

Form factors averaged over particle sizes and orientations

Incomplete or withdrawn chapter of Physics Reference

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0.1 TODO

0.1.1 Literature

Schulz distribution [?, 1]

 Orientational averages: sphere, rod, disk [?] spheroid (approximative) [1].

 Porod limit [?]

0.2

0.2.1 General formalism for form factor averages

The *form factor amplitude* of particle Π at wave vector \mathbf{q} is

$$F(\mathbf{q}) := \int_{\Pi} d^3r e^{i\mathbf{q}\mathbf{r}}. \quad (1)$$

Its squared modulus shall be designated as *form factor intensity*,

$$P(\mathbf{q}) := |F(\mathbf{q})|^2. \quad (2)$$

The scattering of a particles mixture depends on the averages $\langle F(\mathbf{q}) \rangle^2$ and $\langle P(\mathbf{q}) \rangle$.

Förster et al [2] studied averages under a distribution $h(R)$ of the particle size R and a distribution $f(\Omega)$ of the particle orientation Ω ,

$$\langle A(\Pi) \rangle_{R,\Omega} := \int_0^\infty dR h(R) \int_{4\pi} d\Omega f(\Omega) A(\Pi(R, \Omega)). \quad (3)$$

Here we generalize, and at the same time simplify notation, by considering an operator Γ with associated matrix $\mathbf{\Gamma}$ that may rotate, stretch, or deform a simpler geometric body Π ,

$$\Gamma\Pi := \{\mathbf{r} \mid \mathbf{\Gamma}^{-1}\mathbf{r} \in \Pi\}. \quad (4)$$

Let $\mathbf{\Gamma}$ have the distribution $g(\mathbf{\Gamma})$. The average form factor amplitude is

$$\langle F(\mathbf{q}; \mathbf{\Gamma} \Pi) \rangle_{\Gamma} = \int d\mathbf{\Gamma} g(\mathbf{\Gamma}) \int_{\Pi} d^3r e^{i\mathbf{q}\mathbf{r}} \quad (5)$$

$$= \int d\mathbf{\Gamma} g(\mathbf{\Gamma}) \int_{\Pi} d^3r' |\mathbf{\Gamma}| e^{i\mathbf{q}\mathbf{\Gamma}\mathbf{r}'} \quad (6)$$

$$= \int d\mathbf{\Gamma} g(\mathbf{\Gamma}) |\mathbf{\Gamma}| F(\mathbf{\Gamma}^T \mathbf{q}; \Pi). \quad (7)$$

By the same reasoning, the average form factor intensity is

$$\langle P(\mathbf{q}) \rangle_{\Gamma} = \int d\mathbf{\Gamma} g(\mathbf{\Gamma}) \left| F(\mathbf{\Gamma}^T \mathbf{q}; \Pi) \right|^2. \quad (8)$$

0.2.2 Size distribution

The particle size R shall be quantified by its ratio

$$\rho := R/R_0 \quad (9)$$

relative to a reference size R_0 . In the formalism of Sec. 0.2.1, this is described by the matrix

$$\mathbf{\Gamma}_{\rho} = \rho \mathbf{1}, \quad (10)$$

which transforms a particle Π of size R_0 into a particle $\mathbf{\Gamma}_{\rho} \Pi$ of size R . It contributes a factor $|\mathbf{\Gamma}_{\rho}| = \rho^3$ to the substitution (6). If the form factor amplitude is $F_{\Pi}(\mathbf{q})$ for the reference particle, then its average under the size distribution is

$$\langle F(\mathbf{q}; \mathbf{\Gamma}_{\rho} \Pi) \rangle_{\rho} = \int d\rho \rho^3 h(\rho) F(\rho \mathbf{q}; \Pi). \quad (11)$$

Averages over particle sizes can easily be combined with averages over particle orientations because $\mathbf{\Gamma}$ is just a multiple of the unit matrix and therefore commutes with any other matrix.

0.2.3 Gamma distribution

From here on, we need to assume a specific distribution h . Following Refs [2], we choose the Schulz-Zimm distribution

$$h(\rho) \equiv p_{\gamma}(\rho; \kappa, \kappa), \quad (12)$$

which is just a gamma distribution

$$p_{\gamma}(x; \alpha, \beta) := \frac{\beta^{\alpha}}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}, \quad (13)$$

scaled such that $\langle \rho \rangle = \alpha/\beta = 1$. It has the variance $\alpha/\beta^2 = 1/\kappa$. In polymer physics, it is parameterized through the dispersity $z := \langle \rho^2 \rangle = 1 + 1/\kappa$.

Straightforward computation yields the average

$$\langle x^m e^{i\eta x} \rangle = \frac{\Gamma(\alpha + m)}{\Gamma(\alpha)} \frac{\beta^{\alpha}}{(\beta - i\eta)^{\alpha+m}} = \alpha^{\overline{m}} \frac{\beta^{\alpha}}{(\beta - i\eta)^{\alpha+m}} = \frac{\alpha^{\overline{m}}}{\beta^{\overline{m}}} \frac{1}{(1 - i\eta/\beta)^{\alpha+m}} \quad (14)$$

with the raising factorial $a^{\overline{n}} := a(a+1) \cdots (a+n-1)$.

0.2.4 Sphere

The form factor of a sphere with radius R is

$$F(q; R) = \frac{4\pi}{q^3} \tilde{F}(qR) \quad (15)$$

with

$$\tilde{F}(x) = \sin x - x \cos x. \quad (16)$$

To make contact with Ref. [2], we note that $\tilde{F}(x) = x^2 j_1(x)$ with the spherical Bessel function

$$j_1(x) \equiv \sqrt{\frac{\pi}{2x}} J_{3/2}(x) = \frac{\sin x - x \cos x}{x^2}, \quad (17)$$

which can also be expressed as generalized hypergeometric series ${}_0F_1(5/2; \cdot)$.

The average form factor amplitude (11) is

$$\langle F(\mathbf{q}; \Gamma_\rho \Pi) \rangle_\rho = \frac{4\pi}{q^3} \int d\rho p_\gamma(\rho; \kappa, \kappa) \tilde{F}(\rho q R_0) \quad (18)$$

$$= -\frac{4\pi}{q^3} \operatorname{Re} \int d\rho p_\gamma(\rho; \kappa, \kappa) (ie^{i\rho q R_0} + (\rho q R_0)e^{i\rho q R_0}), \quad (19)$$

which has the right form to apply (14):

$$\langle F(\mathbf{q}; \Gamma_\rho \Pi) \rangle_\rho = -\frac{4\pi}{q^3} \operatorname{Re} \left[\frac{i}{(1 - iqR_0/\kappa)^\kappa} + \frac{1}{(1 - iqR_0/\kappa)^{\kappa+1}} \right] \quad (20)$$

$$= -\frac{4\pi}{q^3} \operatorname{Re} \frac{i + (\kappa + 1)qR_0/\kappa}{(1 - iqR_0/\kappa)^{\kappa+1}}. \quad (21)$$

Bibliography

- [1] M. Kotlarchyk and S.-H. Chen, J. Chem. Phys. **79**, 2461 (1983). [1](#)
- [2] M. Wagener and S. Förster, Sci. Rep. **13**, 780 (2023). [1](#), [2](#), [3](#)