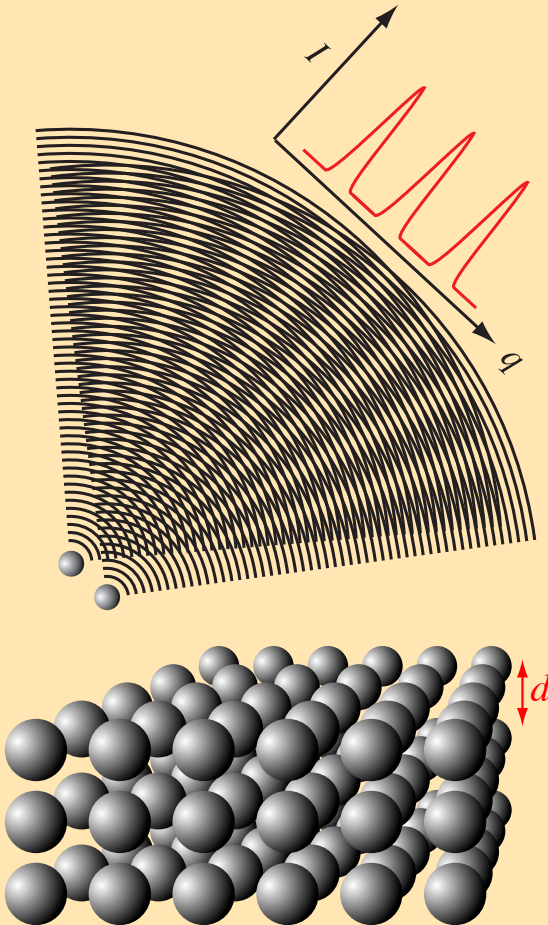
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Si pour $q^* L = n2\pi \rightarrow$ phase

Alors $(q^* + \Delta q)L = (n + \frac{1}{2}) 2\pi \rightarrow$ opposition

$$\Delta q = \pi/L$$



Milieu homogène, diffusion et diffraction

Milieu homogène : $\rho = b/v = Cst$

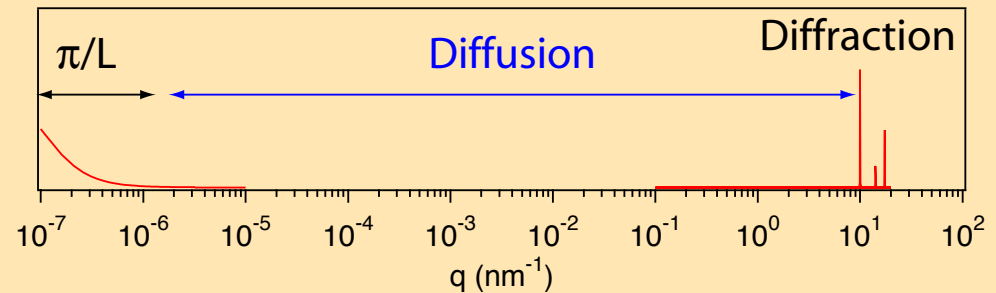
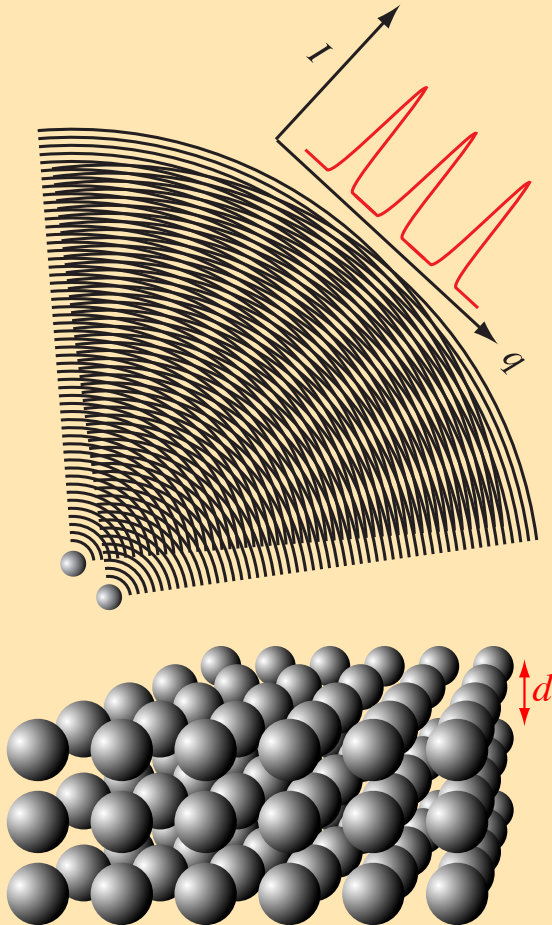
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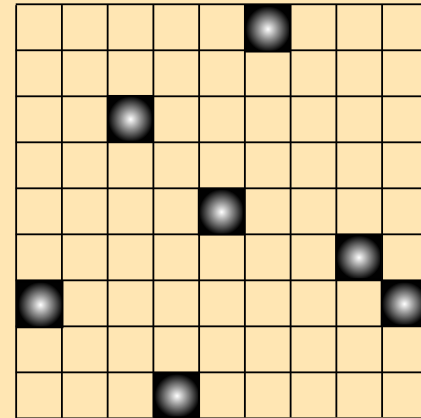
$$\Delta q = \pi/L$$



Un milieu homogène ne diffuse pas

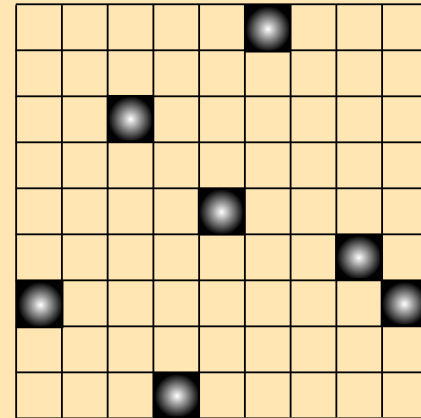
Diffusion et fluctuations

$$\begin{aligned}\mathcal{S}(q) &= \left\langle \sum_i^{V/v} \sum_j^{V/v} b_i b_j e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \right\rangle \\ &= \sum_i^{V/v} \sum_j^{V/v} \langle b_i b_j \rangle \times e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}\end{aligned}$$



Diffusion et fluctuations

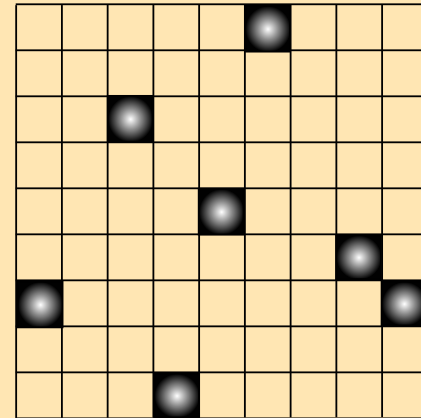
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$$\left. \begin{aligned}\langle b \rangle &= \langle b \rangle \\ \Delta b_i &= b_i - \langle b \rangle \\ \langle \Delta b_i \rangle &= 0 \\ \langle b_i b_j \rangle &= \langle (\Delta b_i + \langle b \rangle) \cdot (\Delta b_j + \langle b \rangle) \rangle\end{aligned} \right\} \Rightarrow \langle b_i b_j \rangle = \langle \Delta b_i \Delta b_j \rangle + \langle b \rangle^2$$

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$$\mathcal{S}(q) = \sum_i^{V/v} \sum_j^{V/v} \langle \Delta b_i \Delta b_j \rangle e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

Seul les fluctuations, spatiales ou temporelles, de longueur de diffusion contribuent à l'intensité diffusée.

Diffusion et fluctuations (suite)

$$\mathcal{S}(q) = \sum_i^{V/v} \sum_j^{V/v} \langle \Delta b_i \Delta b_j \rangle e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

$$\langle \Delta b_i \Delta b_j \rangle / b^2 = \langle \Delta x_i \Delta x_j \rangle$$

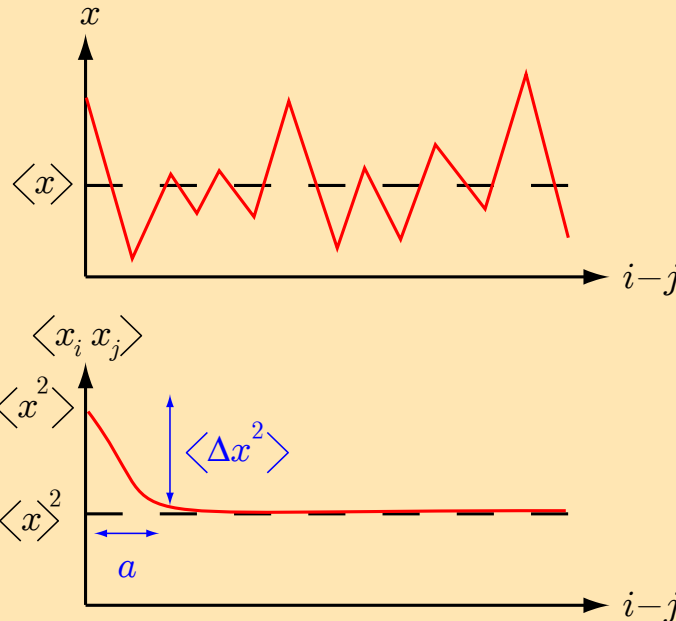
fonction de corrélation de paire

Diffusion et fluctuations (suite)

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fonction de corrélation de paire



$$\langle \Delta x_i \Delta x_j \rangle = 0 \text{ sauf pour } i = j$$

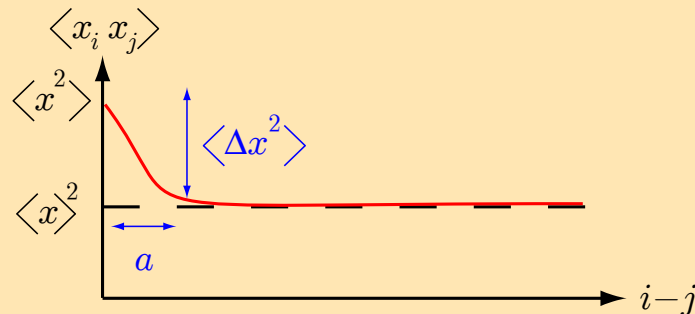
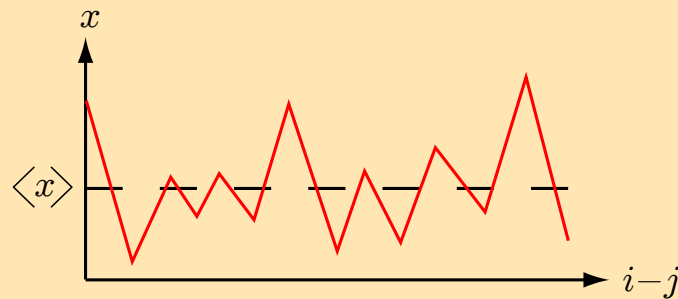
$$\mathcal{S}(q) = b^2 \frac{V}{v} \langle \Delta x^2 \rangle$$

Diffusion et fluctuations (suite)

$$\mathcal{S}(q) = \sum_i^{V/v} \sum_j^{V/v} \langle \Delta b_i \Delta b_j \rangle e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

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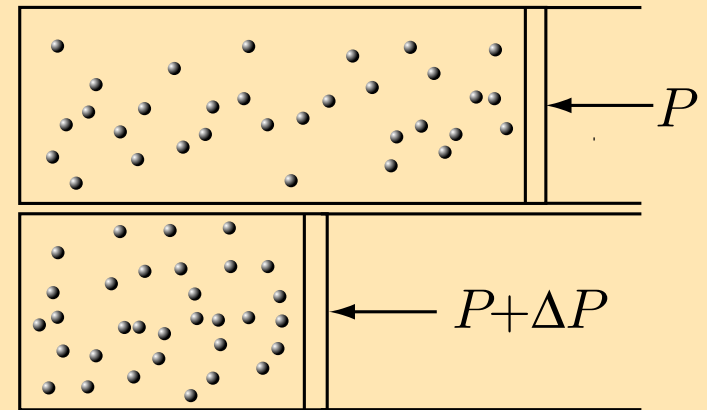
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$$\langle \Delta x_i \Delta x_j \rangle = 0 \text{ sauf pour } i = j$$

$$\mathcal{S}(q) = b^2 \frac{V}{v} \langle \Delta x^2 \rangle$$

$$\kappa_T = \left[\frac{1}{V} \cdot \frac{dP}{d(1/V)} \right]^{-1} = \frac{v}{kT} \frac{\langle \Delta x^2 \rangle}{\langle x \rangle^2}$$



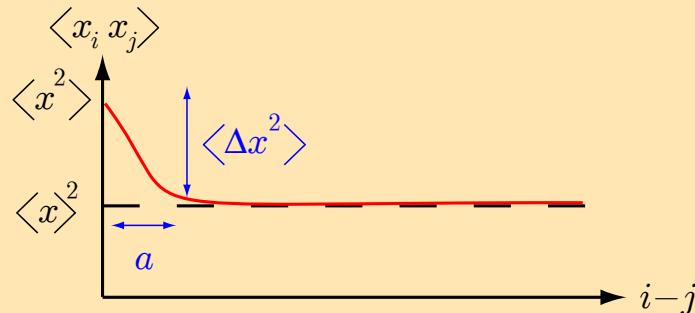
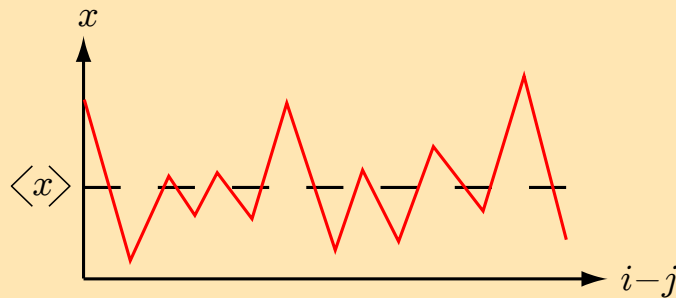
$$\frac{\mathcal{S}(q \rightarrow 0)}{V} = b^2 \left(\frac{n}{V} \right)^2 kT \kappa_T$$

Diffusion et fluctuations (suite)

$$\mathcal{S}(q) = \sum_i^{V/v} \sum_j^{V/v} \langle \Delta b_i \Delta b_j \rangle e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

$$\langle \Delta b_i \Delta b_j \rangle / b^2 = \langle \Delta x_i \Delta x_j \rangle$$

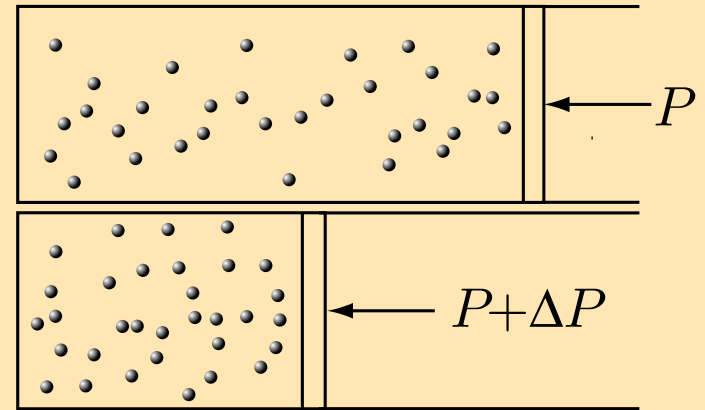
fonction de corrélation de paire



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$$\frac{\mathcal{S}(q \rightarrow 0)}{V} = b^2 \left(\frac{n}{V} \right)^2 kT \kappa_T$$

Gaz parfait : $P = kT / \text{molécule}$

$$\Rightarrow \left[\frac{\mathcal{S}(q \rightarrow 0)/V}{n/V} \right]_{n/V \rightarrow 0} = b^2$$

Solvant-soluté : notion de contraste

$$\langle \rho \rangle = \rho x + \rho_0 x_0$$

$$\Delta \rho_i = (\rho x_i + \rho_0 x_{0i}) - \langle \rho \rangle$$

$$= \rho \Delta x_i + \rho_0 \Delta x_{0i}$$

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$$= \rho \Delta x_i + \rho_0 \Delta x_{0i}$$

Incompressible : $\Delta x_{0i} = -\Delta x_i$

$$\Delta \rho_i = (\rho - \rho_0) \Delta x_i$$

\Downarrow

$$\langle \Delta \rho_i \Delta \rho_j \rangle = (\rho - \rho_0)^2 \langle \Delta x_i \Delta x_j \rangle$$

$$= (\rho - \rho_0)^2 \langle \Delta x_{0i} \Delta x_{0j} \rangle$$

Solvant-soluté : notion de contraste

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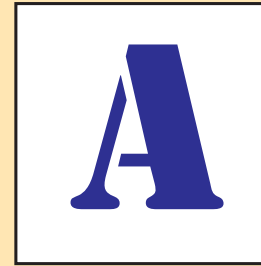
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$$\Delta \rho_i = (\rho - \rho_0) \Delta x_i$$

\Downarrow

$$\langle \Delta \rho_i \Delta \rho_j \rangle = (\rho - \rho_0)^2 \langle \Delta x_i \Delta x_j \rangle$$

$$= (\rho - \rho_0)^2 \langle \Delta x_{0i} \Delta x_{0j} \rangle$$



$$v^2 \rho^2 \mathcal{S}_{\text{soluté}}(q)$$



$$v^2 \rho_0^2 \mathcal{S}_{\text{soluté}}(q)$$



$$v^2 (\rho - \rho_0)^2 \mathcal{S}_{\text{soluté}}(q)$$

$$\mathcal{S}(q) = v^2 (\rho - \rho_0)^2 \mathcal{S}_{\text{soluté}}(q)$$

$$v^2 (\rho - \rho_0)^2 = (b - b_0 v / v_0)^2$$

contraste soluté/solvant

Macromolécules en solution, limite $q \rightarrow 0$

Compressibilité osmotique : $(Cd\pi/dC)^{-1}$, $C = nM/V$

$$\frac{\mathcal{S}(q \rightarrow 0)}{V} = (b - b_0 v/v_0)^2 \left(\frac{C}{M} \right)^2 kT \left(C \frac{d\pi}{dC} \right)^{-1}$$

Solution idéale :

$$\pi = kT/\text{molécule} \quad \left[\frac{\mathcal{S}(q \rightarrow 0)/V}{C} \right]_{C \rightarrow 0} = \left(\frac{b - b_0 v/v_0}{M} \right)^2 M$$

Macromolécules en solution, limite $q \rightarrow 0$

Compressibilité osmotique : $(Cd\pi/dC)^{-1}$, $C = nM/V$

$$\frac{\mathcal{S}(q \rightarrow 0)}{V} = (b - b_0 v/v_0)^2 \left(\frac{C}{M} \right)^2 kT \left(C \frac{d\pi}{dC} \right)^{-1}$$

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$$\left[\frac{\mathcal{S}(q \rightarrow 0)/V}{C} \right]_{C \rightarrow 0} = \left(\frac{b - b_0 v/v_0}{M} \right)^2 M$$

$$\left. \begin{array}{l} M = Nm_1 \\ v = Nv_1 \\ b = Nb_1 \end{array} \right\} \Rightarrow \left[\frac{\mathcal{S}(q \rightarrow 0)/V}{C} \right]_{C \rightarrow 0} = \underbrace{K^2}_{\left(\frac{b_1 - b_0 v_1/v_0}{m_1} \right)^2} \times M$$

Macromolécules en solution, limite $q \rightarrow 0$

Compressibilité osmotique : $(Cd\pi/dC)^{-1}$, $C = nM/V$

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Développement du viriel : $\pi = \pi_{C \rightarrow 0}(1 + MA_2C + \dots)$

$$\frac{\mathcal{S}(q \rightarrow 0)/V}{C} = \left[\frac{\mathcal{S}(q \rightarrow 0)/V}{C} \right]_{C \rightarrow 0} (1 - 2MA_2C + \dots)$$

Ex 1 : Compressibilité de la myoglobine

C. Loupiac et al. (2002), *Eur. J. Biochem.*, 269 : 4731-4737

(PACE, LLB, Saclay)

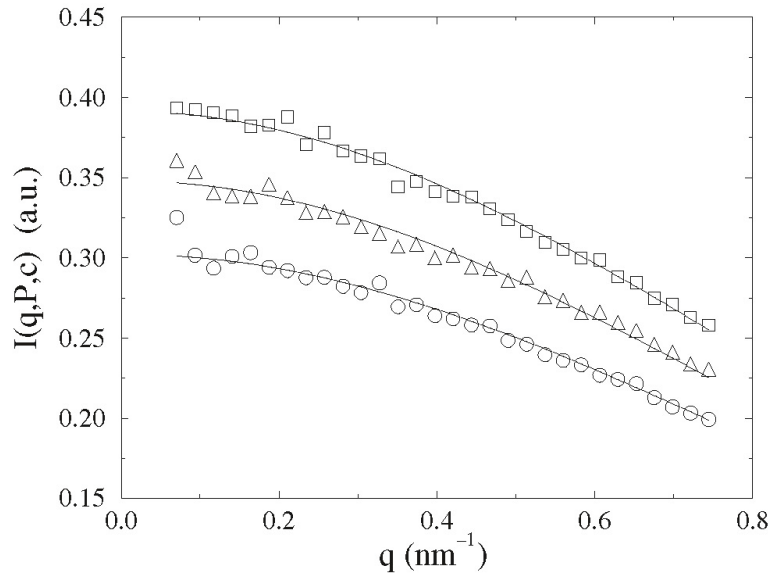


Fig. 1. Scattering spectra $I(q, P, c)$ of MbN_3 at p^2H 6.6, as a function of the wave-number transfer q . The measurements were performed at room temperature. The protein concentration, c , at atmospheric pressure is $11.7 \text{ mg}\cdot\text{cm}^{-3}$ and the pressures, P , are: 54 (○), 154 (△), and 302 (□) MPa. Fits of Eqn 6 to the data are shown as full lines.

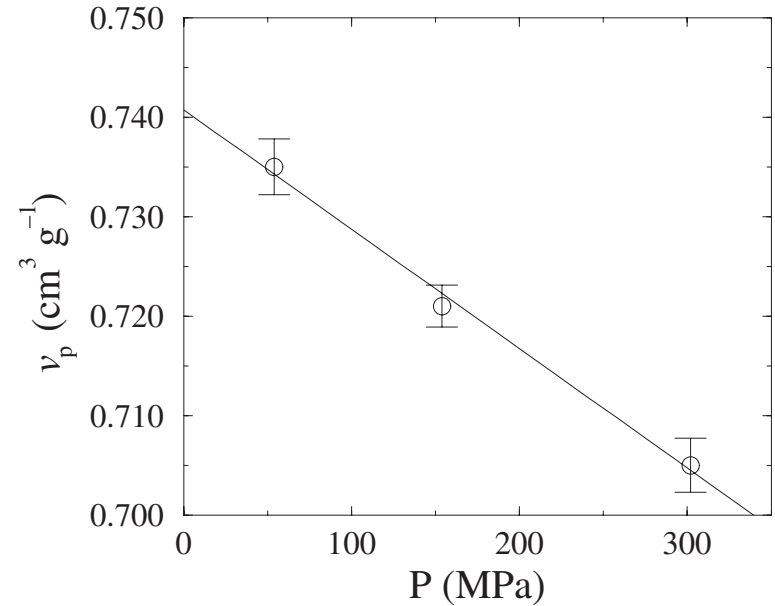


Fig. 7. Partial specific volume $v_p(P)$, of MbN_3 as a function of pressure, P . The almost linear variation of $v_p(P)$ with P allows the isothermal compressibility of the hydrated protein to be computed: $\kappa_{T,p} = (1.6 \pm 0.1) \cdot 10^{-4} \text{ MPa}^{-1}$.

$$\left[\frac{\mathcal{S}(q \rightarrow 0)/V}{C(P)} \right]_{C \rightarrow 0} = \left(\frac{b}{M} - \rho_0(P)v'(P) \right)^2 M$$

Ex 2 : Interactions et cristallisation des protéines

$$P(q \rightarrow 0) = 1 - \frac{\mathcal{L}(q \rightarrow 0)/V}{C} = K^2 M (1 - 2MA_2C + \dots)$$

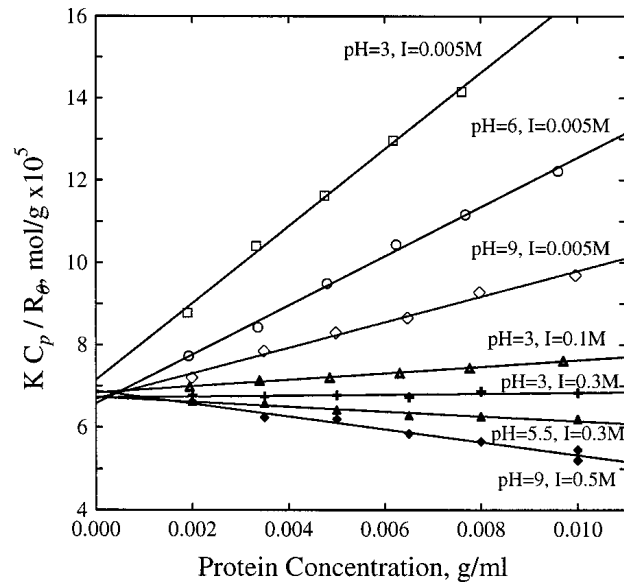


FIGURE 1 Typical plots of lysozyme SLS data according to Eq. 7. The variation of the virial coefficient (given by the slope of the lines) with pH and electrolyte concentration is evident.

Ex 2 : Interactions et cristallisation des protéines

$$P(q \rightarrow 0) = 1 \quad \frac{\mathcal{L}(q \rightarrow 0)/V}{C} = K^2 M (1 - 2MA_2C + \dots)$$

$$S(q \rightarrow \infty) = 1 \quad \frac{\mathcal{L}(q \rightarrow 0)/V}{C} = K^2 MP(q)$$

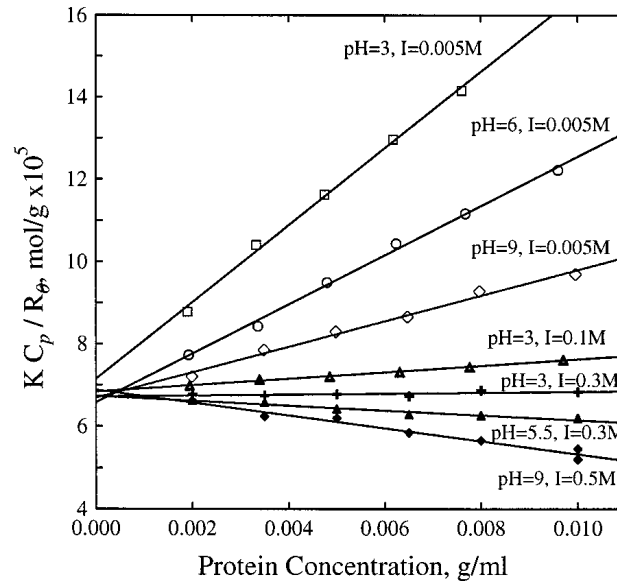


FIGURE 1 Typical plots of lysozyme SLS data according to Eq. 7. The variation of the virial coefficient (given by the slope of the lines) with pH and electrolyte concentration is evident.

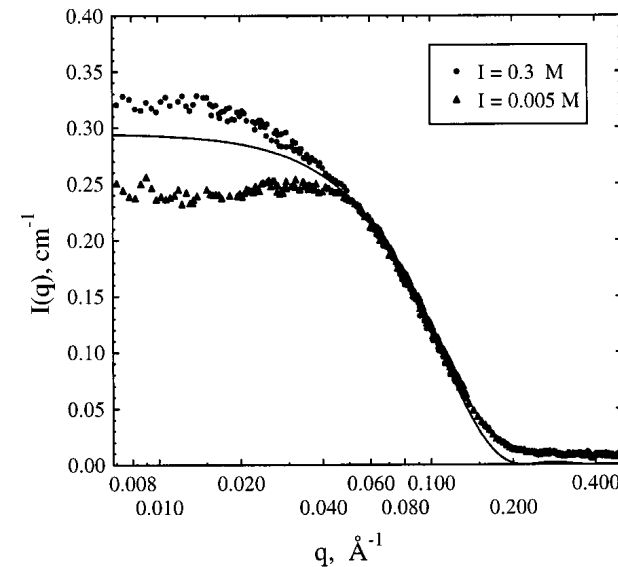


FIGURE 7 Intensity I versus scattering vector q for SANS measurements on chymotrypsinogen at pH 3 and two different electrolyte concentrations. The solid curve is the form factor function fitted by approximating the protein shape by a sphere. Positive deviations from this curve in the low q region indicate attractive interactions and negative deviations indicate repulsions.

Facteur de forme

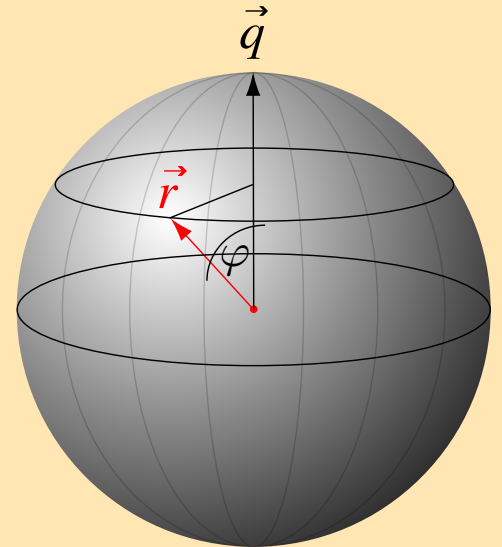
Objets ayant des orientations aléatoires

$$\langle e^{i\vec{q} \cdot \vec{r}} \rangle_{\text{orientations}} = \langle \cos(\vec{q} \cdot \vec{r}) \rangle$$

Facteur de forme

Objets ayant des orientations aléatoires

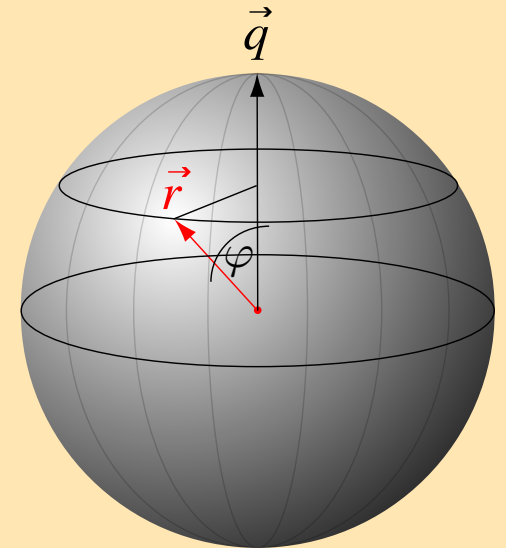
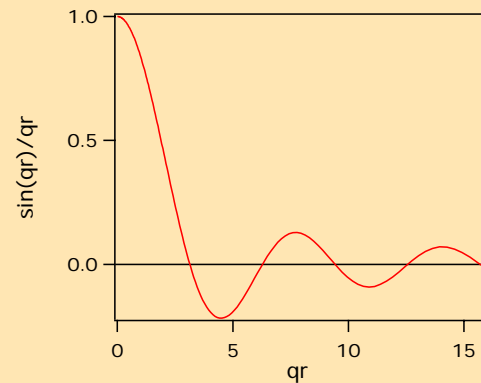
$$\begin{aligned}\langle e^{i\vec{q} \cdot \vec{r}} \rangle_{\text{orientations}} &= \langle \cos(\vec{q} \cdot \vec{r}) \rangle \\ &= \frac{1}{2} \int_0^\pi \cos(qr \cos(\varphi)) \sin(\varphi) d\varphi\end{aligned}$$



Facteur de forme

Objets ayant des orientations aléatoires

$$\begin{aligned}
 \langle e^{i\vec{q} \cdot \vec{r}} \rangle_{\text{orientations}} &= \langle \cos(\vec{q} \cdot \vec{r}) \rangle \\
 &= \frac{1}{2} \int_0^\pi \cos(qr \cos(\varphi)) \sin(\varphi) d\varphi \\
 &= \frac{\sin(qr)}{qr} = j_0(qr)
 \end{aligned}$$



$$P(q) = \frac{1}{N^2} \sum_i^N \sum_j^N \langle e^{i\vec{q} \cdot \vec{r}_{ij}} \rangle = \frac{1}{N^2} \sum_i^N \sum_j^N \frac{\sin(qr_{ij})}{qr_{ij}}$$

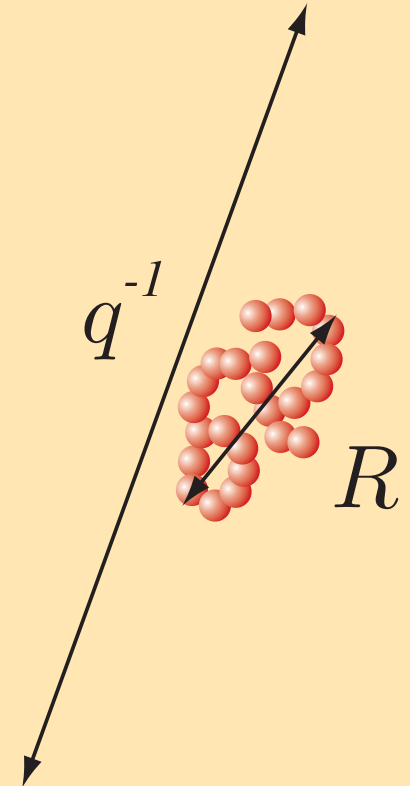
Petits vecteurs de diffusion

$$\frac{\sin(qr)}{qr} = 1 - \frac{(qr)^2}{6} + \dots$$

$$P_{\text{Guinier}}(q) = 1 - \frac{q^2}{3} \underbrace{\left[\frac{1}{2N^2} \sum_i^N \sum_j^N r_{ij}^2 \right]}_{R_g^2} + \dots$$

$$= 1 - \frac{q^2 R_g^2}{3} + \dots$$

$$\approx e^{-q^2 R_g^2/3}$$



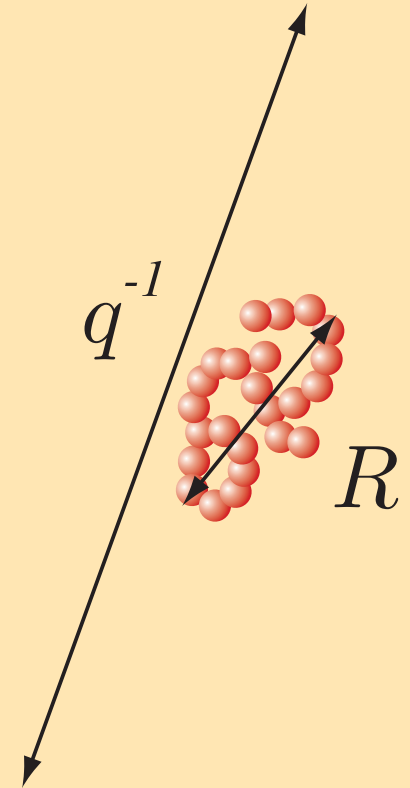
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$$\approx e^{-q^2 R_g^2/3}$$



Rayon de giration : $R_g^2 = \frac{1}{N} \sum_i^N r_i^2 = \langle r_i^2 \rangle$

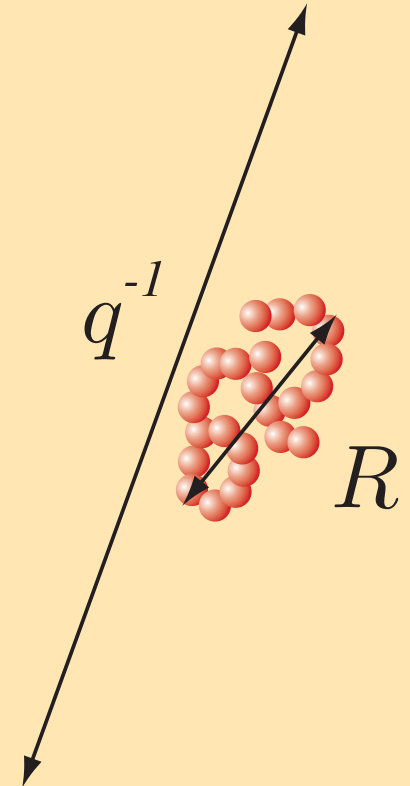
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Rayon de giration : $R_g^2 = \frac{1}{N} \sum_i^N r_i^2 = \langle r_i^2 \rangle$

Boule : $R_g^2 = \left[\int_0^R 4\pi r^2 \times r^2 \times dr \right] / \frac{4}{3}\pi R^3 = \frac{3}{5} R^2$

Bâton : $R_g^2 = L^2/12$

Exemples de formes analytiques : sphères...

Ne dépend pas de l'orientation :

$$P(q) = \frac{1}{N^2} \sum_i^N \sum_j^N e^{i\vec{q} \cdot \vec{r}_{ij}} = \left[\frac{1}{N} \sum_i^N e^{i\vec{q} \cdot \vec{r}_i} \right]^2$$

Exemples de formes analytiques : sphères...

Ne dépend pas de l'orientation :

$$\begin{aligned} P(q) &= \frac{1}{N^2} \sum_i^N \sum_j^N e^{i\vec{q} \cdot \vec{r}_{ij}} = \left[\frac{1}{N} \sum_i^N e^{i\vec{q} \cdot \vec{r}_i} \right]^2 \\ &= \left[\frac{1}{V} \int_0^R j_0(qr) \rho(r) 4\pi r^2 dr \right]^2 \end{aligned}$$

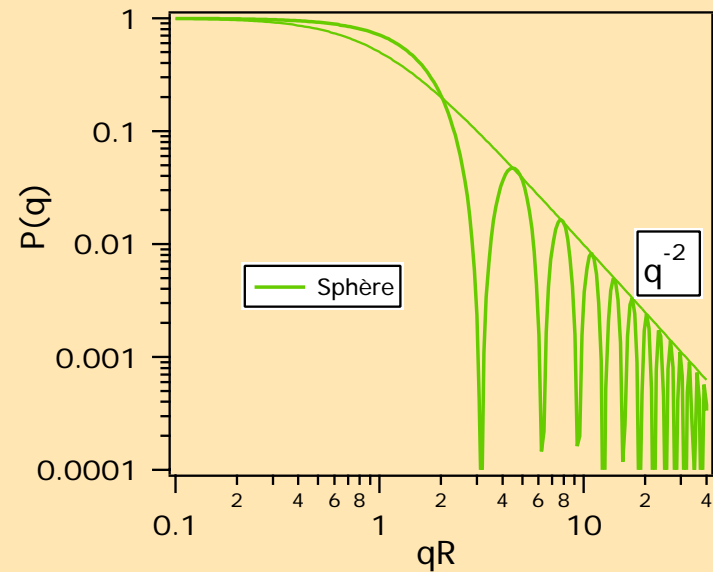
Exemples de formes analytiques : sphères...

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$$P_{\text{sphère}} = \left[\frac{\sin(qR)}{qR} \right]^2 = [j_0(qR)]^2$$



Exemples de formes analytiques : sphères...

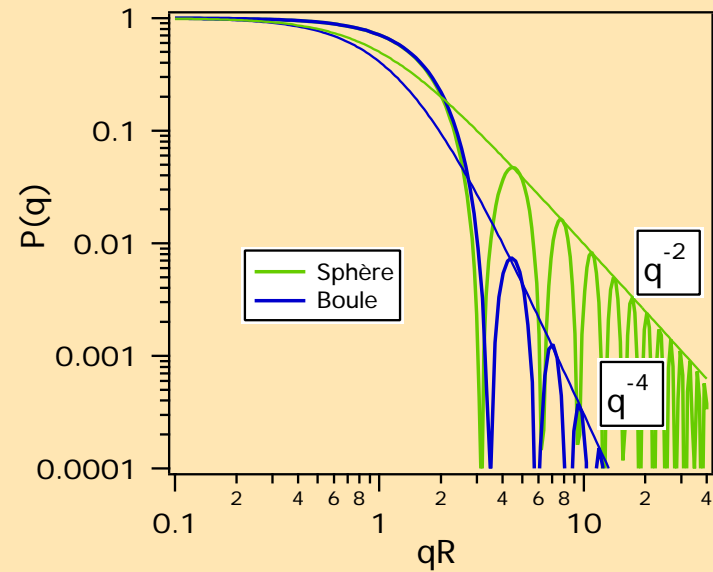
Ne dépend pas de l'orientation :

$$P(q) = \frac{1}{N^2} \sum_i^N \sum_j^N e^{i\vec{q} \cdot \vec{r}_{ij}} = \left[\frac{1}{N} \sum_i^N e^{i\vec{q} \cdot \vec{r}_i} \right]^2$$

$$= \left[\frac{1}{V} \int_0^R j_0(qr) \rho(r) 4\pi r^2 dr \right]^2$$

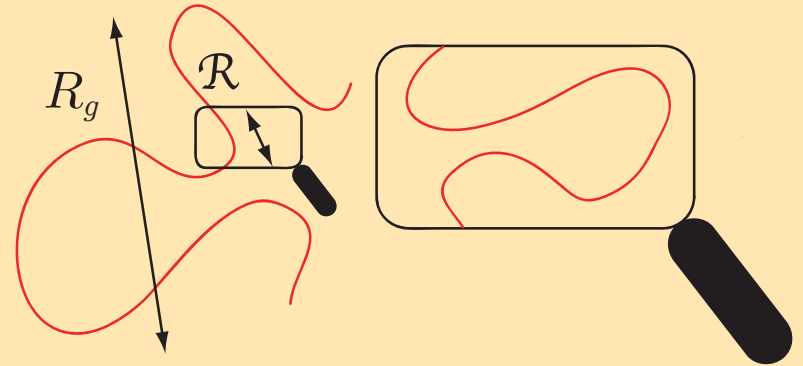
$$P_{\text{sphère}} = \left[\frac{\sin(qR)}{qR} \right]^2 = [j_0(qR)]^2$$

$$P_{\text{boule}}(q) = \left[\frac{3j_1(qR)}{qR} \right]^2$$



Vecteurs de diffusion intermédiaires : loi d'échelle

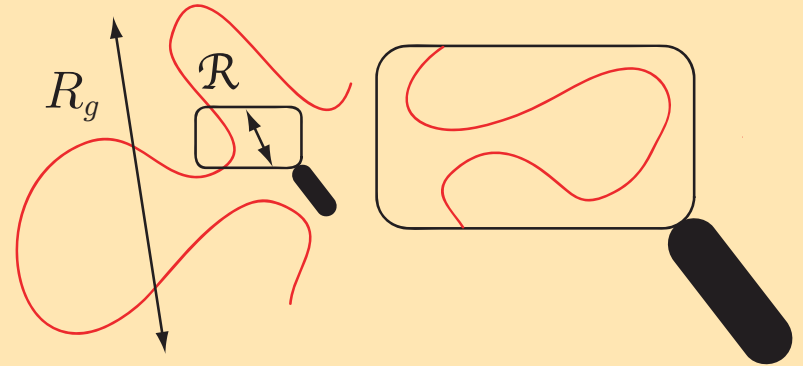
Fractales : $M = m_1 \left(\frac{R}{a} \right)^{\mathcal{D}}$



Vecteurs de diffusion intermédiaires : loi d'échelle

Fractales : $M = m_1 \left(\frac{R}{a} \right)^{\mathcal{D}}$

$$m \left(\frac{R_g}{\mathcal{R}} \right) = M \cdot \begin{cases} f \left(\frac{R_g}{\mathcal{R}} \right) \\ f(x < 1) = 1 \\ f(x \geq 1) = x^{-\alpha} \end{cases}$$



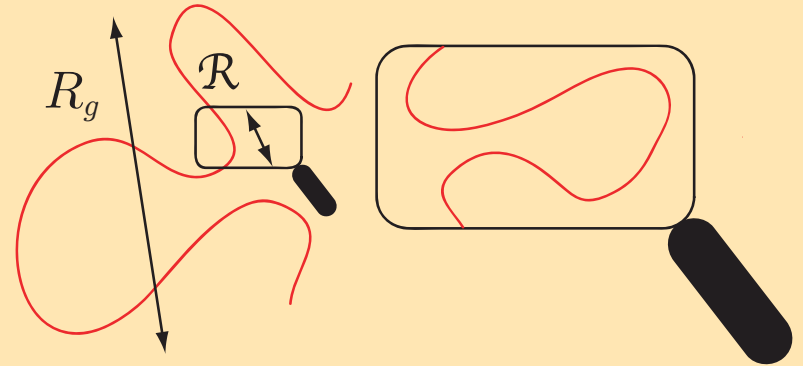
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$$f(x < 1) = 1$$

$$f(x \geq 1) = x^{-\alpha}$$



1. Une seule longueur est pertinente.
 2. A fort grossissement, la mesure est insensible à M .
- $\left| \Rightarrow \alpha = \mathcal{D} \right.$

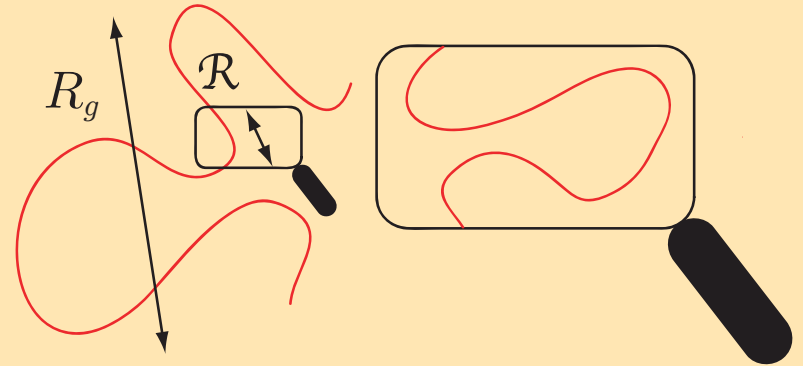
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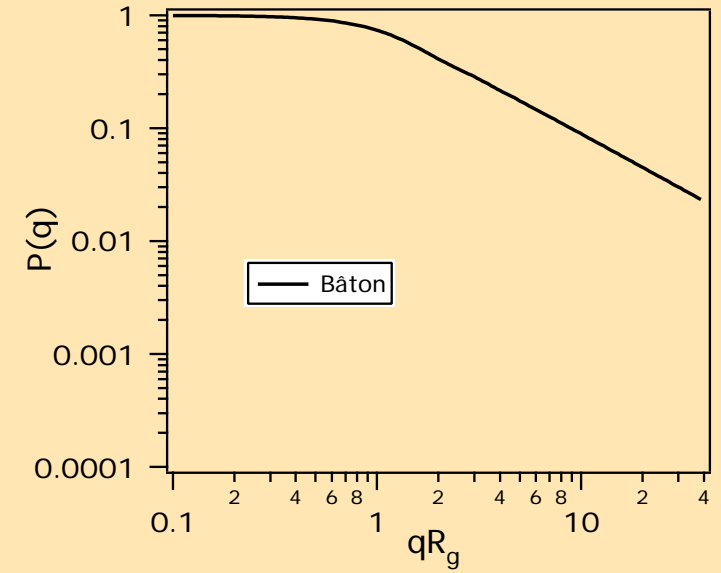
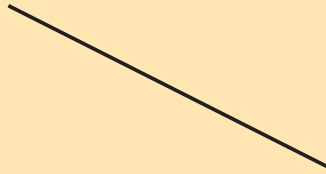
1. Une seule longueur est pertinente.
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$$\left[\frac{\mathcal{S}(q)}{(CVK^2)} \right]_{C \rightarrow 0} = M \cdot P(qR_g) \quad \text{avec} \quad \begin{cases} P(qR_g < 1) = 1 \\ P(qR_g \geq 1) = (qR_g)^{-\mathcal{D}} \end{cases}$$

$$\left[\frac{\mathcal{S}(q)}{(CVK^2)} \right]_{\substack{C \rightarrow 0 \\ qR_g > 1}} = M \cdot (qR)^{-\mathcal{D}} = m_1 \left(\frac{q^{-1}}{a} \right)^{\mathcal{D}}$$

Loi d'échelle (suite)

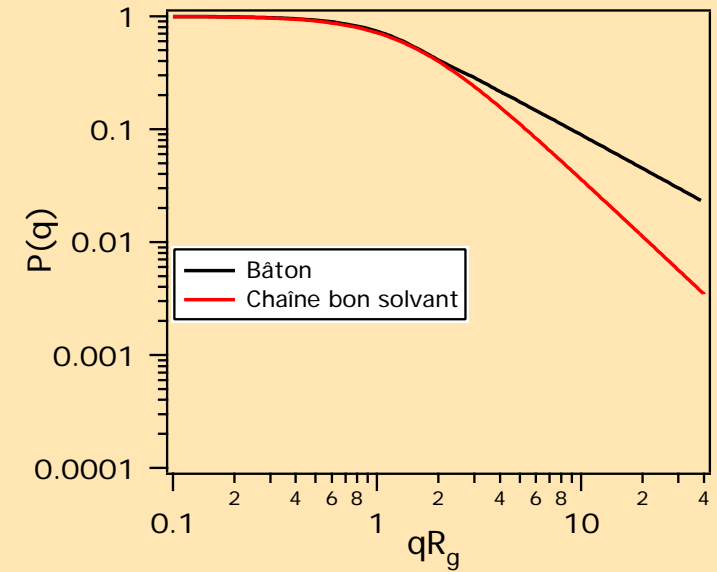
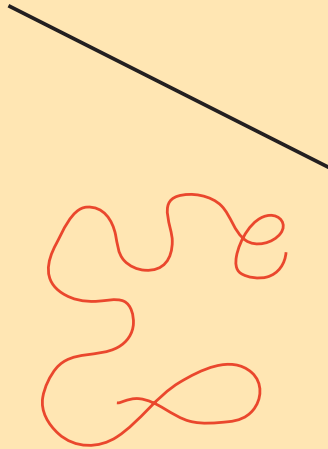
Bâton : $\mathcal{D} = 1$



Loi d'échelle (suite)

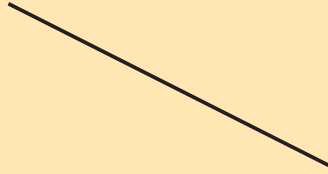
Bâton : $\mathcal{D} = 1$

Chaîne en bon sol-
vant : $\mathcal{D} = 5/3$

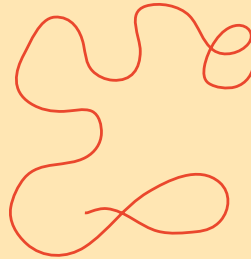


Loi d'échelle (suite)

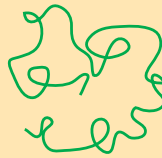
Bâton : $\mathcal{D} = 1$



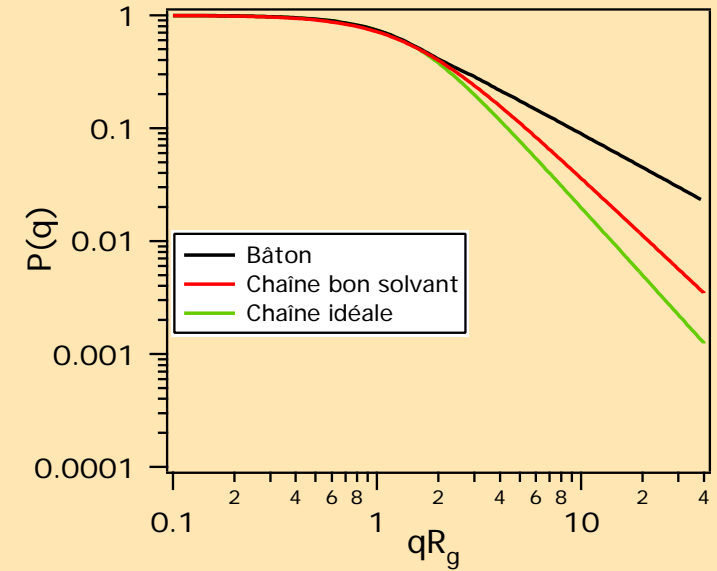
Chaîne en bon sol-
vant : $\mathcal{D} = 5/3$



Chaîne idéale :
 $\mathcal{D} = 2$

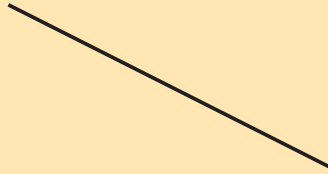


Sphère : $\mathcal{D} = 2$

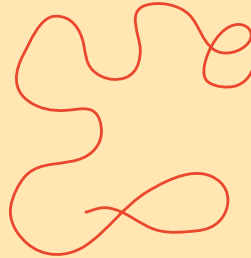


Loi d'échelle (suite)

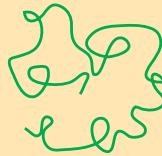
Bâton : $\mathcal{D} = 1$



Chaîne en bon sol-
vant : $\mathcal{D} = 5/3$

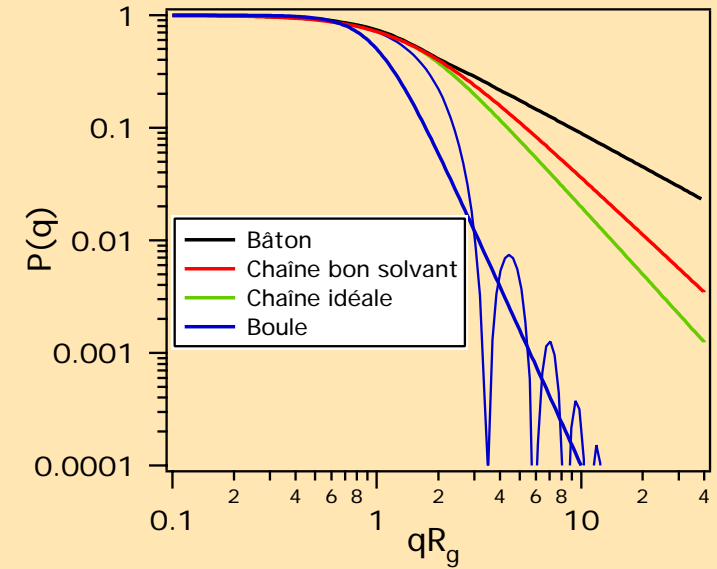


Chaîne idéale :
 $\mathcal{D} = 2$



Sphère : $\mathcal{D} = 2$

Boule : $\mathcal{D}_{\text{surface}} = 2$



Loi d'échelle (suite)

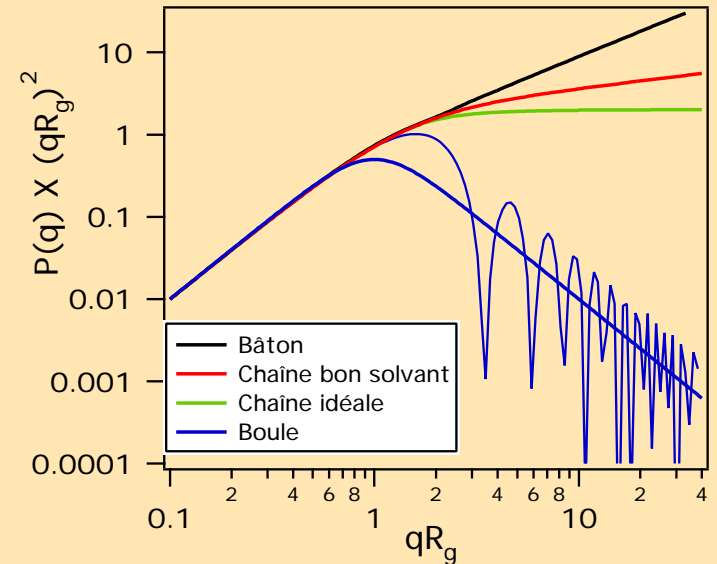
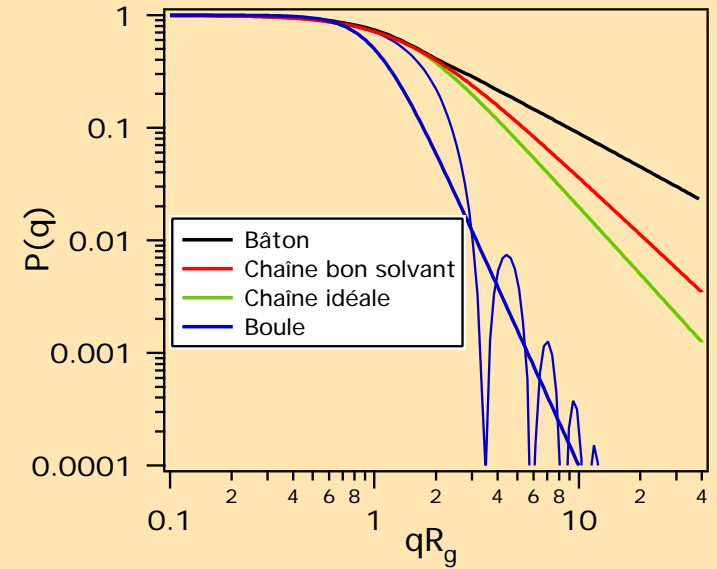
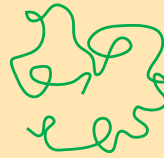
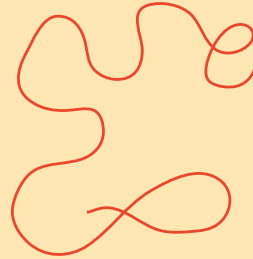
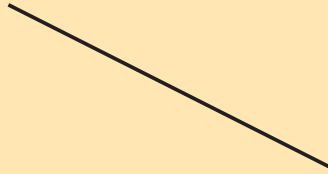
Bâton : $\mathcal{D} = 1$

Chaîne en bon sol-
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Chaîne idéale :
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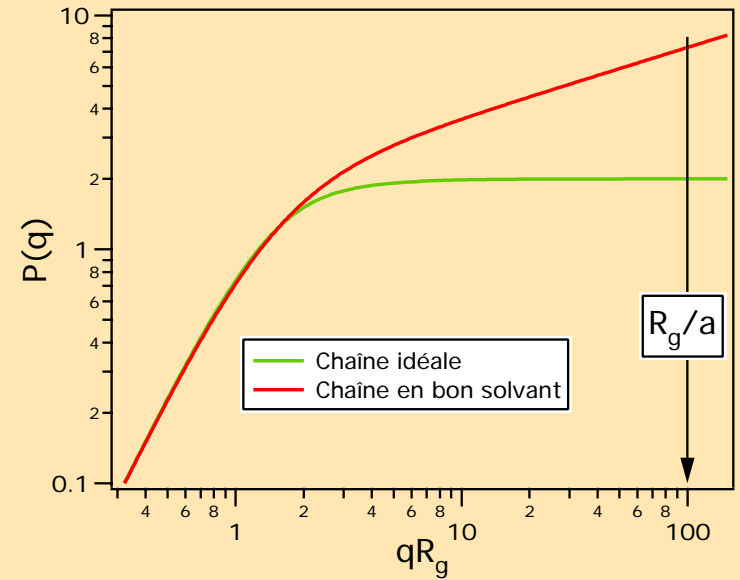
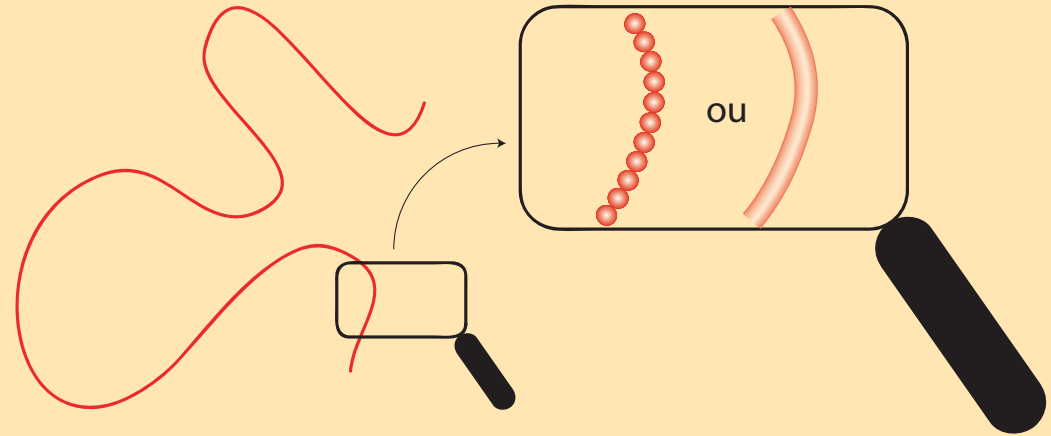
Sphère : $\mathcal{D} = 2$

Boule : $\mathcal{D}_{\text{surface}} = 2$



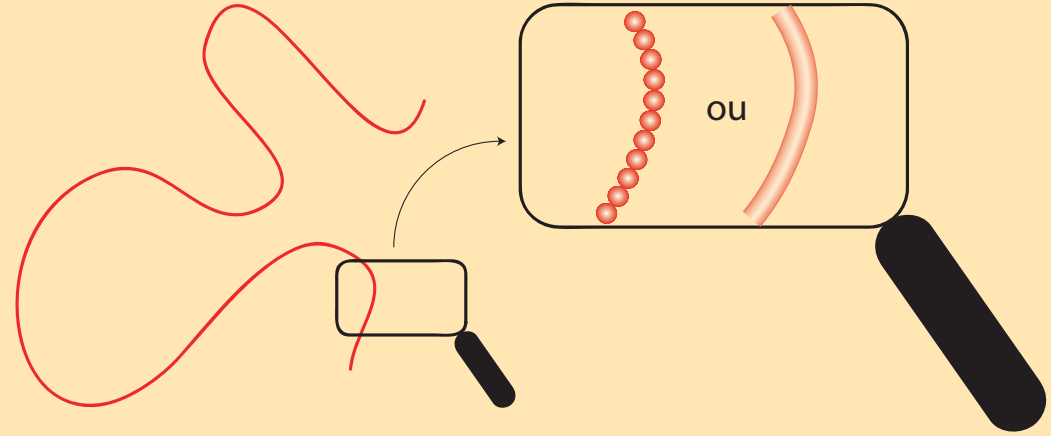
Fonction de coupure à grand q

Le mesure est sensible à la structure locale.



Fonction de coupure à grand q

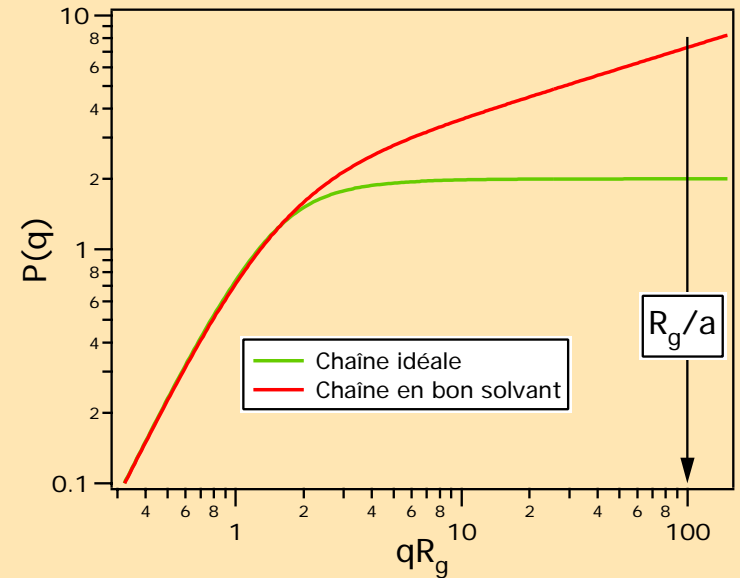
Le mesure est sensible à la structure locale.



Si cette structure locale a une symétrie sphérique :

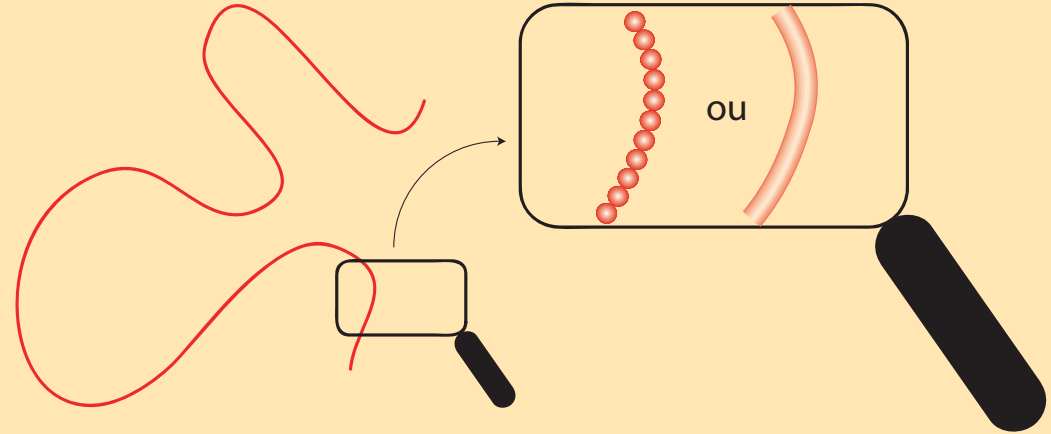
$$P(q) = P_{\text{global}}(q) \times P_{\text{local}}(q)$$

$$P_{qa < 1}(q) = P_{\text{global}}(q) \times e^{-q^2 a^2 / 3}$$



Fonction de coupure à grand q

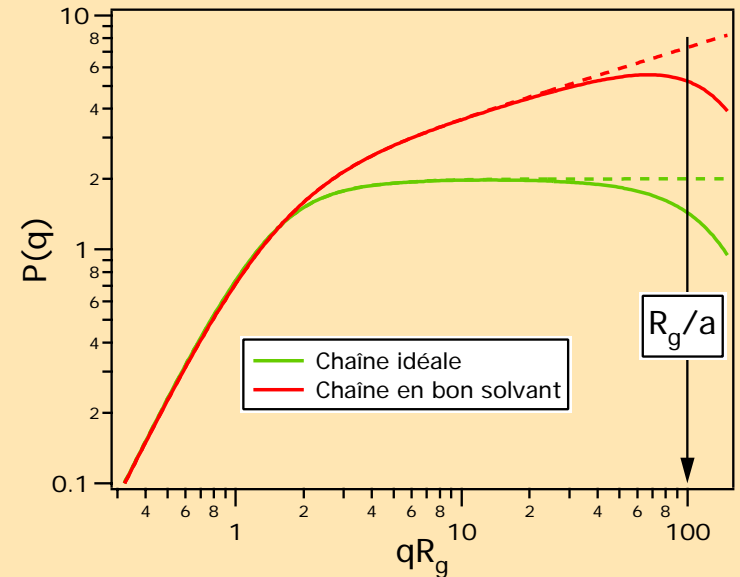
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Ex 3 : Facteurs d'élongation de la traduction

T.V. Budkevich et al. (2002), *Biochemistry*, 41 : 15342-15349

(PSI, Suisse)

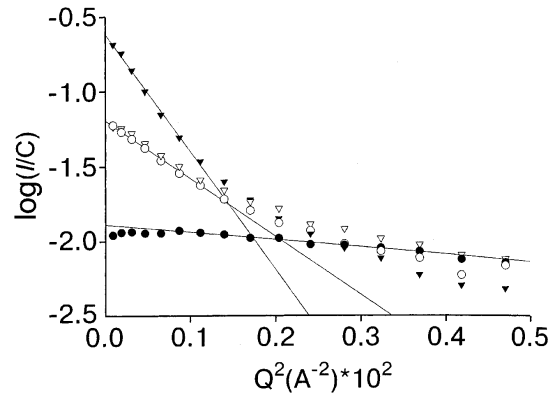


FIGURE 5: Dependence of neutron scattering intensity I on scattering vector Q in Guinier coordinates to tRNA (●), eEF1A (○), eEF1A:tRNA = 1:3 (▽), and eEF1A:tRNA=3:1 (▼).

Guinier :

$$\log(I/C) = \log(M) - q^2 R_g^2/3 + \dots$$

Ex 3 : Facteurs d'élongation de la traduction

T.V. Budkevich et al. (2002), *Biochemistry*, 41 : 15342-15349

(PSI, Suisse)

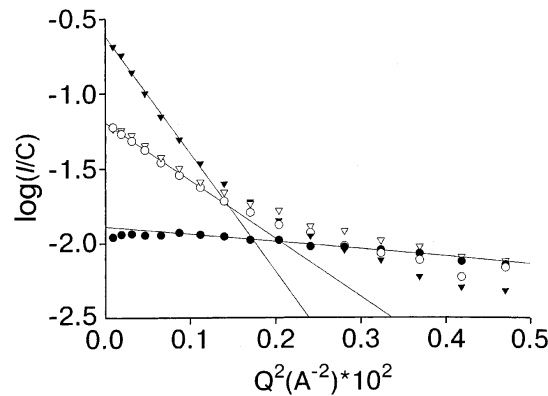


FIGURE 5: Dependence of neutron scattering intensity I on scattering vector Q in Guinier coordinates to tRNA (●), eEF1A (○), eEF1A:tRNA = 1:3 (▽), and eEF1A:tRNA=3:1 (▼).

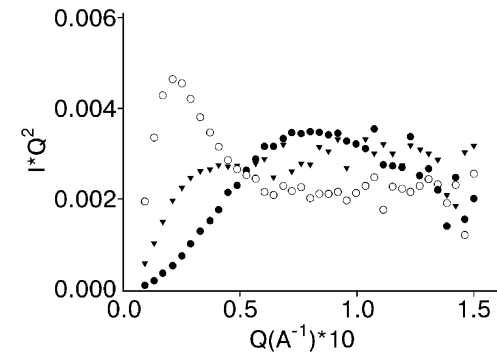


FIGURE 6: Dependence of neutron scattering intensity I on scattering vector Q in Kratky coordinates for tRNA (●), eEF1A (▼), and eEF1A:tRNA = 3:1 (○).

Guinier :

$$\log(I/C) = \log(M) - q^2 R_g^2/3 + \dots$$

Pelote

$$P(q) \approx (1 - (qR_g)^2)^{-1}$$

Boule

$$P(q) \approx (1 - (qR_g)^4)^{-1}$$

Ex 4 : Repliement d'une protéine multidomaine

D. Lairez et al. (2003), *Biophys. J.*, 84 : 3904-3916

(PACE, LLB, Saclay)

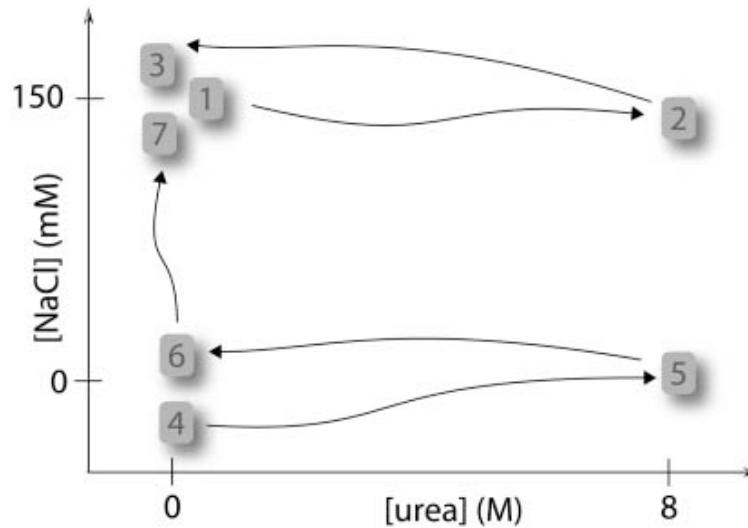


FIGURE 1 The seven samples here studied and their history.

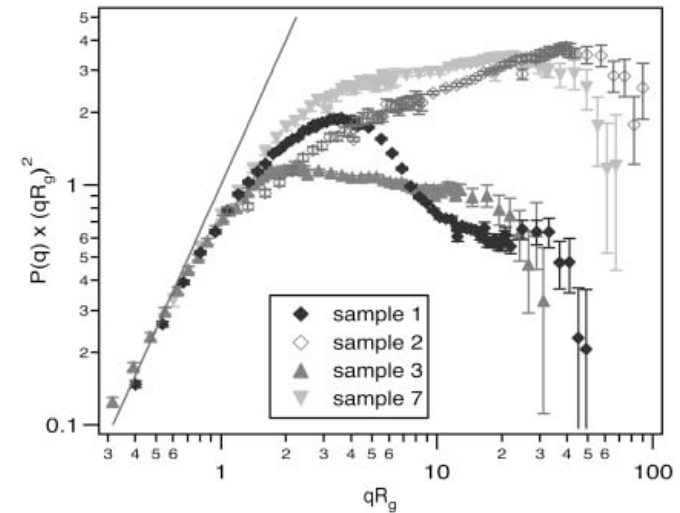


FIGURE 4 Form factors of samples in salt-containing solution in a Kratky representation $P(q) \times (qR_g)^2$ versus qR_g . The symbols meaning is the same as in Fig. 2. The straight line corresponds to $(qR_g)^2$.

Ex 4 : Repliement d'une protéine multidomaine (suite)

D. Lairez et al. (2003), *Biophys. J.*, 84 : 3904-3916

(PACE, LLB, Saclay)

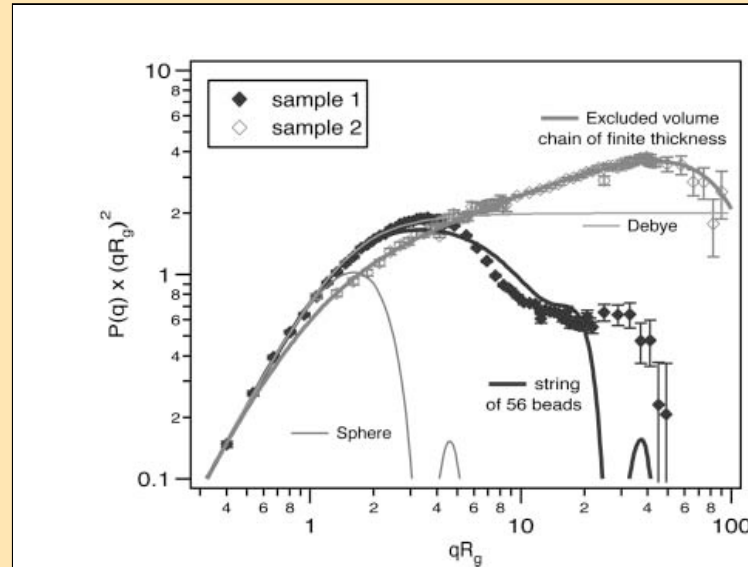


FIGURE 6 Form factor of the native and unfolded fibronectin plotted in a Kratky representation: $P(q) \times (qR_g)^2$ versus qR_g . The full lines correspond to the theoretical expectation for a sphere (Eq. 8), a string of 56 beads (Eq. 12), a Gaussian chain with infinitely small monomer (Debye function, Eq. 9), and a swollen chain with a finite thickness (Eq. 13).

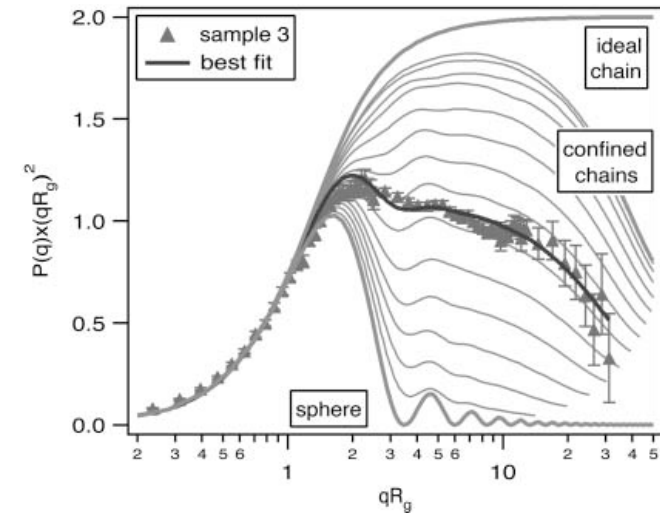
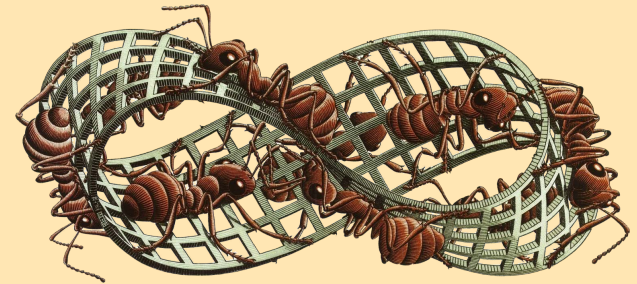


FIGURE 8 $P(q) \times (qR_g)^2$ versus qR_g for fibronectin refolded in salt-containing solution (data points) compared to confined chains (lines). (Top to bottom), lines correspond to: Debye function (unconfined Gaussian chain with infinitely small monomer); confined chains with radius of confinement, R_c from 30- to 4-step-length unit; and compact sphere. The line fitting the data corresponds to $\bar{R}_c = 16 \pm 2$ step-length unit.

Ex 5 : Superhélice d'ADN

$$P_{\text{superhélice}} = P_{\text{global}}(q) \times P_{\text{local}}(q)$$

$$\propto q^{-1} \times \left(1 + \frac{\sin(qd)}{qd}\right)$$



M. Hammermann et al. (1998), *Biophys. J.*, 75 : 3057-3063

(D22, ILL, Grenoble)

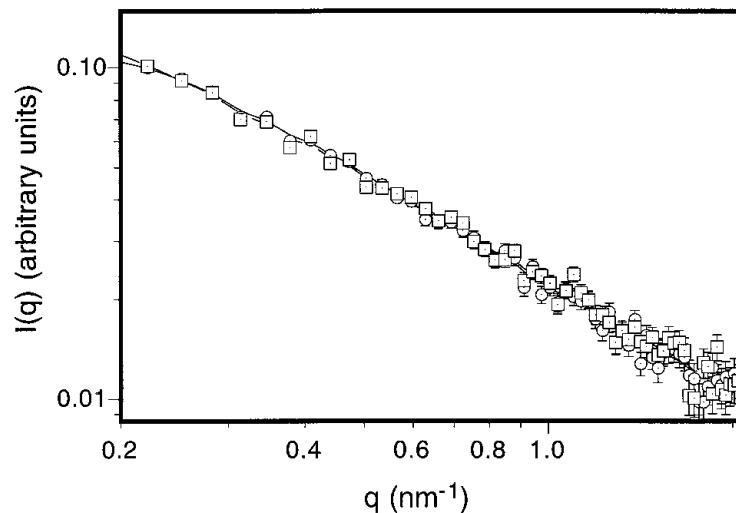


FIGURE 4 Measured scattering intensity $I(q)$ of pUC18, relaxed, in H_2O , 10 mM Tris, at 0 mM (\circ) and 100 mM (\square) NaCl concentrations.

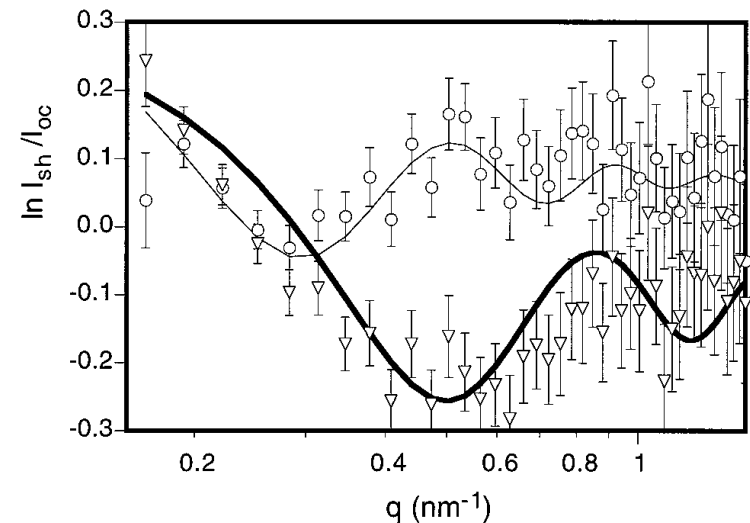
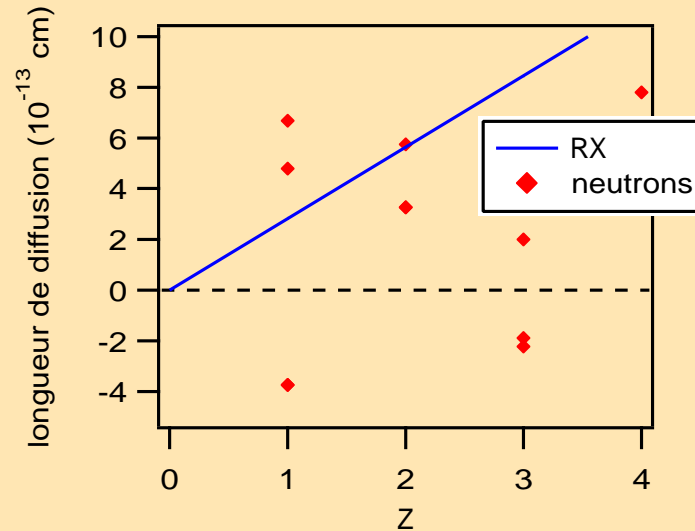
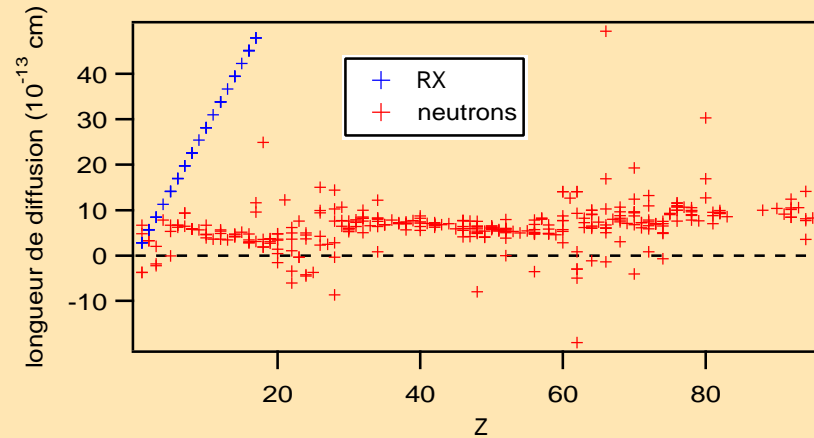


FIGURE 5 Ratio of the measured scattering intensities $I(q)$ of pUC18, supercoiled, in H_2O , 10 mM Tris, at 0 mM (\circ), and 100 mM (∇) Na^+ concentrations and relaxed pUC18 DNA at 100 mM Na^+ concentration. The solid lines are the scattering form factors of a pair of point scatterers at a distance $r = 16.0$ nm (thin line) and $r = 9.0$ nm (thick line).

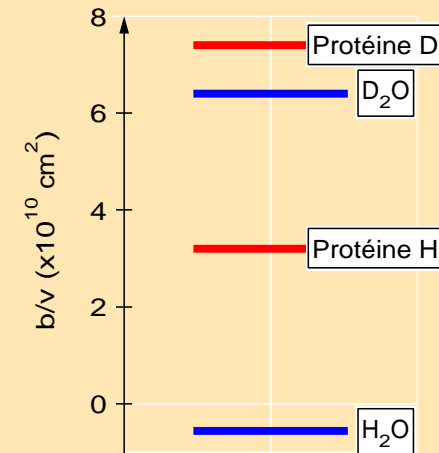
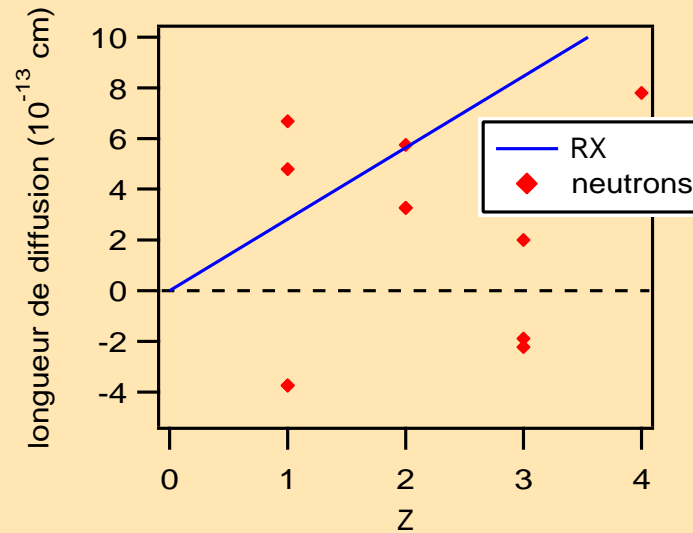
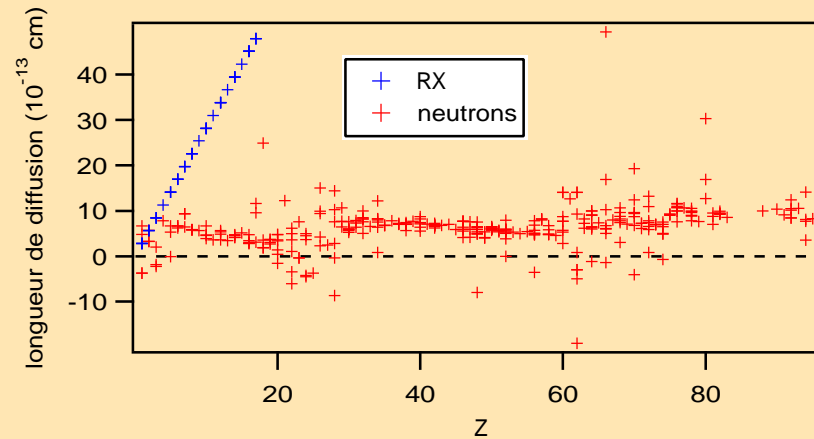
Variations sur le contraste

Marquage isotopique

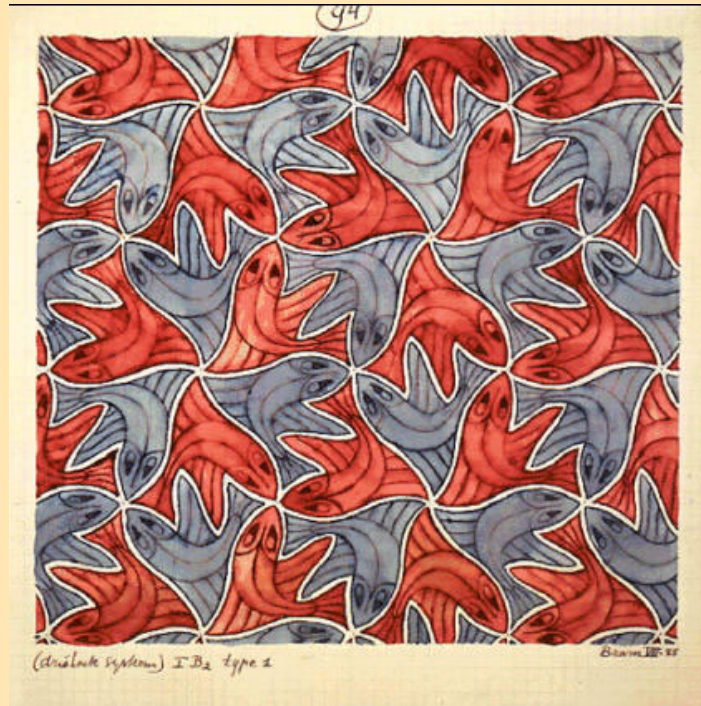


Variations sur le contraste

Marquage isotopique

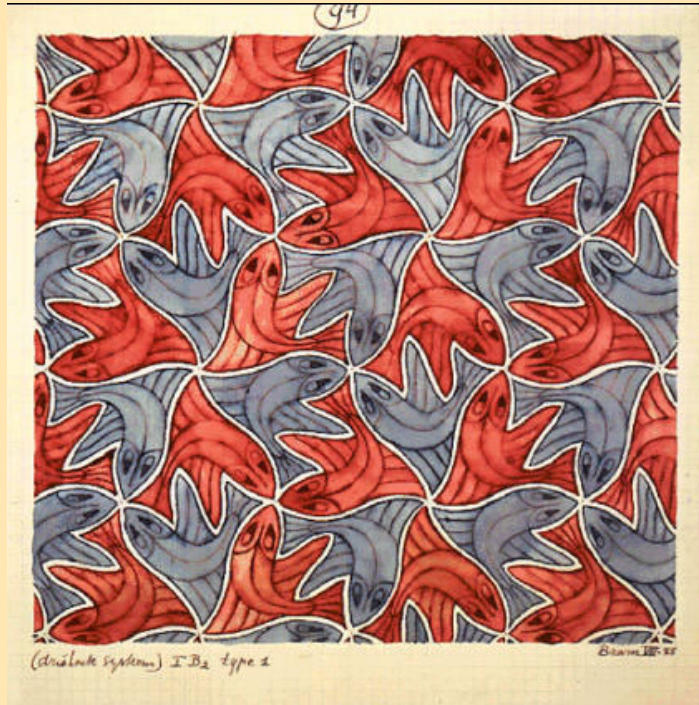


Mélange de deux espèces identiques



Mélange de deux espèces identiques

$$\begin{aligned}\mathcal{S}(q) &= (b_H - b_D)^2 \times \mathcal{S}_{DD} \\ &= (b_H - b_D)^2 \times \\ &\quad [x_D n N^2 P(q) + x_D^2 n^2 N^2 Q(q)]\end{aligned}$$



Mélange de deux espèces identiques



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idem avec \mathcal{S}_{HH}

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$$\text{or } x_H = 1 - x_D$$

\Downarrow

$$P(q) = -nQ(q)$$

Mélange de deux espèces identiques



$$\begin{aligned}\mathcal{S}(q) &= (b_H - b_D)^2 \times \mathcal{S}_{DD} \\ &= (b_H - b_D)^2 \times \\ &\quad [x_D n N^2 P(q) + x_D^2 n^2 N^2 Q(q)]\end{aligned}$$

idem avec \mathcal{S}_{HH}

$$\begin{aligned}\mathcal{S}(q) &= (b_H - b_D)^2 \times \mathcal{S}_{HH} \\ &= (b_H - b_D)^2 \times \\ &\quad [x_H n N^2 P(q) + x_H^2 n^2 N^2 Q(q)]\end{aligned}$$

$$\text{or } x_H = 1 - x_D$$

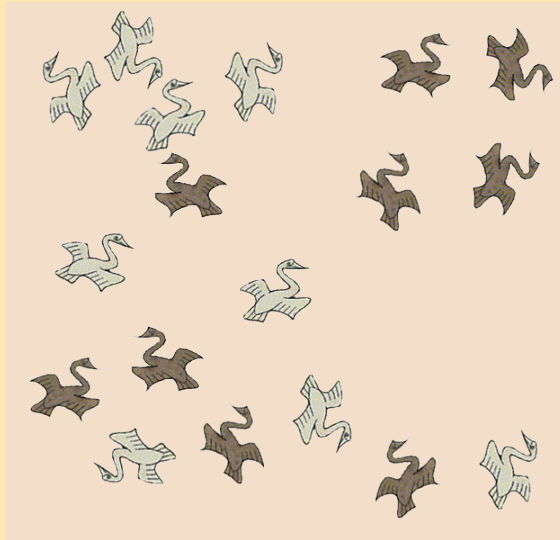
\Downarrow

$$P(q) = -nQ(q)$$

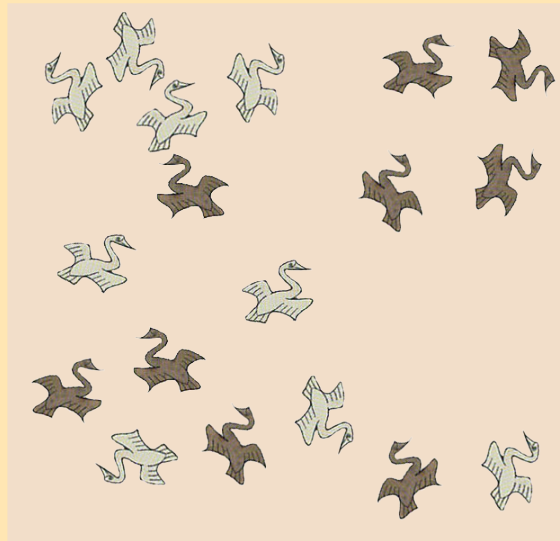
$$\mathcal{S}(q) = (b_H - b_D)^2 \times x_D(1 - x_D) \times nN^2 P(q)$$

On accède directement au facteur de forme.

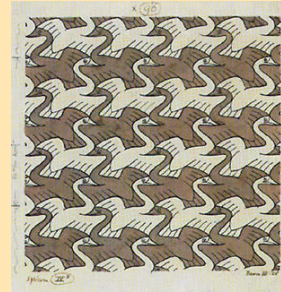
Contraste moyen nul



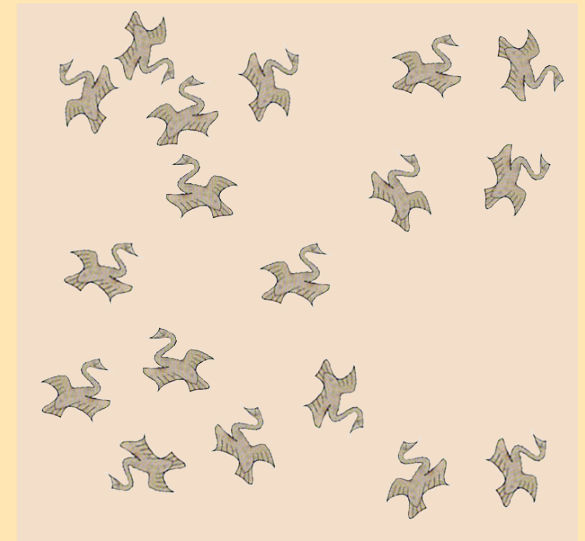
Contraste moyen nul



=

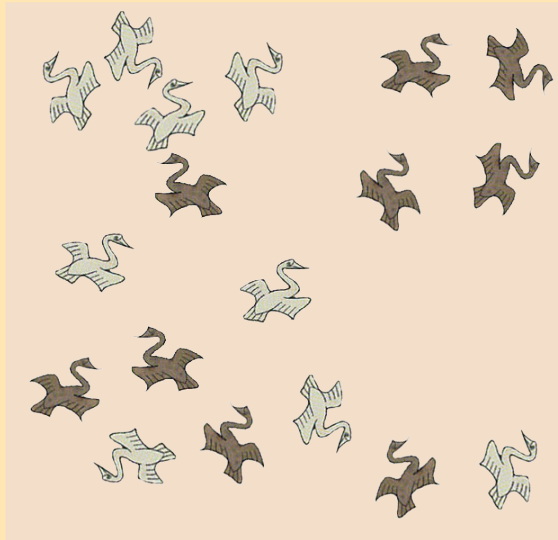


+

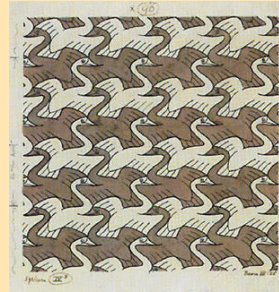


$$\langle b \rangle = x_D b_D + (1 - x_D) b_H$$

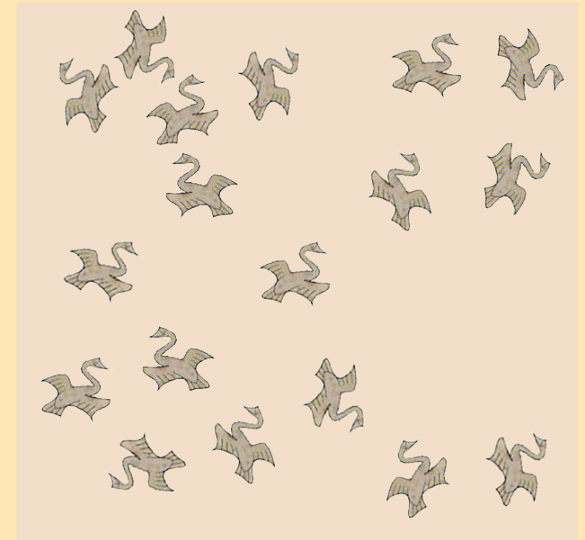
Contraste moyen nul



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+

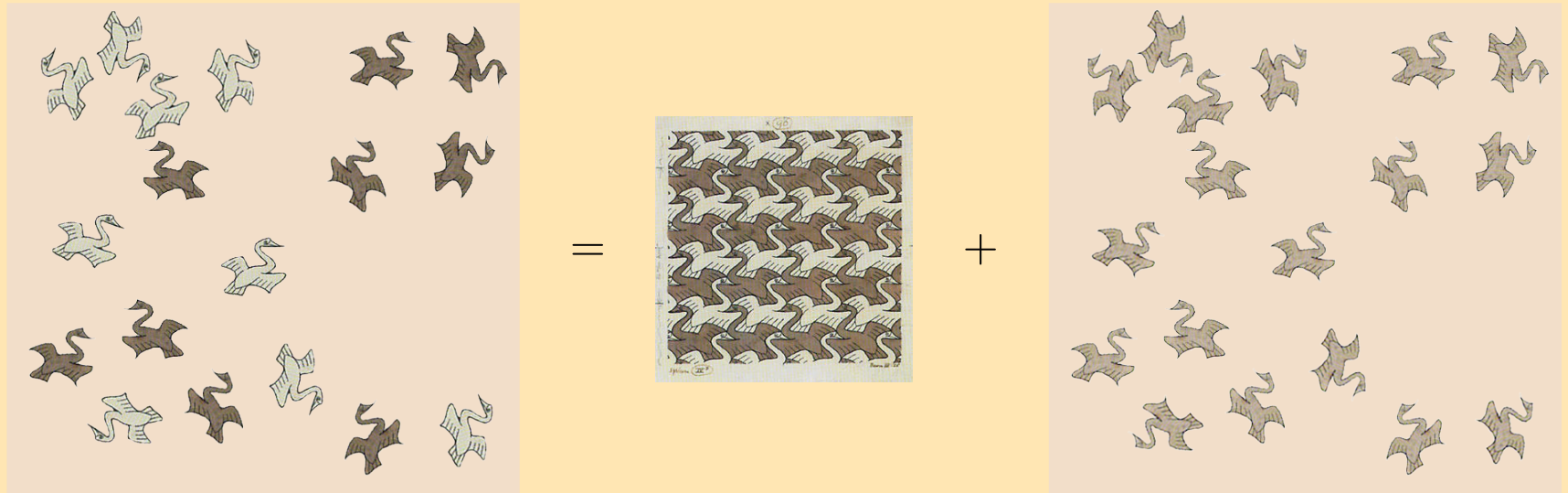


$$\langle b \rangle = x_D b_D + (1 - x_D) b_H$$

$$\begin{aligned} \mathcal{S}(q) = & \left[(b_H - b_D)^2 \times x_D (1 - x_D) n N^2 P(q) \right] \\ & + (\langle b \rangle - b_0)^2 \left[n N^2 P(q) + n^2 N^2 Q(q) \right] \end{aligned}$$

Si $\langle b \rangle - b_0 = 0$, alors $\mathcal{S}(q) \propto P(q)$

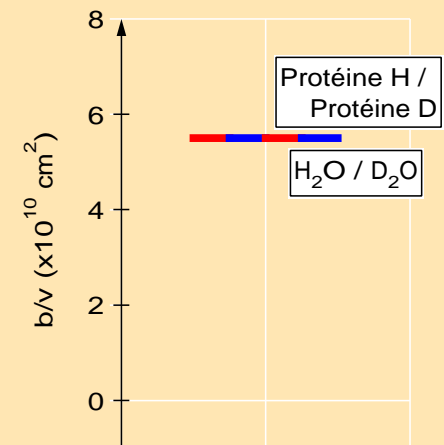
Contraste moyen nul



$$\langle b \rangle = x_D b_D + (1 - x_D) b_H$$

$$\mathcal{S}(q) = [(b_H - b_D)^2 \times x_D(1 - x_D)nN^2P(q)] + (\langle b \rangle - b_0)^2 [nN^2P(q) + n^2N^2Q(q)]$$

Si $\langle b \rangle - b_0 = 0$, alors $\mathcal{S}(q) \propto P(q)$



Mélange de trois espèces, variation de contraste

$$\rho = \rho_A x_A + \rho_B x_B + \rho_0 x_0$$

$$\Delta \rho_i = \rho_A \Delta x_{Ai} + \rho_B \Delta x_{Bi} + \rho_0 \Delta x_{0i}$$

Incompressible : $\Delta x_{0i} = -\Delta(x_{Ai} + x_{Bi})$

$$\Delta \rho_i = (\rho_A - \rho_0) \Delta x_{Ai} + (\rho_B - \rho_0) \Delta x_{0i}$$

$$\begin{aligned} \langle \Delta \rho_i \Delta \rho_j \rangle &= (\rho_A - \rho_0)^2 \langle \Delta x_{Ai} \Delta x_{Aj} \rangle \\ &+ (\rho_B - \rho_0)^2 \langle \Delta x_{Bi} \Delta x_{Bj} \rangle \\ &+ 2(\rho_A - \rho_0)(\rho_B - \rho_0) \langle \Delta x_{Ai} \Delta x_{Bj} \rangle \end{aligned}$$

Mélange de trois espèces, variation de contraste

$$\rho = \rho_A x_A + \rho_B x_B + \rho_0 x_0$$

$$\Delta \rho_i = \rho_A \Delta x_{Ai} + \rho_B \Delta x_{Bi} + \rho_0 \Delta x_{0i}$$

Incompressible : $\Delta x_{0i} = -\Delta(x_{Ai} + x_{Bi})$

$$\Delta \rho_i = (\rho_A - \rho_0) \Delta x_{Ai} + (\rho_B - \rho_0) \Delta x_{0i}$$

$$\begin{aligned} \langle \Delta \rho_i \Delta \rho_j \rangle &= (\rho_A - \rho_0)^2 \langle \Delta x_{Ai} \Delta x_{Aj} \rangle \\ &+ (\rho_B - \rho_0)^2 \langle \Delta x_{Bi} \Delta x_{Bj} \rangle \\ &+ 2(\rho_A - \rho_0)(\rho_B - \rho_0) \langle \Delta x_{Ai} \Delta x_{Bj} \rangle \\ &\downarrow \end{aligned}$$

$$\begin{aligned} \mathcal{S}(q) &= v^2 [(\rho_A - \rho_0)^2 \mathcal{S}_{AA}(q) \\ &+ (\rho_B - \rho_0)^2 \mathcal{S}_{BB}(q) \\ &+ 2(\rho_A - \rho_0)(\rho_B - \rho_0) \mathcal{S}_{AB}(q)] \end{aligned}$$

3 mesures avec des contrastes différents : $\rightarrow \mathcal{S}_{AA}, \mathcal{S}_{BB}$ et \mathcal{S}_{AB}

Mélange de trois espèces, variation de contraste

$$\rho = \rho_A x_A + \rho_B x_B + \rho_0 x_0$$

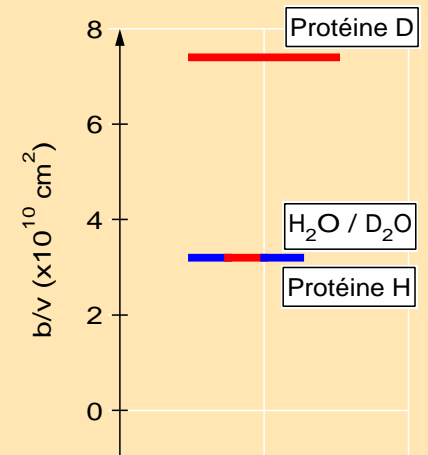
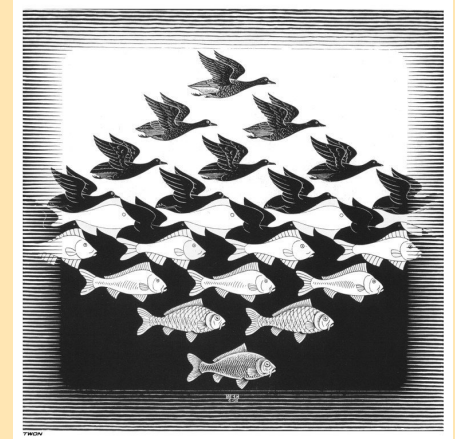
$$\Delta \rho_i = \rho_A \Delta x_{Ai} + \rho_B \Delta x_{Bi} + \rho_0 \Delta x_{0i}$$

Incompressible : $\Delta x_{0i} = -\Delta(x_{Ai} + x_{Bi})$

$$\Delta \rho_i = (\rho_A - \rho_0) \Delta x_{Ai} + (\rho_B - \rho_0) \Delta x_{0i}$$

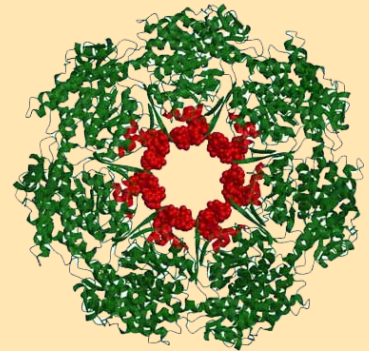
$$\begin{aligned} \langle \Delta \rho_i \Delta \rho_j \rangle &= (\rho_A - \rho_0)^2 \langle \Delta x_{Ai} \Delta x_{Aj} \rangle \\ &+ (\rho_B - \rho_0)^2 \langle \Delta x_{Bi} \Delta x_{Bj} \rangle \\ &+ 2(\rho_A - \rho_0)(\rho_B - \rho_0) \langle \Delta x_{Ai} \Delta x_{Bj} \rangle \\ &\quad \downarrow \end{aligned}$$

$$\begin{aligned} \mathcal{S}(q) &= v^2 [(\rho_A - \rho_0)^2 \mathcal{S}_{AA}(q) \\ &+ (\rho_B - \rho_0)^2 \mathcal{S}_{BB}(q) \\ &+ 2(\rho_A - \rho_0)(\rho_B - \rho_0) \mathcal{S}_{AB}(q)] \end{aligned}$$



3 mesures avec des contrastes différents : $\rightarrow \mathcal{S}_{AA}, \mathcal{S}_{BB}$ et \mathcal{S}_{AB}

Ex 6 : Etude d'un chaperon moléculaire, GroEL



S. Krueger et al. (2003), *J. Struct. Biol.*, 141 : 240-258 (30 m SANS, NCNR, Gaithersburg)

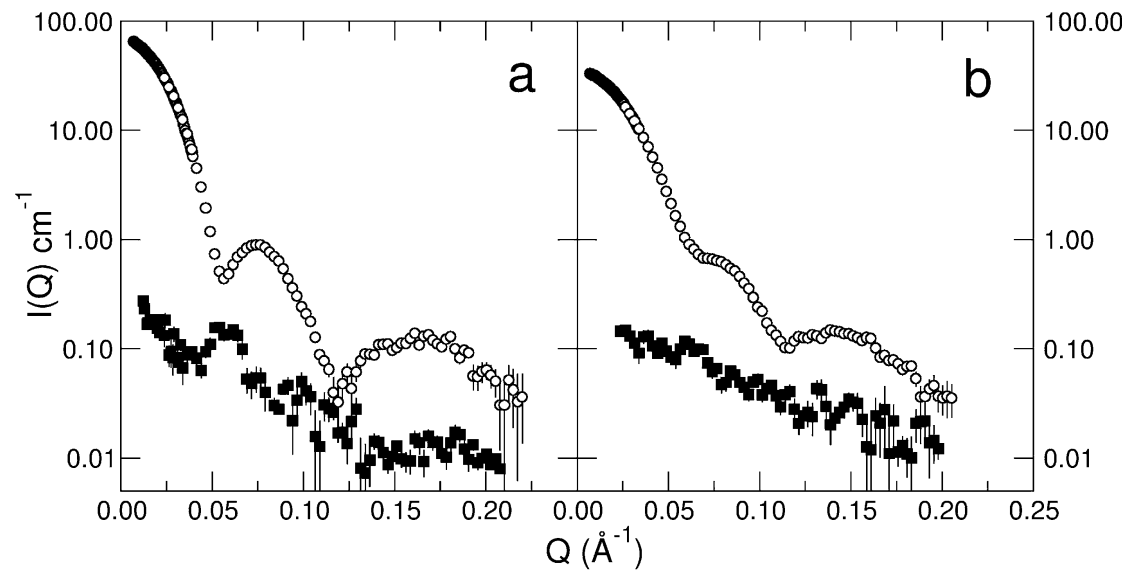


Fig. 6. Scattered intensities of the GroEL ($I_{EL}(Q)$) (○) and dPJ9 ($I_{dPJ9}(Q)$) (■) components as bound in (a) the GroEL/dPJ9 complex and (b) the srGroEL/dPJ9 complex.

Marquage sélectif

$$\mathcal{S} = \sum_i^n \sum_j^n b_i b_j \mathcal{S}_{ij}$$

$$\begin{aligned} \mathcal{S}(b_1, b_2) = & 2b_1 b_2 \mathcal{S}_{12} + b_1^2 \mathcal{S}_{11} + b_2^2 \mathcal{S}_{22} \\ & + 2b_1 \sum_{i=3}^n b_i \mathcal{S}_{1i} \\ & + 2b_2 \sum_{i=3}^n b_i \mathcal{S}_{2i} \\ & + \sum_{i=3}^n \sum_{j=3}^n b_i b_j \mathcal{S}_{ij} \end{aligned}$$

Marquage sélectif

$$\mathcal{S} = \sum_i^n \sum_j^n b_i b_j \mathcal{S}_{ij}$$

$$\begin{aligned} \mathcal{S}(b_1, b_2) = & 2b_1 b_2 \mathcal{S}_{12} + b_1^2 \mathcal{S}_{11} + b_2^2 \mathcal{S}_{22} \\ & + 2b_1 \sum_{i=3}^n b_i \mathcal{S}_{1i} \\ & + 2b_2 \sum_{i=3}^n b_i \mathcal{S}_{2i} \\ & + \sum_{i=3}^n \sum_{j=3}^n b_i b_j \mathcal{S}_{ij} \end{aligned}$$

$$\mathcal{S}(b_{1D}, b_{2D})$$

$$+ \mathcal{S}(b_{1H}, b_{2H})$$

$$- \mathcal{S}(b_{1D}, b_{2H})$$

$$- \mathcal{S}(b_{1H}, b_{2D})$$

$$= 2(b_{1D} - b_{1H})(b_{2D} - b_{2H}) \mathcal{S}_{12}(q)$$

$$\mathcal{S}_{12}(q) \approx \sin(qd_{12})$$

Marquage sélectif

$$\mathcal{S} = \sum_i^n \sum_j^n b_i b_j \mathcal{S}_{ij}$$

$$\mathcal{S}(b_1, b_2) = 2b_1 b_2 \mathcal{S}_{12} + b_1^2 \mathcal{S}_{11} + b_2^2 \mathcal{S}_{22}$$

$$+ 2b_1 \sum_{i=3}^n b_i \mathcal{S}_{1i} \\ + 2b_2 \sum_{i=3}^n b_i \mathcal{S}_{2i} \\ + \sum_{i=3}^n \sum_{j=3}^n b_i b_j \mathcal{S}_{ij}$$

$$\mathcal{S}(b_{1D}, b_{2D})$$

$$+ \mathcal{S}(b_{1H}, b_{2H})$$

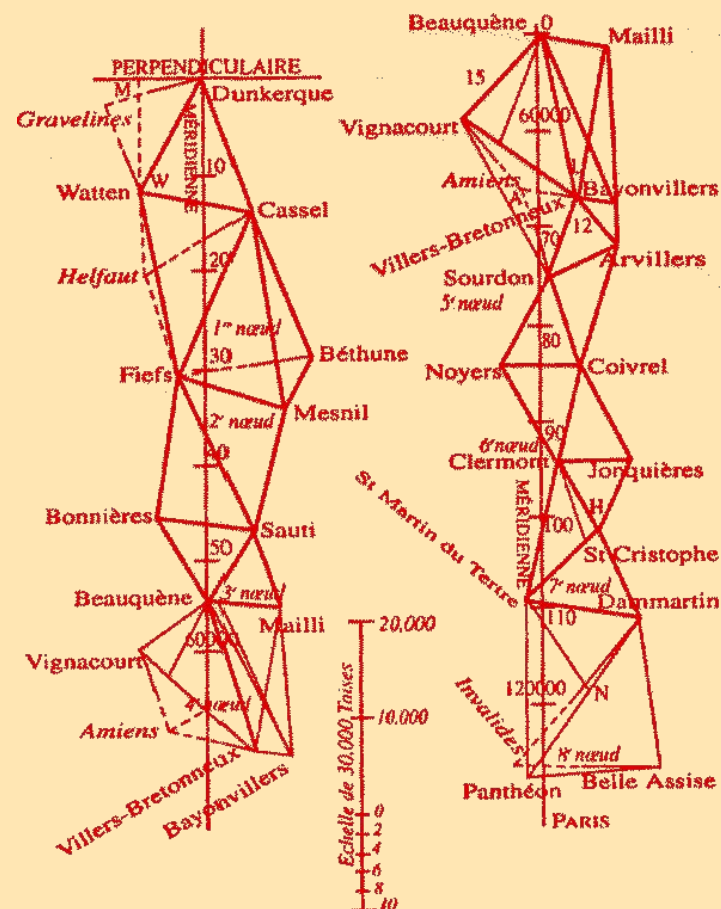
$$- \mathcal{S}(b_{1D}, b_{2H})$$

$$- \mathcal{S}(b_{1H}, b_{2D})$$

$$= 2(b_{1D} - b_{1H})(b_{2D} - b_{2H}) \mathcal{S}_{12}(q)$$

$$\mathcal{S}_{12}(q) \approx \sin(qd_{12})$$

Triangulation



Ex 7 : Triangulation et structure quaternaire des sous-unités ribosomales

M.S. Capel et al. (1987), *Science*, 238 : 1403-1406

(Brookhaven)

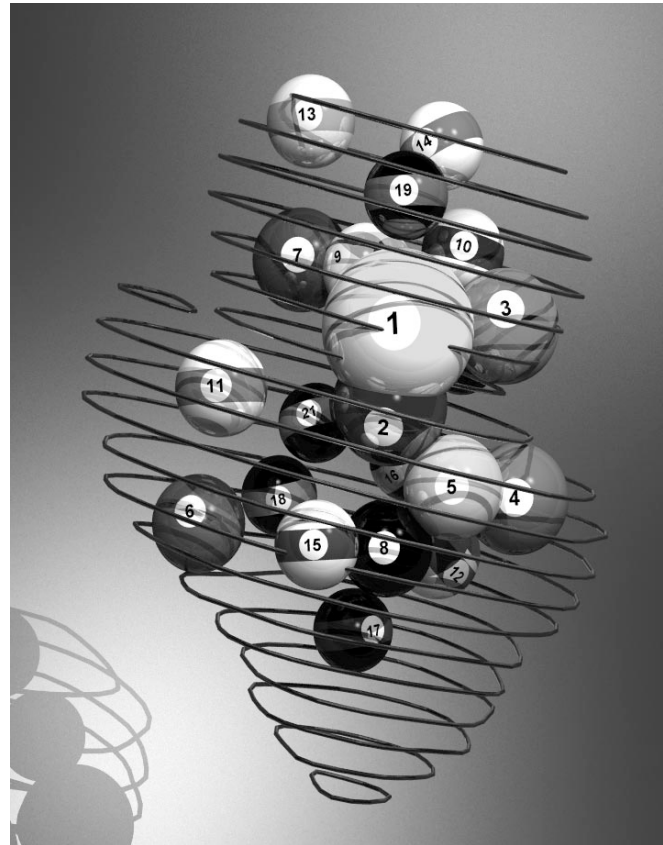


Figure 2 The placement of proteins within the 30S subunit. Proteins are shown as spheres the volumes of which are proportional to molecular weight. Their placement was determined by neutron scattering (10). The protein array is superimposed on the outline of the 30S subunit in a manner that maximizes its overlap with epitope positions determined by immunoelectron microscopy. This figure was provided by Malcolm Capel.