UNIVERSIDADE FEDERAL
DO RIO DE JANEIRO

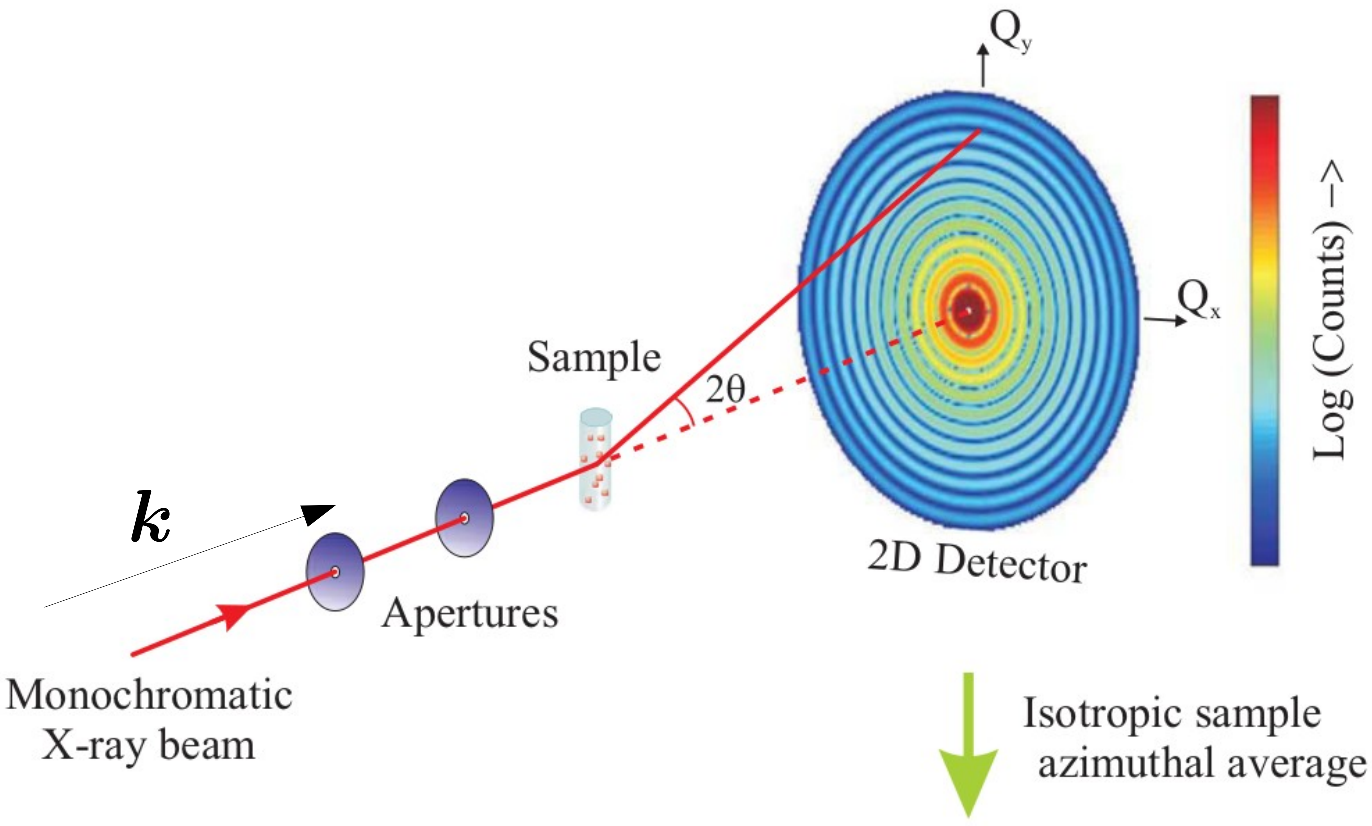
Espalhamento em baixo ângulo

para sistemas coloidais

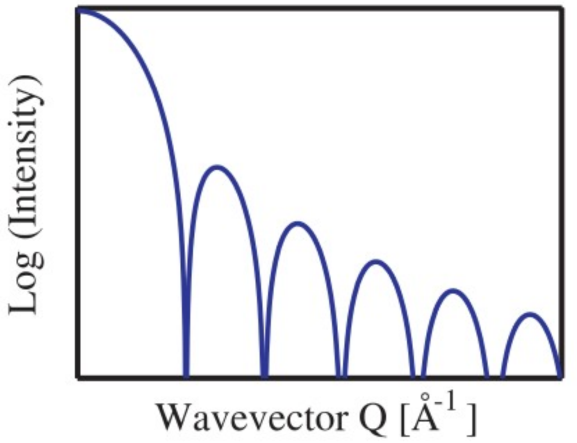
Elvis do A. Soares @ATMOS

elvis.asoares@gmail.com

Motivação



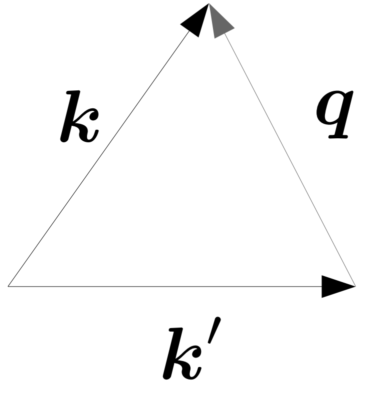
$$q = |\boldsymbol{q}| = 2k \sin\theta$$

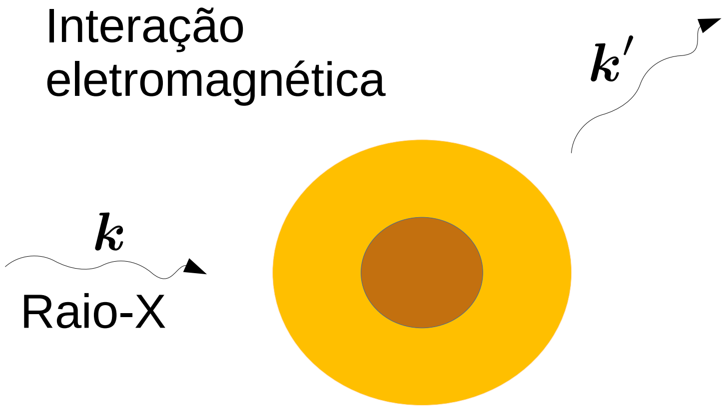


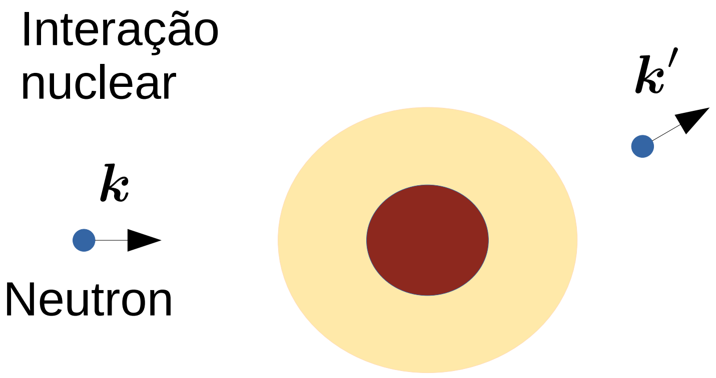
$$k = \frac{2\pi}{\lambda}$$

Als-Nielsen, Jens, and Des McMorrow. Elements of modern X-ray physics. John Wiley & Sons, 2011.

Teoria de Espalhamento





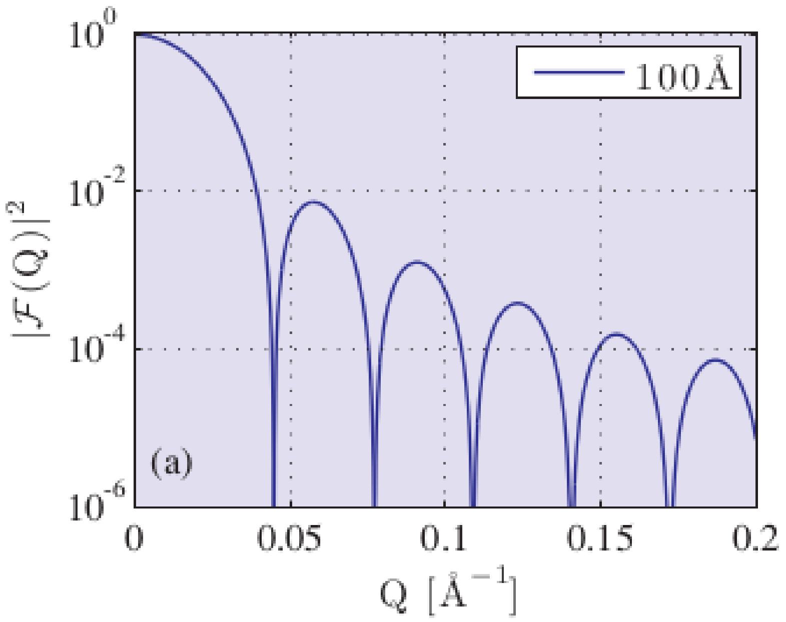


$$I(q) = nV_p^2\Delta\rho_e^2|F(q)|^2S(q) + B(q)$$

- Intensidade espalhada
- Fator de Estrutura
- Densidade de partículas
- Volume da partícula
- Diferença de densidade *específica* entre a partícula e o solvente
- Fator de forma
- Background

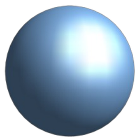
Fator de forma

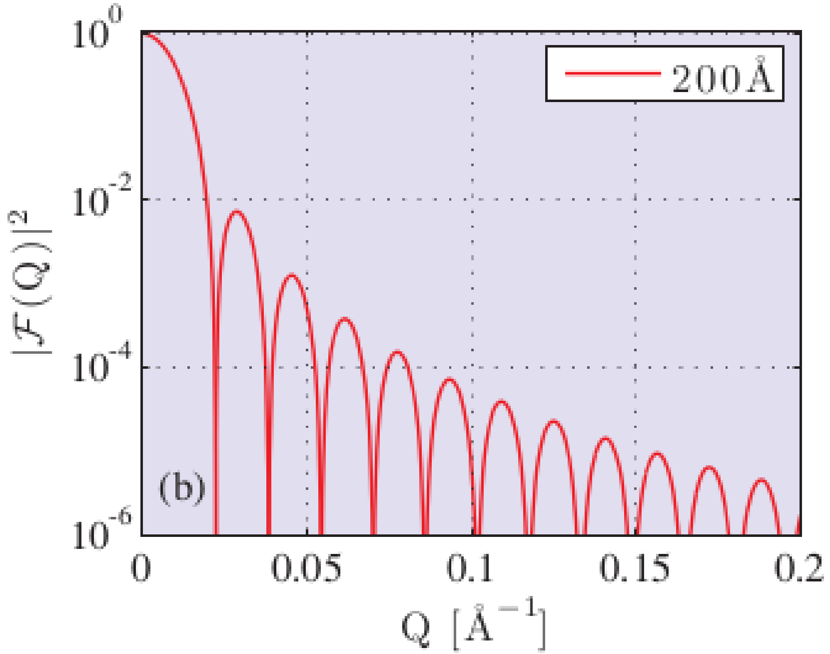
$$F(q) = \frac{1}{V_p} \int_{V_p} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \, \mathrm{d}V_p$$



Para esferas

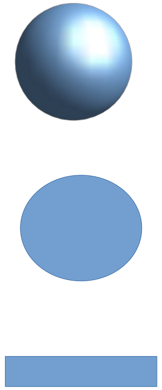
$$F(q) = 3\left[\frac{\sin(qR) - qR\cos(qR)}{(qR)^3}\right]$$

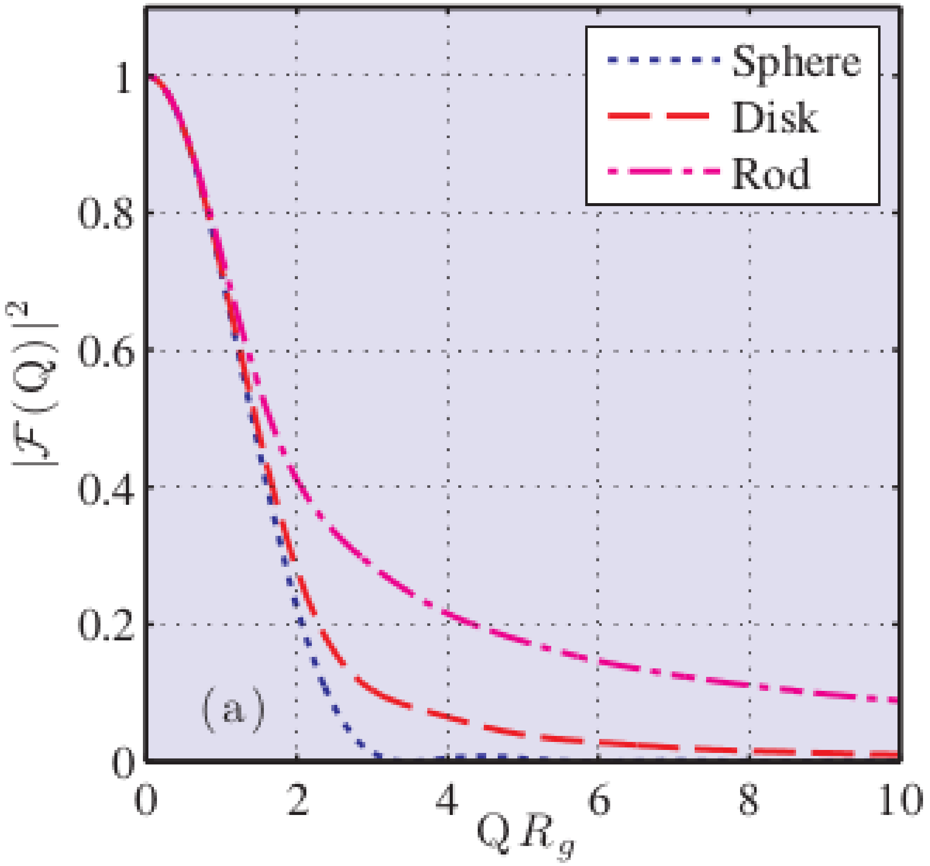


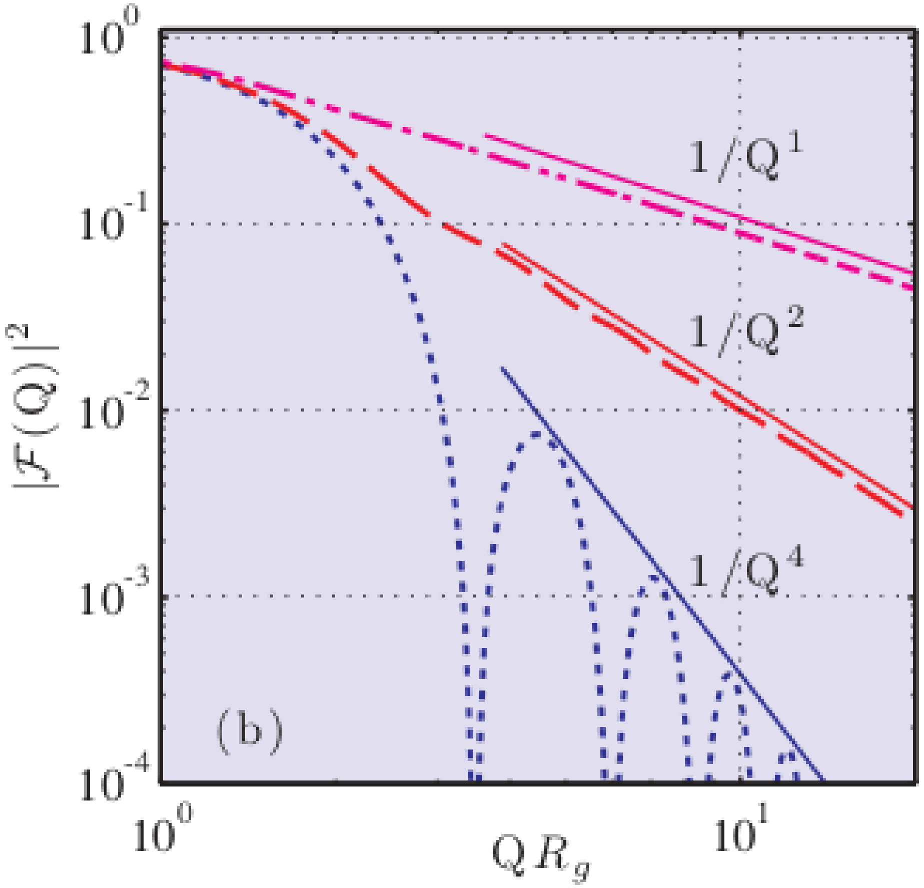


Als-Nielsen, Jens, and Des McMorrow. Elements of modern X-ray physics. John Wiley & Sons, 2011.

Outros formatos

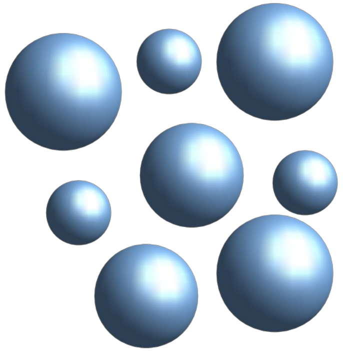






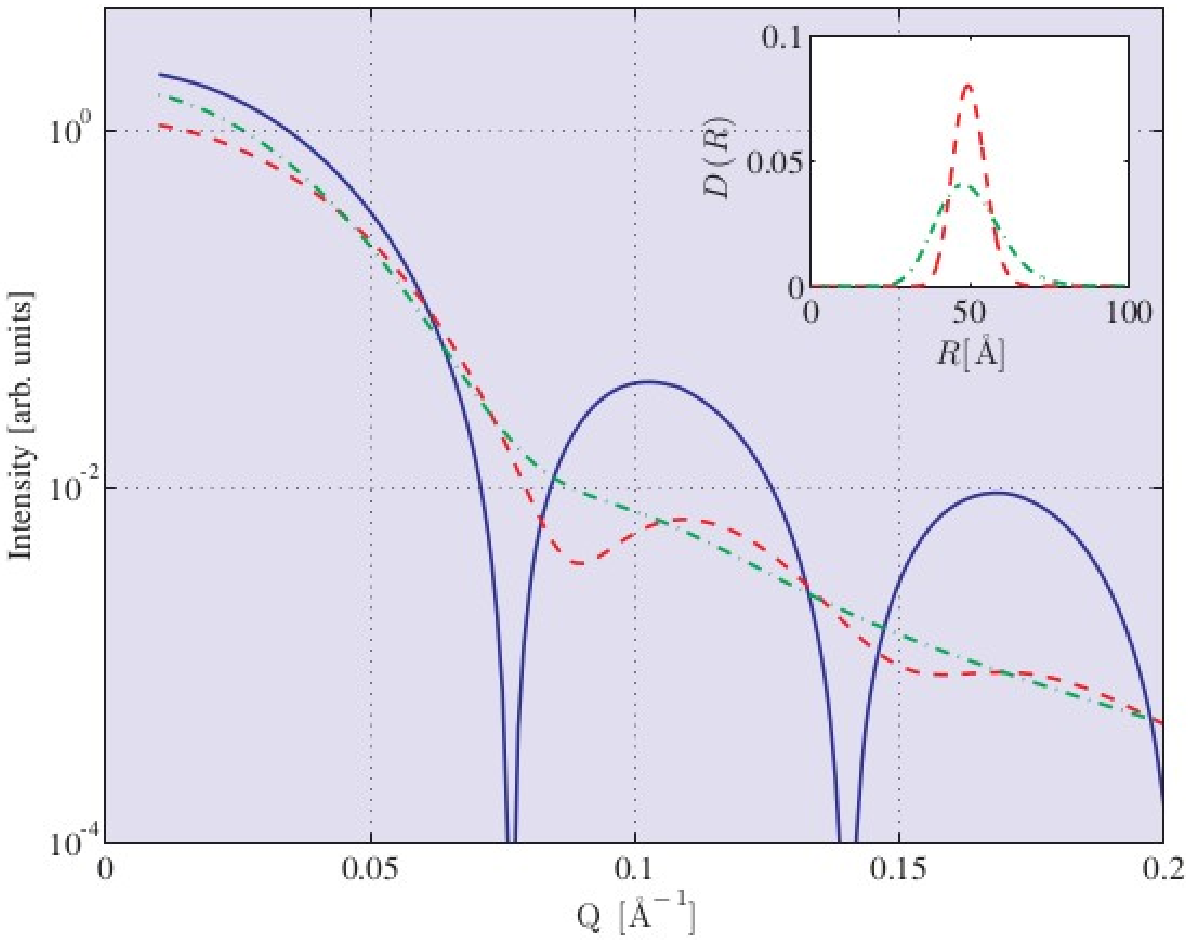
Als-Nielsen, Jens, and Des McMorrow. Elements of modern X-ray physics. John Wiley & Sons, 2011.

Polidispersividade



Distribuição de
tamanho de partículas

$$I(q) = \Delta\rho_e^2 \int_0^\infty D(R) V_p(R)^2 |F(q,R)|^2 S(q,R) + B(q)$$



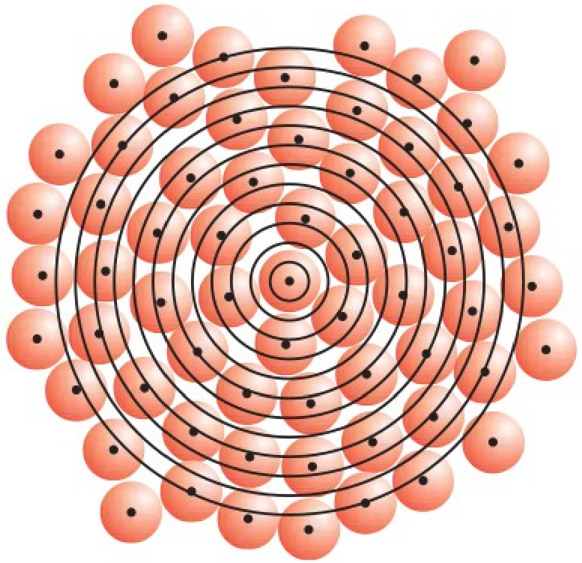
Als-Nielsen, Jens, and Des McMorrow. Elements of modern X-ray physics. John Wiley & Sons, 2011.

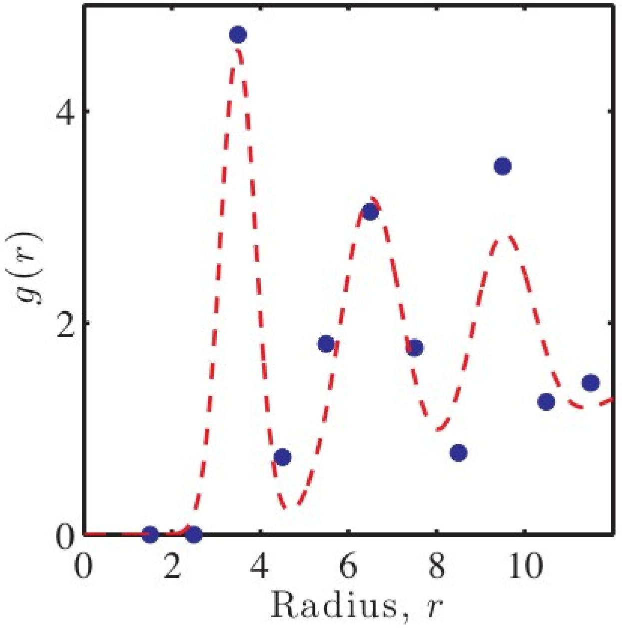
Fator de estrutura

$$S(q) = \frac{1}{N}\langle\widetilde{\rho}_{-\boldsymbol{q}}\widetilde{\rho}_{\boldsymbol{q}}\rangle = \frac{1}{N}\left\langle\sum_{i,j} e^{iq(r_j - r_i)}\right\rangle$$

Relacionado diretamente às interações entre partículas

$$S(q) = 1 + \rho\int(g(r) - 1)e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\,\mathrm{d}r^3$$





Als-Nielsen, Jens, and Des McMorrow. Elements of modern X-ray physics. John Wiley & Sons, 2011.

Equação de Ornstein-Zernike

$$h(r) = g(r) - 1 = c(r) + \rho \int c(|\boldsymbol{r} - \boldsymbol{r}'|)h(r')\,\mathrm{d}^3 r'$$

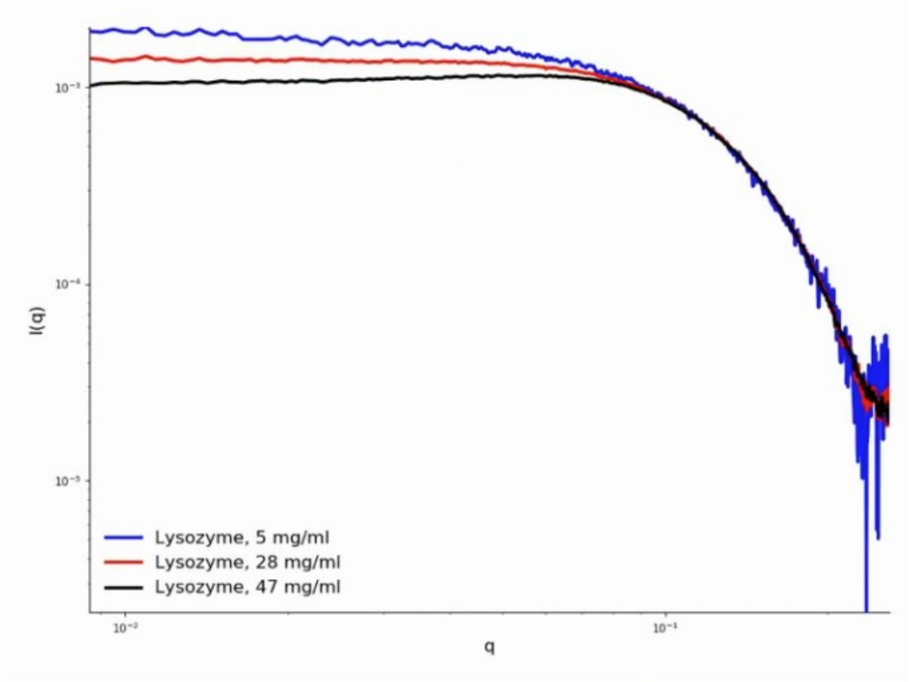
Relação com o potencial de pares

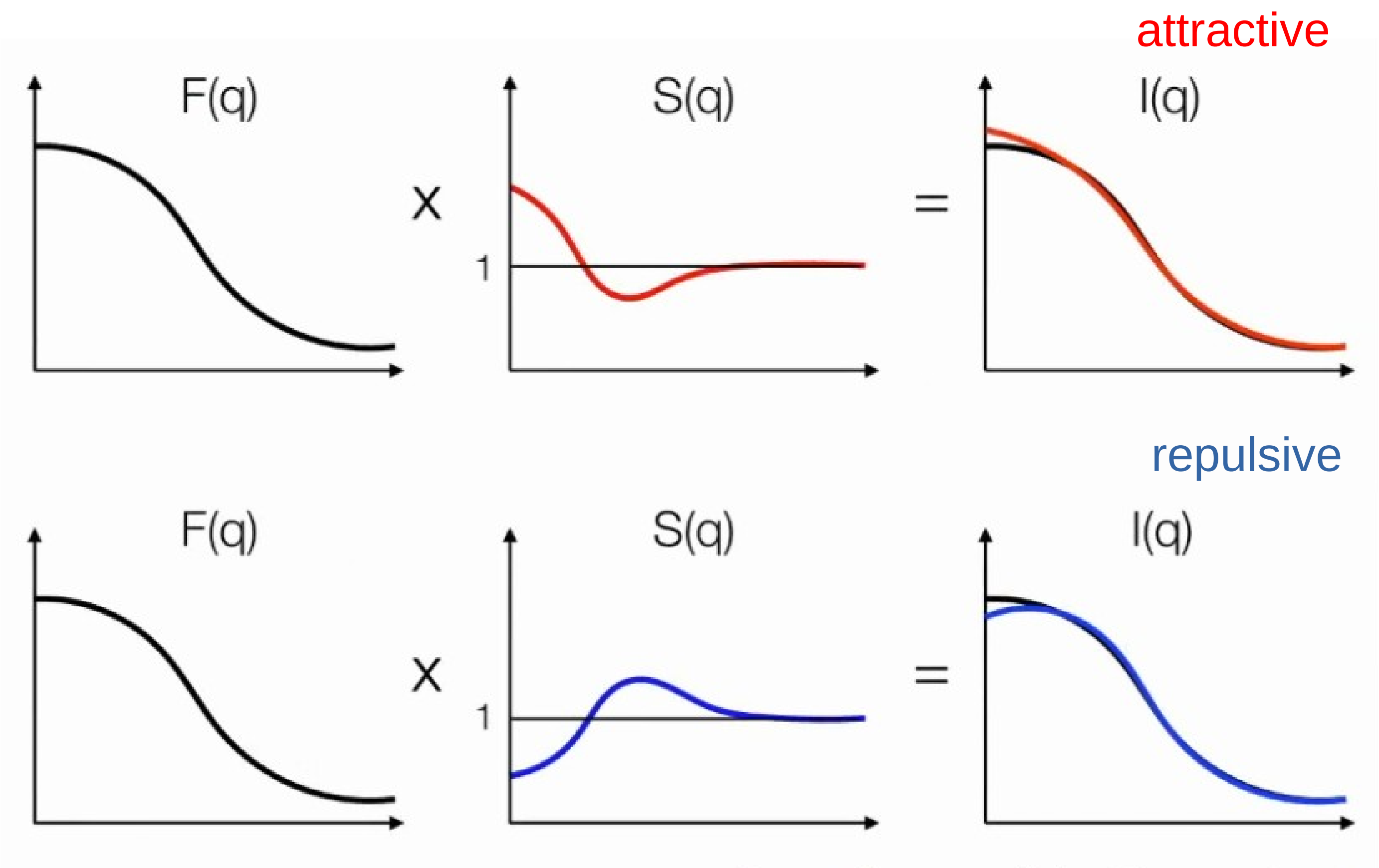
Relações de fechamento:

- **RPA** (**R**andom **P**hase **A**pproximation**):** $c(r) = -\beta u(r)$
-
- **MSA** (**M**ean-**S**pherical **A**pproximation): $c(r) = \begin{cases} g(r)(1 - e^{-\beta u(r)}), r < \sigma \\ -\beta u(r), r > \sigma \end{cases}$
- **PY** (**P**ercus-**Y**evic): $c(r) = (1 - e^{-\beta u(r)})(h(r) + 1)$
- **HNC** (**H**yper**n**eted-**C**hain) $c(r) = -\beta u(r) + h(r) - \ln(1 + h(r))$
- SCOZA, SMSA, HMSA, RY, ...

C. Caccamo, Integral Equation Theory Description of Phase Equilibriain Classical Fluids, Physics Report 274, 1-105

Interparticle interaction

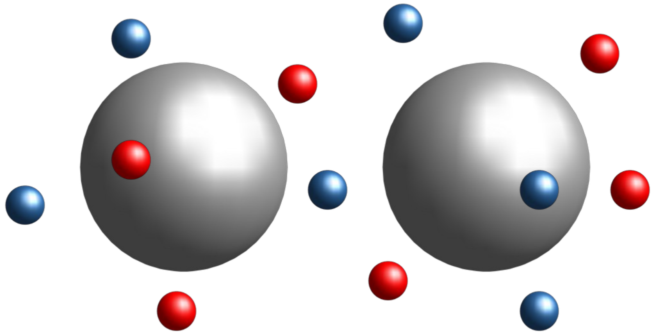


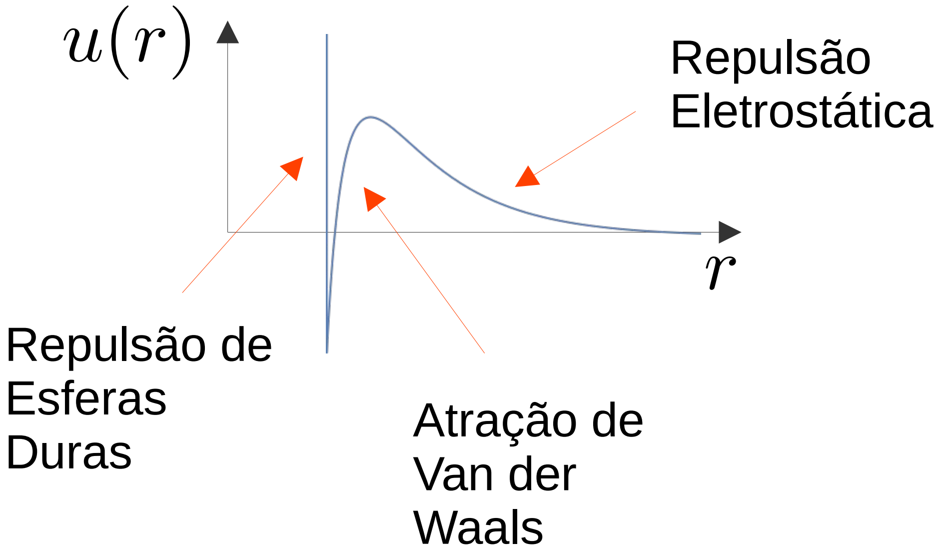


$$S(q) = \frac{1}{1 - \rho \widetilde{c}(q)} = \frac{1}{1 + \rho \beta \widetilde{u}(q)}$$ (RPA)

Hansen, Jean-Pierre, and Ian Ranald McDonald. Theory of simple liquids. Academic Press, 2013.

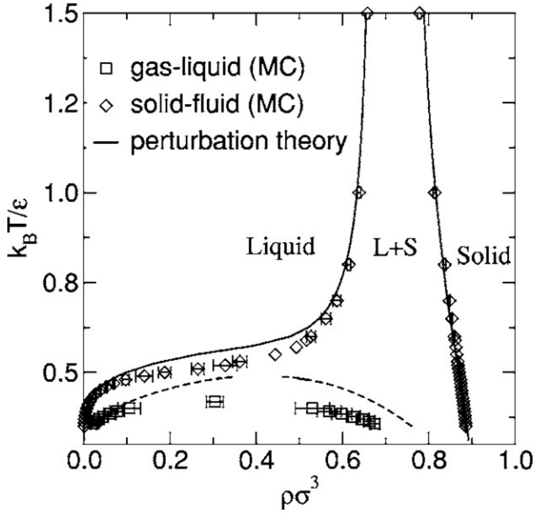
Aplicação a sistemas coloidais





- Propriedades das partículas:
  Carga, formato, Hamaker

- Sistema coletivo:
  Gás, líquido, sólido, (?)



- Potenciais de pares
- Esferas duras (hard-spheres):

$$u(r) = \begin{cases} \infty, r < \sigma \\ 0, r > \sigma \end{cases}$$

- Yukawa

$$u(r) = K\frac{e^{-\kappa(r-\sigma)}}{r}$$

- Van der Waals

$$u(r) = -\frac{A}{12}\left[\frac{\sigma^2}{r^2-\sigma^2} + \frac{\sigma^2}{r^2} + 2\ln\left(\frac{r^2-\sigma^2}{r^2}\right)\right]$$

E. J. W. Verweyand J. TH. G. Overbeek, Theory of the Stability of Lyophobic Colloids, Elsevier, Amsterdam, (1948)