

Form and structure factors with complex scattering vector

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In condensed-matter scattering, especially under grazing incidence, complex scattering vectors account for absorption and evanescent waves. Form and structure factors, by definition, are analytic functions of the scattering vector $\mathbf{q}$ and therefore can be continued from real to complex $\mathbf{q}$. Specifically, $|\mathbf{q}|$ must be continued as $\sqrt{\mathbf{q} \cdot \mathbf{q}}$. For an isotropic scatterer, the square root is spurious as $F(\mathbf{q})$ is an entire function of $\mathbf{q} \cdot \mathbf{q}$. This justifies the existing implementation in *IsGISAXS* and *BornAgain* and confirms that one must not take the sesquilinear product $\mathbf{q}^* \cdot \mathbf{q}$.

1. Complex wavenumber

When waves propagate through a medium, absorption and other forms of attenuation can be described by an imaginary wavevector component. Nonetheless, in the standard treatment of neutron and X-ray scattering, the scattering vector $\mathbf{q}$ is usually assumed to be real. Attenuation terms are drawn out of the computation of the differential cross section and are treated, if at all, by classical transport theory, on par with multiple scattering (Sears, 1989).

This approximation loses all justification if the incident or scattered wavefield arises as the sum of partial waves that represent different radiation trajectories. Essentially the same condition decides whether the standard Born approximation must be replaced by the distorted-wave Born approximation (DWBA).

A literature search for ‘complex scattering vector’ returned papers on synthetic-aperture radar polarimetry. In that field, however, a ‘scattering vector’ (López-Martínez & Pottier, 2021) encodes a scattering matrix that expresses scattering amplitudes and phases; it has nothing to do with our $\mathbf{q}$. To date, the only important application of form and structure factors of complex $\mathbf{q}$ seems to be grazing-incidence small-angle scattering (GISAS), a standard method to study nanostructures in stratified materials (Renaud *et al.*, 2009).

In GISAS, incident (Vineyard, 1982) and scattered (Dietrich & Wagner, 1984) radiation undergo refraction and reflection, so the radiation is a superposition of two plane waves with vertical wavevector components pointing up and down. The two partial waves follow different trajectories and hence suffer different attenuation. For small grazing angles, path lengths within a layer can become large, making attenuation quantitatively significant. As scattering amplitudes from different partial waves add coherently, attenuation cannot be a common prefactor but yields a different complex factor for each of the four DWBA terms. Furthermore, even in the absence of attenuation, $\mathbf{q}$ acquires an imaginary component if the incident (Marra *et al.*, 1979) or scattered (Dietrich

$$q = \sqrt{\mathbf{q} \cdot \mathbf{q}}$$



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& Wagner, 1984) wave is evanescent in a classically forbidden sample layer.

For these reasons, form and structure factors must admit complex scattering vectors $\mathbf{q} \in \mathbb{C}^3$.

2. Form or structure factor

The form factor of an embedded particle, or the structure factor of a particle assembly, can be written as

$$F(\mathbf{q}) := \int d^3r \exp(i\mathbf{q} \cdot \mathbf{r}) g(\mathbf{r}), \quad (1)$$

where $g(\mathbf{r})$ is the indicator function of a hard particle, or the scattering-length density of a soft particle, or the pair distribution function of an assembly. We take for granted that the decay $g \rightarrow 0$ for $r \rightarrow \infty$ is sufficiently fast so that convergence is not an issue.

Repeating an argument from Wuttke (2021), by equation (1) and Leibniz's rule for differentiating under the integral, $F(\mathbf{q})$ is infinitely complex-differentiable for all $\mathbf{q} \in \mathbb{C}^3$. Thereby it is entire in each Cartesian component of $\mathbf{q}$, i.e. holomorphic (= analytic) everywhere. By the same token, $F: \mathbb{C}^3 \rightarrow \mathbb{C}$ is an analytic continuation of the more standard $\tilde{F}: \mathbb{R}^3 \rightarrow \mathbb{C}$ that is well known for many specific density distributions $g(\mathbf{r})$.

However, closed expressions for $\tilde{F}$ often involve the absolute value $q := |\mathbf{q}|$, which is not an analytic function. Therefore, in this note, it is shown how to rewrite $\tilde{F}$ so that it can be analytically continued as F . To arrive at closed solutions, I consider the special cases of an isotropic scatterer and a scatterer with cylindrical symmetry.

3. Isotropic densities

I consider isotropic densities, $g(\mathbf{r}) \equiv g(r)$ with $r := |\mathbf{r}|$. This comprises the form factor of hard and soft spheres, and the structure factor of liquid-like random assemblies.

The standard computation for real $\mathbf{q}$ starts from the observation that the isotropy of g allows us to freely choose the orientation of the $\mathbf{r}$ coordinate system. With the z axis chosen along $\hat{\mathbf{q}} := \mathbf{q}/q$, equation (1) becomes

$$\tilde{F}(\mathbf{q}) = \int d^3r \exp(iqz) g(r). \quad (2)$$

With $\mathbf{r}$ expressed in spherical coordinates, two of the three integrals can be resolved:

$$\tilde{F}(\mathbf{q}) = 2\pi \int_0^\infty dr r^2 \int_0^\pi d\vartheta \sin \vartheta \exp(iqr \cos \vartheta) g(r) \quad (3)$$

$$= \frac{4\pi}{q} \int_0^\infty dr r \sin(qr) g(r). \quad (4)$$

The appearance of a q^{-1} singularity is misleading as it is compensated by the first term in the power series of the sine

function. The regularity of $\tilde{F}(\mathbf{q})$ becomes clearer if one uses the cardinal sine function $\text{sinc } x := (\sin x)/x$:

$$\tilde{F}(\mathbf{q}) = 4\pi \int_0^\infty dr r^2 \text{sinc}(qr) g(r). \quad (5)$$

As anticipated in Section 2, this result involves $q = |\mathbf{q}|$, which precludes a straightforward analytic continuation of $\tilde{F} \mapsto F$. Worse, the above derivation cannot be justified for complex $\mathbf{q}$ because a complex $\hat{\mathbf{q}}$ does not specify a coordinate direction in $\mathbb{R}^3$.

From equation (1) with isotropic g , I infer $F(\Gamma\mathbf{q}) = F(\mathbf{q})$ for any $\Gamma \in \text{SO}(3)$ and all $\mathbf{q} \in \mathbb{C}^3$. For any real $\mathbf{q} \neq 0$, there exists $\Gamma \in \text{SO}(3)$ with $\Gamma\mathbf{q} = (q, 0, 0)$, so $F(\mathbf{q}) = F(q, 0, 0) =: A(q)$. Since $A(-q) = F(-q, 0, 0) = A(q)$, A is even, and its Taylor series is $A(q) = \sum_k a_k q^{2k} = \sum_k a_k (\mathbf{q} \cdot \mathbf{q})^k$. The right-hand side is entire and agrees with F on $\mathbb{R}^3$, so by analytic continuation $F(\mathbf{q}) = \sum_k a_k (\mathbf{q} \cdot \mathbf{q})^k$ for all $\mathbf{q} \in \mathbb{C}^3$. In view of equation (5), I conclude that

$$F(\mathbf{q}) = 4\pi \int_0^\infty dr r^2 \text{sinc}(qr) g(r), \quad (6)$$

provided the scalar q be defined as

$$q := \sqrt{\mathbf{q} \cdot \mathbf{q}}. \quad (7)$$

The resulting q reduces to $|\mathbf{q}|$ when $\mathbf{q}$ is real.

For the complex square root in equation (7), one would normally have to choose a branch. Here, however, it does not matter because the square root is spurious; its appearance is only due to the conventional definition of the sinc function. As sinc is an even entire function, its power series involves only squares of the function argument, here $(qr)^2 = (\mathbf{q} \cdot \mathbf{q})r^2$.

4. Densities with cylindrical symmetry

I now consider densities with cylindrical symmetry, $g(\mathbf{r}) \equiv g(r_\parallel, z)$ where $r_\parallel := \sqrt{x^2 + y^2}$. This comprises the form factor of cylinders, cones and other shapes with a symmetry axis.

For real $\mathbf{q}$, I choose the z axis along the cylinder axis. Let $\mathbf{r}_\parallel := (x, y)$ be the in-plane component of $\mathbf{r}$, and similarly $\mathbf{q}_\parallel := (q_x, q_y)$ with magnitude $q_\parallel := |\mathbf{q}_\parallel|$. Cylindrical symmetry resolves one of the three integrals in equation (1):

$$\tilde{F}(\mathbf{q}) = \int dz \exp(iq_z z) \int d^2r_\parallel \exp(i\mathbf{q}_\parallel \cdot \mathbf{r}_\parallel) g(r_\parallel, z) \quad (8)$$

$$= \int dz \exp(iq_z z) \int_0^\infty dr_\parallel r_\parallel \int_0^{2\pi} d\varphi \exp(iq_\parallel r_\parallel \cos \varphi) g(r_\parallel, z) \quad (9)$$

$$= 2\pi \int dz \exp(iq_z z) \int_0^\infty dr_{\parallel} r_{\parallel} J_0(q_{\parallel} r_{\parallel}) g(r_{\parallel}, z). \quad (10)$$

This is as far as one can go for generic g ; for specific g , one or both of the remaining integrals may be solvable analytically.

For the analytic continuation, the same reasoning as in the isotropic case applies. Since $F(\mathbf{q})$ is entire and invariant under rotations about the z axis, its power series contains only rotation-invariant homogeneous polynomials. These depend only on q_z and $\mathbf{q}_{\parallel} \cdot \mathbf{q}_{\parallel} = q_x^2 + q_y^2$. Therefore, $F(\mathbf{q})$ depends on $\mathbf{q}_{\parallel}$ only through $\mathbf{q}_{\parallel} \cdot \mathbf{q}_{\parallel}$. Since $\tilde{F}$ from equation (10) has this property when $\mathbf{q} \in \mathbb{R}^3$, and since analytic continuation is unique, the analytic continuation is

$$F(\mathbf{q}) = 2\pi \int dz \exp(iq_z z) \int_0^\infty dr_{\parallel} r_{\parallel} J_0(q_{\parallel} r_{\parallel}) g(r_{\parallel}, z), \quad (11)$$

provided

$$q_{\parallel} := \sqrt{\mathbf{q}_{\parallel} \cdot \mathbf{q}_{\parallel}} = \sqrt{q_x^2 + q_y^2}. \quad (12)$$

Again, the square root is spurious because J_0 is even and entire.

5. Conclusions

Complex scattering vectors $\mathbf{q}$ are needed whenever absorption affects the coherent superposition of partial waves. Software for simulating GISAS must at least support a complex component q_z , as does the program *IsGISAXS* (Lazzari, 2002, 2006). Our program *BornAgain* supports fully complex $\mathbf{q}$, which facilitates the rotation of particles [Pospelov *et al.*, 2020; Scientific Computing Group of Heinz Maier-Leibnitz Zentrum, Garching, 2014–2026; for polyhedral form factors, see Wuttke (2021)]. The present communication documents and justifies the mathematics implemented in this software long ago.

Form factors $F(\mathbf{q})$ are given by integral (1), which is an analytic function of $\mathbf{q}$. If a solution $\tilde{F}(\mathbf{q})$ is known for $\mathbf{q} \in \mathbb{R}^3$, then $F(\mathbf{q})$ can be obtained by analytic continuation of $\tilde{F}$. This holds even if the derivation of $\tilde{F}$ involves a concept like the direction of $\mathbf{q}$ that has no unique generalization from $\mathbf{q} \in \mathbb{R}^3$ to $\mathbf{q} \in \mathbb{C}^3$. However, if a closed expression for $\tilde{F}$

contains a non-analytic function like $|\mathbf{q}|$ or $|\mathbf{q}_{\parallel}|$, then it must be replaced by an analytic function (like $|\mathbf{q}| = \sqrt{\mathbf{q} \cdot \mathbf{q}}$, which agrees for $\mathbf{q} \in \mathbb{R}$). Alternatively, to get rid of the spurious square root, one could replace conventional function notations like $\text{sinc}(z)$ or $J_0(z)$ by equivalent functions of z^2 .

One must not use the standard norm $\|\mathbf{q}\|$, almost everywhere in mathematics defined via the sesquilinear (Hermitian) product $\mathbf{q}^* \cdot \mathbf{q}$, which is not an analytic function of $\mathbf{q}$. The bilinear form $\mathbf{q} \cdot \mathbf{q}$ is not positive definite, and therefore equation (7) is not a norm, but it is the correct analytic continuation of $q = |\mathbf{q}|$ from real to complex $\mathbf{q}$.

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References

- Dietrich, S. & Wagner, H. (1984). *Z. Phys. B Condens. Matter* **56**, 207–215.
- Lazzari, R. (2002). *J. Appl. Cryst.* **35**, 406–421.
- Lazzari, R. (2006). *IsGISAXS*, Version 2.6, <http://www.insp.jussieu.fr/oxydes/IsGISAXS/isgisaxs.htm>.
- López-Martínez, C. & Pottier, E. (2021). *Basic Principles of SAR Polarimetry*, in *Polarimetric Synthetic Aperture Radar: Principles and Application*, edited by I. Hajnsek & Y.-L. Desnos, Remote Sensing and Digital Image Processing, Vol. 25, pp. 1–58. Cham: Springer.
- Marra, W. C., Eisenberger, P. & Cho, A. Y. (1979). *J. Appl. Phys.* **50**, 6927–6933.
- Pospelov, G., Van Herck, W., Burle, J., Carmona Loaiza, J. M., Durniak, C., Fisher, J. M., Ganeva, M., Yurov, D. & Wuttke, J. (2020). *J. Appl. Cryst.* **53**, 262–276.
- Renaud, G., Lazzari, R. & Leroy, F. (2009). *Surf. Sci. Rep.* **64**, 255–380.
- Scientific Computing Group of Heinz Maier-Leibnitz Zentrum, Garching (2014–2026). *BornAgain*, <https://www.bornagainproject.org>, <https://doi.org/10.5281/zenodo.20312089>.
- Sears, V. P. (1989). *Neutron Optics*. Oxford University Press.
- Vineyard, G. H. (1982). *Phys. Rev. B* **26**, 4146–4159.
- Wuttke, J. (2021). *J. Appl. Cryst.* **54**, 580–587.