Form factors of particle systems in dilute solutions

Munirat Idris
250998407
Chemistry
https://github.com/midris28/Final-Project-Munirat-Idris.git

1 Introduction

Static Light Scattering (SLS), also known as laser light scattering, is a versatile and powerful technique used to measure the size and shape (form factor) of particles in a sample, as well as their spatial arrangement and interaction (structure factor) [6] . SLS can be applied to many particle systems, from simple colloids to complex macromolecules, making it a valuable tool in many scientific disciplines. SLS illuminates a sample with monochromatic light (often from a laser) and measures the intensity of the scattered light as a function of the scattering angle. The variation in scattering intensity with angle can be related to variations in the density of the scatterers within the sample, thus providing insights into both the individual properties of the scatterers (via the form factor) and their collective arrangement (via the structure factor).

SLS is a non-invasive and powerful technique to study the structural properties of particles and macromolecules in a solution [1]. It involves measuring the intensity of light scattered by a sample as a function of scattering angle or time, providing valuable information about particle size, shape, concentration, and interactions. When a beam of light passes through a solution containing particles, the particles scatter the incident light in all directions. The intensity of scattered light depends on particle size, shape, and concentration. By analyzing the scattering pattern, SLS can provide quantitative information about these properties. Briefly, SLS experiments typically use a light scattering instrument equipped with a laser or monochromatic light source, a detector, and optical components for collecting and analyzing scattered light. The detector measures the intensity of scattered light at different angles to obtain angular scattering profiles or autocorrelation functions [1]. In static scattering, the intensity of scattered light is measured as a function of scattering angle or time, providing information about particle size, shape, and interactions.

Particle systems are the mathematical and computational models used to simulate the behavior of a collective of particles, such as atoms or photons, in a given physical environment [20]. Particle systems, crucial in materials science, physics, and chemistry, consist of particles with shapes and sizes that can significantly impact the material's properties.

The form factor, $P(q)$, describes how an individual particle scatters light. It is a function of the scattering vector, q, which is related to the scattering angle and the wavelength of the incident light [16]. In light scattering experiments, the measured intensity is directly related to the form factor when particles are sufficiently dilute, so inter-particle interference are neglected. The form factor in particle systems, a fundamental concept in the study of scattering experiments, relates to how individual particles scatter light or other forms of electromagnetic radiation [12]. It is a critical parameter for understanding and interpreting scattering experiment results, offering insights into the particles' size, shape, and internal structure within a given system. The form factor function essentially describes how the scattering intensity varies with the scattering angle for a single particle, assuming the particle is isolated and there are no interparticle interactions. The structure factor, $S(q)$, comes into play when particles are not dilute; hence, there is interference from scattering off different particles. This factor provides information about the spatial distribution of particles within the sample. When particles are closer, their interaction and relative positioning affect the scattering, introducing peaks in the scattered intensity characteristic of ordered structures or showing a more uniform distribution in fluids or amorphous solids [8]. Analyzing these patterns allows for determining the degree of order, the presence of specific lattice structures in crystals, or the characteristics of liquid crystals or glasses. In general, the intensity of scattered light, $I(q)$, measured in any light scattering experiment is proportional to the product of the form factor and the structure factor :

$$I(q) \propto P(q) \cdot S(q) \tag{1}$$

Where P is the form factor, and S is the structure factor
This equation provides information about particle characteristics (size, shape) and their collective arrangement (spacing, order). Scattering data analysis enables delineation of these contributions, although it may require modeling and fitting procedures, especially when dealing with complex or polydisperse systems. When interactions between particles are significant, as in concentrated suspensions or solutions, additional factors, such as the structure factor, come into play, accounting for the particles' spatial arrangement and interaction [11].
The study of particle systems in materials science often focuses on understanding the behavior and properties of systems consisting of monodisperse spheres, bidisperse spheres, and cylindrical rods. These systems are foundational models for various materials, from colloidal suspensions to complex nanocomposite structures. Monodisperse spheres represent a system of uniform particles in size and shape. This idealized system is a benchmark for understanding the fundamental properties of spherical particles without the complexity introduced by size and shape variations. Investigating monodisperse systems allows us to develop models that predict how spherical particles scatter light or radiation. This is crucial for determining particle size distribution and interactions in complex systems [7]. Bidisperse spheres involve two distinct sizes of spherical particles. This system introduces an additional layer of complexity, enabling the study of how size disparity affects the material's packing, stability, and phase behavior. It is possible for particles of different sizes to interact with each other in bidisperse systems, which is different from monodisperse systems. This can create new structures and effects, like phase separation or better mechanical properties [21].
Cylindrical rods, on the other hand, introduce anisotropy due to their elongated shape, which significantly affects their packing behavior, orientation, and flow in a medium. The study of cylindrical rods is essential for understanding fibrous materials, liquid crystals, and other anisotropic systems [22]. Their unique geometry influences materials' mechanical, optical, and thermal properties, making the characterization of their form and structure factors crucial for applications in polymer science and nanotechnology. The form factor provides insights into the individual particle's size, shape, and internal structure.
The focus of this study is to delve into the potential of light scattering in understanding different particle shapes and analyzing their physical and statistical properties, with an emphasis on only the form factors because we are working with dilute solutions. This objective is of utmost importance as it paves the way for a deeper understanding of the underlying physics and chemistry of the systems under investigation. To achieve this, I employ Python code for data analysis. The code is meticulously designed to generate simulated data and perform statistical characterization, thereby advancing our understanding of complex particle systems

2 Theoretical mathematical expressions of the form factor for each geometric shape

Monodisperse spheres form factor

The form factor of monodisperse spheres is a fundamental concept in scattering data analysis, crucial for elucidating the structural properties of materials at the nanoscale. Mathematically, the form factor $P(q)$ of a monodisperse spherical particle is defined as the Fourier transform of its electron density distribution, which reflects how scattering intensity varies with the scattering vector q [5]. The scattering vector is inversely related to the distance over which variations in electron density are observed and is given:

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

where θ is half the scattering angle and λ is the wavelength of the incident radiation.
For spherical particles of radius R, the form factor is given by:

$$P(q) = \left(\frac{3\left[\sin(qR) - (qR)\cos(qR)\right]}{(qR)^3} \right)^2 \quad (3)$$

This equation describes how the intensity of scattered light (or other radiation) diminishes as the scattering angle increases, capturing the particles' spherical symmetry and uniform electron density. It assumes the particles are homogenous and isotropic, meaning they scatter light equally in all directions [8]. The spherical Bessel function is pivotal in defining the form factor, especially in scattering studies where it encapsulates particles' spatial distribution and size. The form factor $P(q)$ is essentially derived from these functions, revealing the scattering profile due to a single particle. For spherical particles, the form factor can be expressed in terms of the spherical Bessel function of the first kind, $j_0(x)$, given as:

$$j_0(x) = \frac{\sin(x)}{x} \quad (4)$$

In the mathematical formulation for the form factor of monodisperse spheres, the spherical Bessel function appears due to the Fourier transform of the spherical particle's spatial electron density. Incorporating the spherical Bessel function into the form factor equation is important because it accurately describes how the intensity of scattered waves diminishes due to the interference effects at different angles for spherical particles [5]. It captures how the physical geometry, particularly the spherical shape and size, affects the scattering pattern.

Form factor for Bi/polydisperse sphere systems.
Bidisperse sphere systems consist of a mixture of spherical particles of two distinct sizes. These systems are more complex than monodisperse systems, which contain particles of only one size because introducing a second particle size introduces new variables and interactions. The characteristics and behavior of bidisperse sphere systems are not merely an average of the two individual components; instead, they exhibit unique properties and phenomena resulting from the interplay between the different-sized particles [2]. One of the defining characteristics of bidisperse systems is how the size disparity affects particle interactions and spatial arrangement. Smaller particles can fit into the spaces between larger ones, affecting the maximum packing density and influencing the system's rheological properties. In a bidisperse system, the overall scattering intensity is influenced by the individual form factors of the small and large spheres and the distribution of these sphere sizes[2]. The form factor of each particle size in a bidisperse system can be described using the same mathematical formulation as for monodisperse spheres. Still, the total scattering intensity observed will be a weighted average of the two, where the weights correspond to the volume fraction and number density of each particle size. Specifically, for spheres, the form factor $P(q)$ is also calculated as in equation (3).
In addition to considering the individual form factors, it is crucial to account for interference effects arising from the spatial arrangement of particles. In bidisperse systems, these effects can be more complex due to the presence of two different sizes of spheres, which can lead to a more intricate interference pattern than monodisperse systems [19]. This complexity is particularly noticeable when the spheres are in close packing conditions or when the size ratio and concentration of the two types of spheres lead to unique structural formations. The overall scattering pattern of a bidisperse sphere system is notably affected by the volume fraction and the size ratio of the two types of spheres [5].
The form factor is calculated separately for each of the two sizes. Since the form factor is dependent on the sphere's radius, the presence of two distinct sizes means performing this calculation twice, once for each radius. The overall scattering intensity from the bidisperse system is a weighted average of the scattering from each sphere size. The weights are typically based on the volume fraction or number density and scattering contrast of each particle size within the mixture [21, 4, 3]. This means calculations must account not just for the differing form factors but also for how much each population of spheres contributes to the total scattering. The interference between scattered

waves from particles of different sizes influences the scattering pattern from a bidisperse system. The variation in radii leads to different phase differences in the scattered waves, which can significantly alter the interference pattern compared to a monodisperse system.
Even though the system is bidisperse, the form factor of each particle size can be described using the same mathematical formulation as for monodisperse spheres, but the interpretation and application of this formulation require consideration of the size distribution; a standard model used for this purpose is the Schulz distribution. The Schulz distribution, a type of size distribution function, is beneficial for modeling the size distribution of particles in polydisperse systems—systems with particles of varying sizes. In a bidisperse system, the normalized Schulz distribution allows for a statistical representation of the spread of the sizes of the small and large spheres. The parameters of the Schulz distribution can be tailored to accurately reflect the proportion and distribution of the two different sphere sizes within the system [13].
In a bidisperse system, considering each particle size's form factor separately allows for analyzing how each population contributes to the overall scattering pattern. However, because the system contains particles of two different sizes, normalizing the form factor by the average volume of the particles becomes crucial for meaningful comparison and integration of the scattering contributions from both sizes. This normalization involves scaling the form factor by the volume fraction of the particles, which accounts for the actual physical volume occupied by the particles of each size in the solution [13]. Despite the particles different sizes, this approach helps quantify the scattered intensity in comparable units. Let's outline the necessary mathematical expressions and their implications to delve into the mathematical aspects of scattering by bidisperse systems, including the Schulz distribution and the normalization of form factors by average volume. The form factor, $P(q)$, for spherical particles as a function of the scattering vector magnitude, q, is given by:

$$P(q,R) = \left(\frac{3[\sin(qR) - qR\cos(qR)]}{(qR)^3} \right)^2 \tag{5}$$

where R is the radius of the sphere, and $q = 4\pi \sin(\theta)/\lambda$ with θ being the scattering angle and λ the wavelength of the incident radiation.
The size distribution of particles in a bidisperse system can be characterized by the Schulz distribution, $Z(R)$, which for the radius R is expressed as:

$$Z(R; z, R_{\text{avg}}) = \frac{1}{R_{\text{avg}}} \left(\frac{z+1}{R_{\text{avg}}} \right)^{(z+1)} \frac{R^z \exp\left(-\frac{(z+1)R}{R_{\text{avg}}} \right)}{\Gamma(z+1)} \tag{6}$$

where R_{avg} is the average radius of the particles,
z is a parameter related to the breadth of the distribution (with larger values of z indicating narrower distributions),
$\Gamma(z+1)$ is the gamma function evaluated at $z+1$.

For a population of spheres with a distribution of sizes, the average form factor is obtained by integrating over the size distribution, $Z(R)$, weighted by the volume each radius contributes, which emphasizes larger particles due to their volume [13]. The normalized form factor by average volume, $\langle P(q) \rangle$, becomes:

$$\langle P(q) \rangle = \frac{\int P(q,R) R^3 Z(R)\, dR}{\int R^3 Z(R)\, dR} \tag{7}$$

Given that $\langle P(q) \rangle$ normalizes the scattering data by the volume distribution of the particles, this expression ensures that the scattering intensity reflects the actual physical contribution of particles of different sizes. For a bidisperse system of small and large spheres, the overall scattering intensity, $I(q)$, can be modeled by summing the contributions from each population (denoted as 1 for small and 2 for large spheres), considering their respective volume fractions (v_1 and v_2) and form factors ($\langle P_1(q) \rangle$ and $\langle P_2(q) \rangle$):

$$I(q) = v_1 \langle P_1(q) \rangle + v_2 \langle P_2(q) \rangle \tag{8}$$

In practice, the volume fractions v_1 and v_2 should sum to 1 ($v_1 + v_2 = 1$) for closed systems or represent the respective proportions for open/dilute systems.

Form factor of monodisperse cylindrical rods

Cylindrical rods, a fundamental geometric shape, are extensively studied in various scientific and engineering disciplines due to their unique geometric attributes and versatile applications ranging from materials science to mechanical engineering. A cylindrical rod is characterized by its length (L) and diameter (D) or radius (r), with the diameter being twice the radius ($D = 2r$). The simplicity of this geometry belies the complexity and the diversity of the applications and theoretical considerations it entails [14]. A cylindrical rod's surface area includes the curved surface and the areas of the two circular ends. The total surface area can be calculated as:

$$A = 2\pi rL + 2\pi r^2 = \pi D(L + \frac{D}{2}) \tag{9}$$

The volume of the cylinder is the product of the base area and the height (length) of the cylinder, which can be expressed as:

$$V = \pi r^2 L = \frac{\pi D^2 L}{4} \tag{10}$$

A necessary dimensionless quantity for cylindrical rods is the aspect ratio, defined as the ratio of the length to the diameter (L/D) or length to the radius (L/r). The derivation of the form factor for cylindrical rods can be intricate, relying on cylindrical coordinates and involving special functions like Bessel functions, which naturally emerge from solving problems with cylindrical symmetry [16]. The axial symmetry of the problem simplifies the form factor $P(q)$ to an integral involving the zero-order Bessel function $J_0(qr)$ due to the radial variation, and a simple cosine function for the length given as follows:

$$P(q) = \frac{1}{V} \int_0^L dz \int_0^R r\, dr\, J_0(qr\sin\theta) \int_0^{2\pi} d\phi\, \cos(qz\cos\theta) \tag{11}$$

Here, V is the volume of the cylinder, J_0 is the zeroth-order Bessel function of the first kind, and $qr\sin\theta$ and $qz\cos\theta$ arise from projecting the scattering vector q onto the radial and axial directions, respectively. Solving the integrals, considering the normalization where $V = \pi R^2 L$, yields:

$$P(q) = 2\frac{J_1(qR\sin\theta)}{qR\sin\theta}\frac{\sin(qL\cos\theta/2)}{qL\cos\theta/2} \tag{12}$$

where J_1 is the first-order Bessel function of the first kind. This expression describes how the cylindrical object scatters radiation as a function of q and the scattering angle θ.

In cylindrical coordinates, a rod can be described by its radius R, length L, and the radial (r), azimuthal (ϕ), and axial (z) coordinates. The scattering vector q is defined as $q = 4\pi\sin(\theta/2)/\lambda$, where θ is the scattering angle, and λ is the wavelength of the incident radiation.

The derivation of the form factor in this context leverages the cylindrical symmetry of the rods, leading to the integral over the cylinder volume that uses Bessel functions due to their appearance in solutions to wave equations in cylindrical coordinates. The form factor $P(q)$ for a cylinder is thus expressed as:

$$P(q) = \int_0^L dz \int_0^R rdr \int_0^{2\pi} d\phi\, e^{-iq\cdot r} \tag{13}$$

Here, $q \cdot r = qr\sin(\theta)\cos(\phi) + qz\cos(\theta)$, with θ between the vector q and the axis of the cylinder, simplifying due to the azimuthal integration to:

$$P(q) = \frac{1}{V} \int_{0}^{L} dz \int_{0}^{R} r dr \, J_0(qr\sin(\theta)) \, e^{-iqz\cos(\theta)} \tag{14}$$

Where V is the volume of the cylinder, and J_0 is the zeroth-order Bessel function of the first kind, reflecting the radial dependence. The axial dependence is evident in the exponential term. The integral can be evaluated to yield the form factor in terms of the scatter vector q and the dimensions of the cylinder:

$$P(q) = 2\frac{J_1(qR\sin(\theta))}{qR\sin(\theta)} \times \frac{\sin\left(\frac{1}{2}qL\cos(\theta)\right)}{\frac{1}{2}qL\cos(\theta)} \tag{15}$$

The aspect ratio (L/D, where $D = 2R$ is the diameter), significantly influences the scattering profile captured by the form factor. The aspect ratio determines the cylindrical rod's elongation and how this geometry scatters light. For rods with a high aspect ratio, the form factor emphasizes the scattering in directions perpendicular to the length of the rod [14]. In the limit of very high q, the form factor highlights the slender nature of the rods, making it sensitive to changes in rod length. Conversely, rods with a low aspect ratio behave more like disks in scattering experiments. Here, the scattering is more sensitive to the rod's diameter, impacting how $P(q)$ behaves at different q values.

3 Methods and methodology

Statistical characterization of selected particle systems

The mean intensity represents the average intensity of scattered light across the scattering pattern for each analyzed shape. It measures the overall strength of the scattering signal. Mathematically, the mean intensity is calculated using the following expression:

$$\overline{I} = \frac{1}{N}\sum_{i=1}^{N} I_i \tag{16}$$

where $\overline{I}$ is the mean intensity, N is the total number of measurements, and I_i is the intensity measured in the ith experiment or observation.

Variance is a statistical measure quantifying the scattering data spread or dispersion of intensity values. It provides insights into the variability or fluctuations in the signal intensity. The mathematical expression for variance is given by:

$$\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(I_i - \overline{I})^2 \tag{17}$$

where σ^2 represents the variance, N is the total number of intensity measurements, I_i is the intensity of the ith measurement, and $\overline{I}$ is the mean intensity of all measurements.

Statistical measures used to describe the distribution of data points are Skewness and Kurtosis, which are given as:

$$\text{Skewness} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{X_i - \overline{X}}{\sigma}\right)^3 \tag{18}$$

Skewness is a measure of distortion from a symmetrical distribution. A symmetric distribution is defined as having zero skewness. S is positive if the distribution is right-skewed and negative if left-skewed. Kurtosis, on the other hand, is a measure of the shape of distribution defined below

$$\text{Kurtosis} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{X_i - \overline{X}}{\sigma}\right)^4 - 3 \tag{19}$$

where N is the number of data points, X_i represents the ith data point, $\overline{X}$ is the mean of the data points, and σ is the standard deviation of the data points.
The subtraction by 3 in the Kurtosis formula adjusts it to a baseline where a normal distribution's kurtosis is 0. A normal distribution (Gauss distribution) is defined as having zero kurtosis. K is positive if the distribution is shaper or narrower than the normal distribution and negative if flattened. These formulas measure the asymmetry (Skewness) and the tailedness (Kurtosis) of the probability distribution of real-valued random variables.

Form factor equations used for particle system calculations implemented in the Python code
i) The form factor of a monodisperse spherical particle with a core structure used is described in the following equation and plotted in Python using the log-log scale
ii) The form factor of polydispersed spherical particles used in this study includes the expression for P (q) for the bimodal polydispersed spherical particles given above plotted in log-log scale
iii) The form factor for a monodisperse rigid cylinder rod with uniform scattering length density is described with the equations discussed earlier and plotted using Python in a log-log scale

Software packages used For this study, all software packages used are already installed in Python, and a few of the packages used are Numpy, panda, Mathplot, Scipy, Plotly, etc

4 Results

A. Statistical properties of monodisperse particle system of spheres

Monodispheres spheres
Monodisperse spheres represent a geometric particle system where each sphere is of uniform size and shape, differing from polydisperse systems where particle sizes vary. The statistical characterization of such systems involves the analysis of statistical metrics. The histogram provided a visual representation of the distribution of particle sizes in Figure 1(b). In the case of monodisperse systems, the histogram typically shows a single, sharp peak, indicating uniformity in particle size. This peak corresponds to the sphere's expected diameter of 50nm, providing immediate insight into the system's monodispersity, displayed in Figure 1(a).

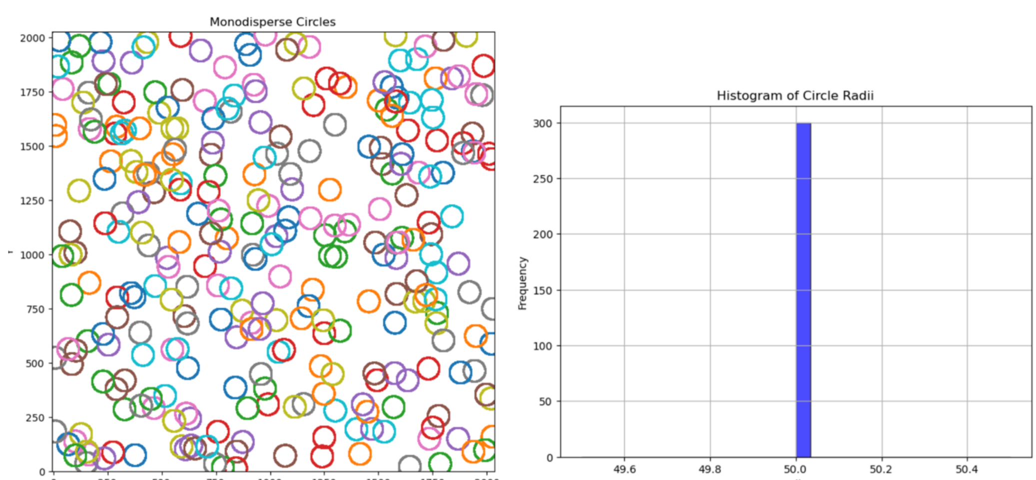

Figure 1: (a) Randomly generated monodisperse circles (b) Histogram of the monodisperse system indicating the uniformity in the system

The mean or average size of the spheres offers a measure of central tendency, which, in monodisperse systems, closely aligns with the size of nearly all particles within the sample. The variance and standard deviation are critical in quantifying the spread of the particle sizes around this mean. However, for monodisperse systems, both these measurements are markedly low, reflecting the minimal particle size variation [9]. Skewness is near zero in ideal monodisperse systems, indicating a symmetrical distribution around the mean. These statistical characteristics collectively offer a comprehensive understanding of the uniformity and dispersion of particle sizes in monodisperse systems.

Bi-disperse particle system In the study of bidisperse sphere systems, particles come in two distinct sizes, offering a richer field for statistical analysis than monodisperse systems, where all particles are the same size. The statistical characterization of these systems requires evaluating several key metrics to understand the distribution and interaction of spherical particle sizes within the system, as shown in Figure 2(a).

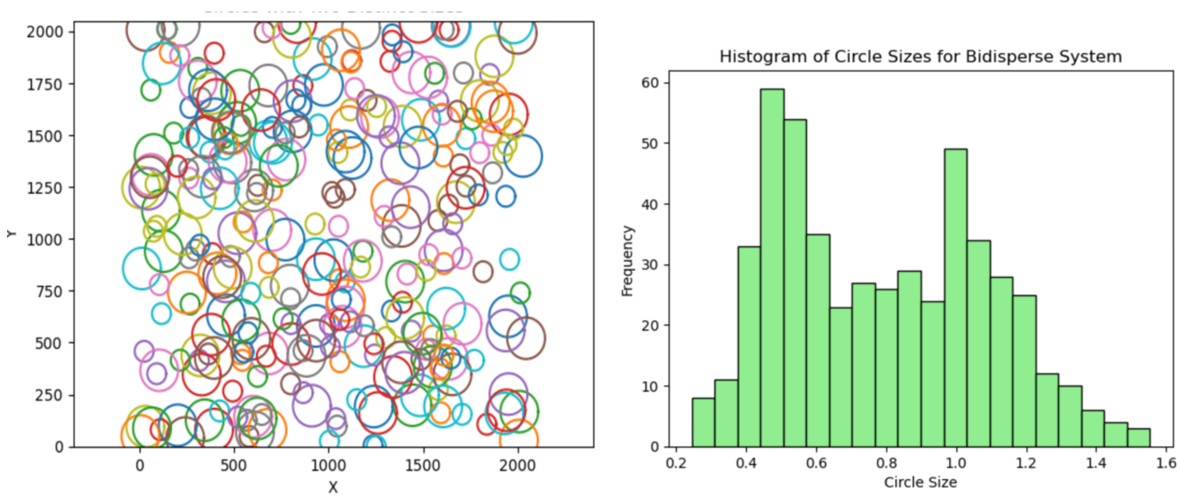

Figure 2: (a) Random bidisperse circles of two different radii (b) Histogram plot of the system, illustrating the randomness in the system

The histogram plot features two pronounced peaks corresponding to the two sizes (figure 2(b)). This bimodal distribution highlights the presence of two distinct particle sizes and is crucial for visualizing the proportion and distribution of each size within the system [17]. The calculated values are summarized in Table 1.

Mean	73.17
Standard deviation	24.93
Variance of length	621.64
Skewness of length	0.15

Table 1: Statistical characterization of bidisperse circle radii

This bidisperse system's mean or average radius measures central tendency, reflecting the system's overall scale. Still, the distribution of sizes is not the same, and this measure becomes less informative without considering the system's bimodality. Variance and standard deviation become particularly interesting in bidisperse systems, as they tend to be higher than in monodisperse systems. These statistics quantify the spread of particle sizes around the mean, showcasing the diversity inherent in bidisperse systems. Skewness in bidisperse distributions can reveal asymmetries in the size distribution, mainly if one particle size is more predominant than the other. However, ideal bidisperse systems where sizes are equally represented may exhibit low skewness, similar to monodisperse systems. For this study, both sizes in the system were equally represented.

Cylindrical rods of finite length

The statistical characterization of systems composed of cylindrical rods of finite length is crucial in understanding materials' structural and dynamical properties, such as liquid crystals, fibrous composites, and colloidal dispersions. Unlike spherical particles, cylindrical rods introduce anisotropy due to their shape, significantly affecting their packing, orientation, and phase behavior, necessitating a comprehensive statistical approach [15]. A histogram for cylindrical rods typically focuses on two key aspects: length and orientation distribution (Figure 3(b)). The length distribution histogram can reveal whether the system is monodisperse, with uniform-length rods, or polydisperse. The orientation distribution, depicted in a polar histogram, indicates the directionality of rods within the system, which is crucial for understanding their collective behavior. The mean length measures central tendency, while the variance and standard deviation quantify the spread of lengths around this mean, offering insight into the system's homogeneity. In purely monodisperse samples, variance and standard deviation are minimal, reflecting uniform rod lengths. However, a finite standard deviation is observed in real systems, indicating size dispersity [14].

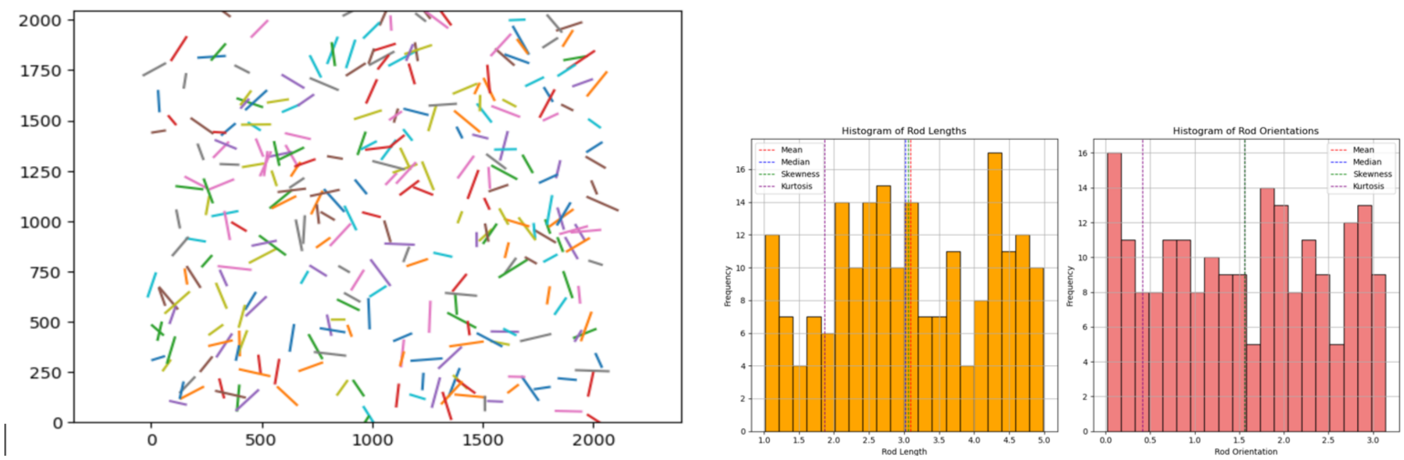

Figure 3: (a) randomly generated rods (b) Histogram of rods length and orientation

Skewness and kurtosis further detail the length distribution's shape and orientation. Skewness assesses the asymmetry, revealing whether shorter or longer rods predominate. At the same time, kurtosis measures the distribution's "tailedness," indicating the presence of outlier rod lengths significantly different from the mean (Table 2) and understanding these statistical characteristics aids in predicting the rods' packing efficiency, orientation order, and rheological properties, which are crucial for designing materials with specific mechanical and optical characteristics [18]. Such statistical analysis forms the backbone of theoretical models and simulations that guide the synthesis and application of rod-like particles in various industrial and scientific fields. We can conclude that the system is random from all the calculated particle values.

Rods	Rod length	Rod orientation
Mean	3.09	1.56
Standard deviation	1.13	0.93
Variance	1.27	0.87
Skewness	-0.03	0.00
Median	3.02	1.56
Kurtosis	-1.09	-1.23

Table 2: Statistical characterization of rod length and orientations

B) Calculated Form factors across the studied particle systems

The form factor is a mathematical function that describes how these particles scatter light or other electromagnetic radiation. This scattering behavior is crucial for analyzing and characterizing the materials' structural properties at the microscopic or nanoscopic level. Typically, form factors depend on the shape, size, and orientation of the particles within the system and the wavelength of the incident radiation.

1. Form Factor Monodisperse particle system

The form factor is well understood for a sphere, as shown in Figure 4. The calculated form factor is given as:

$$P(q) = \frac{3\left(\sin(qr) - qr\cos(qr)\right)}{(qr)^3} \tag{20}$$

where $P(q)$ is the form factor for a sphere, q is the scattering vector magnitude, and r is the radius of the sphere.

There are some exciting features in the plot. The slope of the plot in the high log q range is equal to -4, and it defines the Guinier region, indicating the radius of gyration. This gives the overall size of the particles. The Guiner approximation is only valid for very small angles where the plot is linear. At larger angles, the Porod region shows a periodic behavior with the minima reflecting higher symmetry and the scattering following a power-law decay, providing information about the internal structure. Figure 4 shows the assumption of a uniform density with no internal structure.

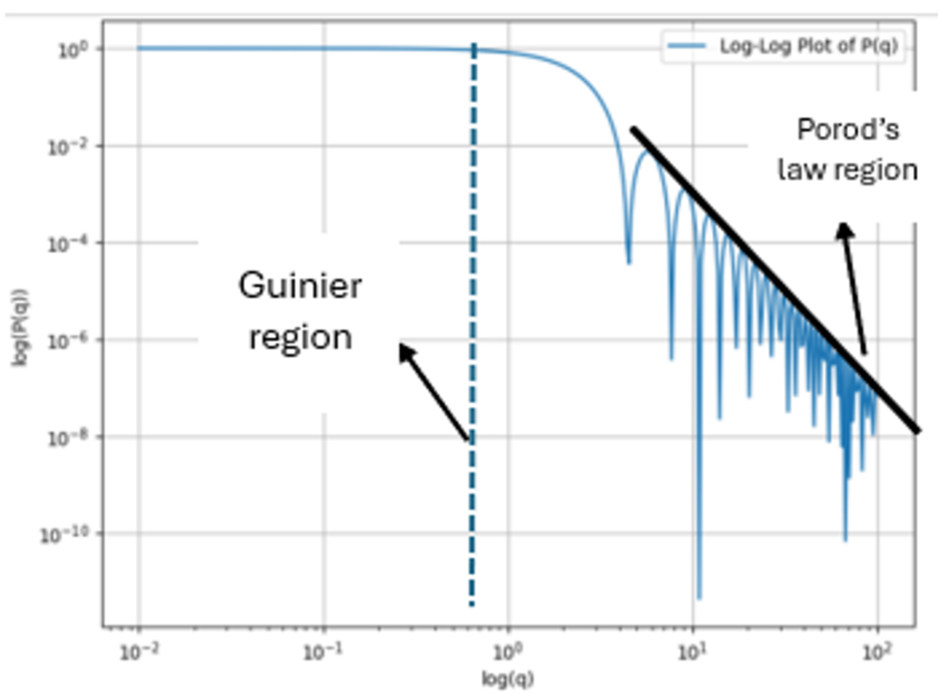

Figure 4: Form factor of a hard sphere

Considering a monodisperse spherical particle with a core shell structure described in equations (2-4) in the theoretical section and as shown in figure 5(a) and plotted in a log-log graph in figure 5(b)

Figure 5(a) shows the sketch of the monodisperse sphere indicating its core, and 5(b) shows the form factor that accounts for the contrast between the core shell and the surrounding medium. We also observe the Guinier region, which indicates that the radius of gyration is similar to that of a sphere.

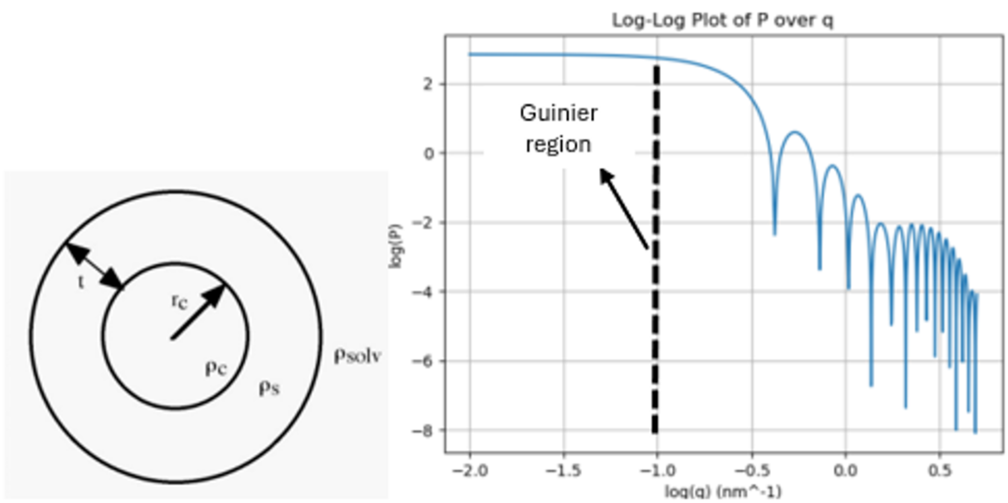

Figure 5: (a) sketch of monodisperse sphere (b) form factor of the monodisperse sphere

2. The form factor of a bidisperse particle system

In bidisperse systems, where two distinct sizes of spheres are present, the form factor becomes a weighted sum of the form factors of each particle size. This leads to a more complex pattern of scattering peaks shown in Figure 6(a), reflecting the coexistence of two different sizes. Observing these patterns provides information on the two-particle size distribution and relative concentrations. In Figure 6(b), the distribution plot indicates the two particle sizes of the circles in the bidisperse system.

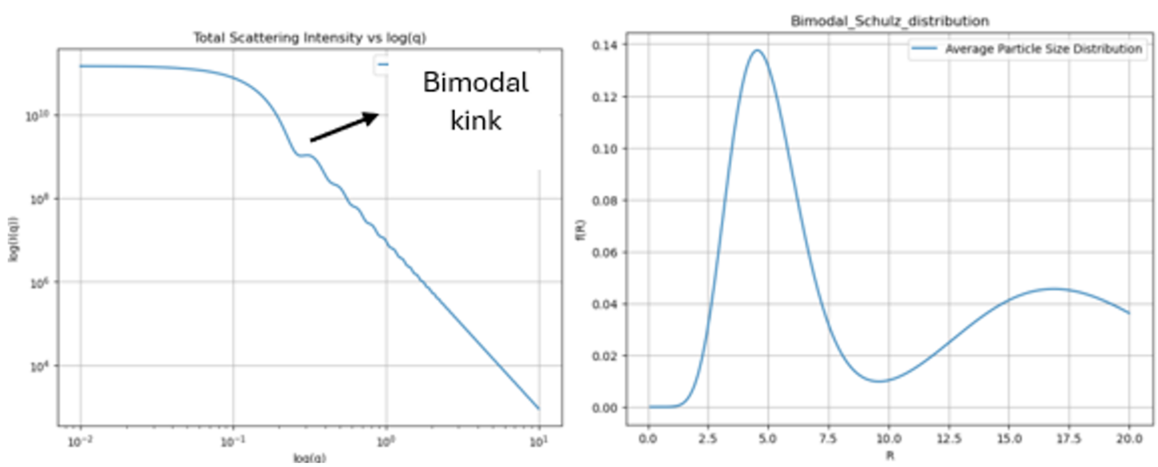

Figure 6: (a) form factor of a bidisperse sphere (b) bimodal Schulz distribution

3. The form factor of a cylindrical rod

Cylindrical rods of finite length introduce anisotropy into the scattering pattern due to their elongated shape. The form factor for cylindrical rods depends on their length, diameter, and orientation relative to the incident radiation [10]. For randomly oriented rods, the scattering intensity differs significantly from that of spheres, often showing a higher degree of anisotropy in the scattering pattern. Theoretical predictions for the scattering by cylindrical particles derived from the solutions to the scattering problem for infinitely long cylinders, modified to account for the finite length of the rods. For this study, the form factor calculated is for a monodisperse right circular cylinder with uniform scattering length density.

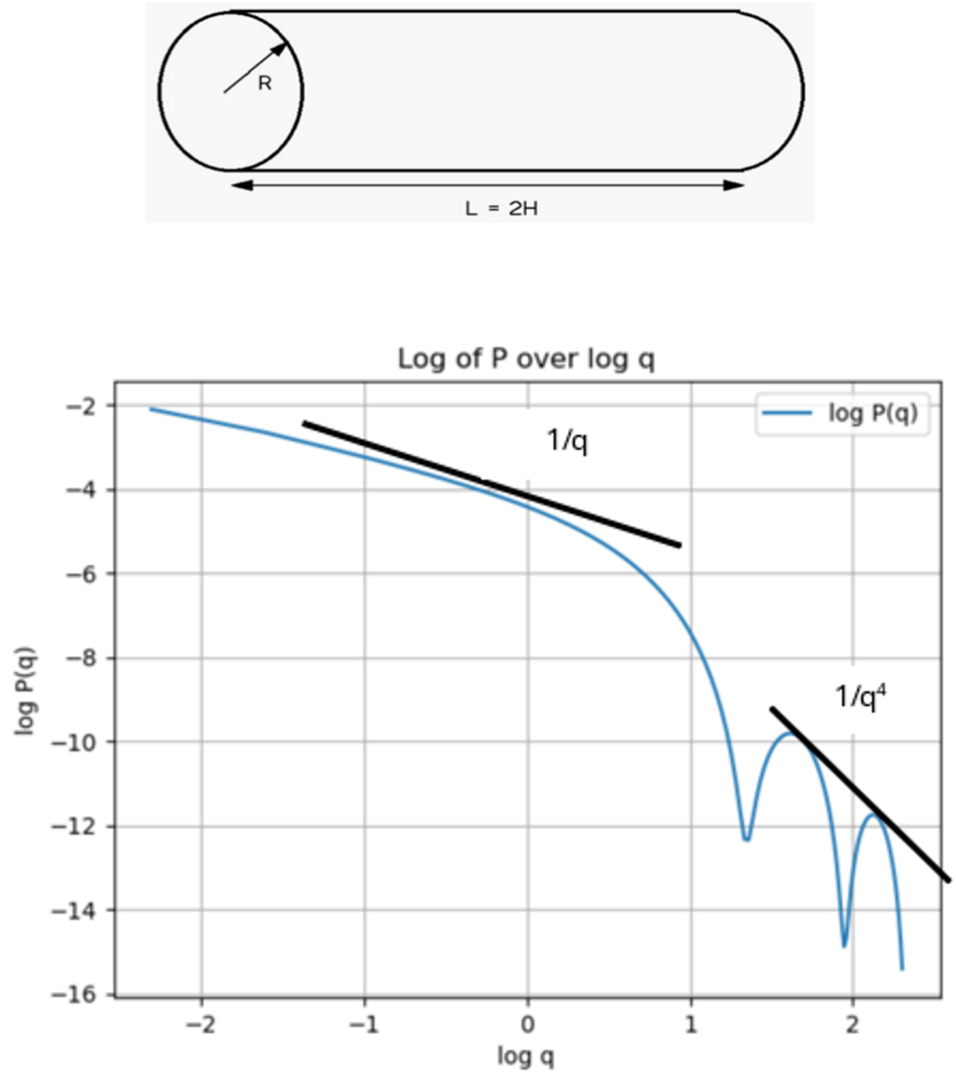

Figure 7: 7(a) schematics of a cylindrical rod (b) form factor for monodisperse right circular cylinder

The Guinier region reveals the cross-sectional radius of gyration for the perpendicular scattering and the length for the parallel scattering. Rod shows characteristic decay in the Porod region, which is proportional to q-1 as illustrated in Figure 7(b) and with a slope of -1, reflecting their elongation, which is typical for a cylindrical rod in similar agreement to a previous study[1].

C). Comparison with theoretical equations for each particle system using Least square methods and Structural Similarity Measurement

We compared our calculated values with each particle system's theoretical values using Least square methods and Structural Similarity Index Measurement (SSIM). The calculated standard error, SSIM values, and the goodness of fit for all the considered particle systems are given in Table 3. The Least square error is a method used to minimize the sum of the square differences between observed and predicted values. In contrast, standard error measures the dispersion of sample mean estimates from the population mean. The bidisperse system error is significantly higher than the rest in all systems. This was expected as the goodness of fit for the system was extremely high, indicating that the calculated model was flawed.

The Structural Similarity Index (SSI), or the Structural Similarity Index Measure (SSIM), is a metric used to assess the similarity between two images. It provides a quantitative evaluation of image quality or the degree of similarity between two images by considering changes in texture, luminance, and contrast rather than focusing

Particle systems	Sphere	Monodisperse sphere	Bidisperse sphere	cylindrical rod
Least square error	3.90e-10	4.88e-8	2.36e24	9.49e-10
Standard error	9.886e-7	9.881e-6	7.68e10	9.74e-07
SSIM	0.72	0.69	0.71	0.73
Mean squared error	0.01	0.02	0.01	0.01
Standard deviation	0.11	0.13	0.10	0.12

Table 3: Summary of calculated errors and SSIM

solely on pixel-level differences. Although initially designed for applications in digital image processing, assessing structural similarity can be extended to comparing theoretical and experimental form factors of various particle systems. When conceptualizing the SSIM in the context of scattering, one can think of it as analogous to assessing the similarity between the calculated and theoretical form factors of particle systems. For a given particle system (e.g., spheres or rods), the theoretical form factor provides a base "image" (a model prediction). In contrast, the experimentally determined form factor offers a "real image" that includes noise, instrument effects, and sample imperfections. This indicates a high similarity between theoretical and experimental form factors, suggesting that the theoretical model accurately describes the particle system under study. For all the studied particle systems, the SSIM was between 0.73 to 0.69 Bidisperse Systems with SSI Values of 0.69, which is lower than the rest of the system, still suggest a reasonably good match between theoretical predictions and experimental data despite the inherent complexity and increased difficulty in accurately modeling bidisperse systems compared to monodisperse ones. The similarity suggests that the theoretical model captures the essential characteristics of the particle sizes and distributions. However, there might still be room for refinement in the model or the interpretation of the experimental data. SSIM value within a close range for complex systems, like bidisperse spheres, indicates that while the model is generally accurate, minor discrepancies might exist due to model assumptions or experimental setup variations. Relative consistency in all the SSI/SSIM values across different systems (spheres, rods, mono, and bidisperse) indicates the robustness of the applied theoretical models, highlighting the potential need for specific adjustments tailored to each system's unique features.

Applications and Practical Implications

Form factors are crucial in characterizing the scattering properties of various particle systems, such as monodisperse spheres, bidisperse spheres, and cylindrical rods. These factors are essential for understanding how particles interact with light, electrons, or neutrons, providing insights into the particles' size, shape, and distribution. The form factor of monodisperse spheres is critical to determining their uniformity and size distribution. A single, sharp peak in the scattering pattern indicates high uniformity, essential for applications requiring consistent particle sizes.

The form factors help analyze the size distribution and spacing within particles for bidisperse systems, where two distinct particle sizes are present. Understanding these aspects is crucial for materials where controlled heterogeneity is desired for enhanced properties. Characterizing cylindrical rods involves understanding how their aspect ratio (length to diameter) and orientation distribution affect their scattering behavior. This is vital for composites and nanotechnology applications, where rods' alignment can significantly impact material properties. Understanding form factors is vital for developing advanced materials and technologies. They provide fundamental insights that guide the design and synthesis of materials with tailored properties for specific applications.

Future trends and potential research areas stem from these analyses, exploring different shape geometries and particle systems. This exploration not only aids in developing novel materials but also in enhancing the functionality of existing ones. Nanoparticles exhibit unique properties due to their size and shape, influencing their optical, electrical, and magnetic behaviors. Future research can delve into synthesizing complex nanoparticle geometries such as rods, stars, and frames and understanding their form factors for photovoltaics, drug delivery, and sensing technologies applications. Investigating the form factors of these materials can lead to the precise control of their micro-phase segregation behavior and the spatial distribution of fillers, respectively.

5 Discussion and conclusions

Understanding form factors is crucial in characterizing particle-based materials, which impacts the development and innovation of advanced materials and technologies. These factors influence how we interpret the scattering data from materials, providing insights into particle size, shape, assembly, and distribution. Form factors for monodisperse spheres provide data on the uniformity and precision of particle sizes within a sample. The sharpness of the scattering peak can indicate the degree of uniformity essential for applications requiring consistent optical or electronic properties across the material. The simplicity of spherical geometry allows for straightforward interpretation of scattering data, making it easier to assess the quality of monodispersity. This is particularly important in applications like drug delivery, where particle size affects distribution and absorption rates.

For bidisperse systems, the presence of two distinct particle sizes adds complexity, requiring careful analysis of form factors to distinguish between the different populations of spheres. Understanding this bi-dispersity is essential in tailor-making materials for specific functionalities, such as catalysis or filtration, where various sizes play roles in reaction rates or pore-blocking mechanisms. Bidisperse systems also provide insight into interparticle interactions based on how the two different-sized particles distribute and organize themselves relative to each other. This is critical in developing composite materials or the pharmaceutical industry, where the efficacy of drug formulations can depend on these interactions.

The form factor of cylindrical rods reveals their anisotropic properties, which are paramount in designing materials with directional dependencies, such as reinforced composites or liquid crystal displays. The orientation and alignment of rods within a matrix or solvent can significantly affect mechanical strength, electrical conductivity, and optical properties. Analysis of cylindrical rods focuses on the aspect ratio and the orientation distribution of the rods. This analysis can guide the synthesis of nanocomposites and the development of advanced fibers with enhanced tensile strength or conductivity.

The importance of understanding form factors cannot be overemphasized in the design of advanced materials. The detailed knowledge of form factors enables the precise design and synthesis of materials with desirable characteristics, including optical clarity, mechanical strength, or chemical reactivity. Knowledge of how form factors affect material properties underpins the development of predictive models that can forecast the behavior of materials under different conditions, significantly reducing the need for trial and error in material development.

In conclusion, the form factors are instrumental in characterizing particles like monodisperse spheres, bidisperse spheres, and cylindrical rods. Their understanding advances our ability to tailor materials for specific applications and pushes the envelope of technological innovations, emphasizing their significant impact on materials science.

References

[1] Masahiko Abe. *Measurement techniques and practices of colloid and interface phenomena*. Springer, 2019.

[2] Carmine Anzivino, Mathias Casiulis, Tom Zhang, Amgad Salah Moussa, Stefano Martiniani, and Alessio Zaccone. Estimating random close packing in polydisperse and bidisperse hard spheres via an equilibrium model of crowding. *The Journal of Chemical Physics*, 158(4), 2023.

[3] R Beetstra, Martin Anton van der Hoef, and JAM Kuipers. Drag force of intermediate reynolds number flow past mono-and bidisperse arrays of spheres. *AIChE journal*, 53(2):489–501, 2007.

[4] Robert S Farr and Robert D Groot. Close packing density of polydisperse hard spheres. *The Journal of chemical physics*, 131(24), 2009.

[5] LA Feigin, Dmitri Iwanowitsch Svergun, et al. *Structure analysis by small-angle X-ray and neutron scattering*, volume 1. Springer, 1987.

[6] Otto Glatter. *Scattering methods and their application in colloid and interface science*. Elsevier, 2018.

[7] Ian W Hamley. *Small-angle scattering: theory, instrumentation, data, and applications*. John Wiley & Sons, 2021.

[8] Jean-Pierre Hansen and Ian Ranald McDonald. *Theory of simple liquids: with applications to soft matter*. Academic press, 2013.

[9] Lucio Isa, Falk Lucas, Roger Wepf, and Erik Reimhult. Measuring single-nanoparticle wetting properties by freeze-fracture shadow-casting cryo-scanning electron microscopy. *Nature communications*, 2(1):438, 2011.

[10] D Izzo. Solutions of rods and spheres: Predictions for the diffusion coefficient. *AIP Advances*, 13(5), 2023.

[11] David A Jacques and Jill Trewhella. Small-angle scattering for structural biology—expanding the frontier while avoiding the pitfalls. *Protein science*, 19(4):642–657, 2010.

[12] Miroslaw Jonasz and Georges Fournier. *Light scattering by particles in water: theoretical and experimental foundations*. Elsevier, 2011.

[13] Steven R. Kline. Reduction and analysis of SANS and USANS data using IGOR Pro. *Journal of Applied Crystallography*, 39(6):895–900, Dec 2006.

[14] Lars Onsager. The effects of shape on the interaction of colloidal particles. *Annals of the New York Academy of Sciences*, 51(4):627–659, 1949.

[15] Christopher D Putnam, Michal Hammel, Greg L Hura, and John A Tainer. X-ray solution scattering (saxs) combined with crystallography and computation: defining accurate macromolecular structures, conformations and assemblies in solution. *Quarterly reviews of biophysics*, 40(3):191–285, 2007.

[16] Manuel Rottereau, Jean Christophe Gimel, Taco Nicolai, and Dominique Durand. Monte carlo simulation of particle aggregation and gelation: Ii. pair correlation function and structure factor. *The European Physical Journal E*, 15(2):141–148, 2004.

[17] Salvatore Torquato and Henry W Haslach Jr. Random heterogeneous materials: microstructure and macroscopic properties. *Appl. Mech. Rev.*, 55(4):B62–B63, 2002.

[18] Gert Jan Vroege and Henk NW Lekkerkerker. Phase transitions in lyotropic colloidal and polymer liquid crystals. *Reports on Progress in Physics*, 55(8):1241, 1992.

[19] Haina Wang and Salvatore Torquato. Designer pair statistics of disordered many-particle systems with novel properties. *The Journal of Chemical Physics*, 160(4), 2024.

[20] Hua Wu and Marco Lattuada. Light scattering: The application of static light scattering: Zimm plot. In *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*. Elsevier, 2013.

[21] Fan Zhang, Andrew J Allen, Lyle E Levine, De-Hao Tsai, and Jan Ilavsky. Structure and dynamics of bimodal colloidal dispersions in a low-molecular-weight polymer solution. *Langmuir*, 33(11):2817–2828, 2017.

[22] Wu-Yang Zhang, Ying Jiang, and Jeff ZY Chen. Solution of the onsager model for the structure of rigid rods confined on a spherical surface. *Physical Review E*, 85(6):061710, 2012.