BornAgain

Software for simulating and fitting
X-ray and neutron small-angle scattering
at grazing incidence

User Manual

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Disclaimer: Software and documentation are work in progress.
We cannot guarantee correctness and accuracy.
If in doubt, contact us for assistance or scientific collaboration.

Contents

Introduction

About BornAgain

`BornAgain` is a software package to simulate and fit reflectometry, off-specular scattering, and grazing-incidence small-angle scattering (GISAS) of X-rays and neutrons. It provides a generic framework for modeling multilayer samples with smooth or rough interfaces and with various types of embedded nanoparticles. Support for neutron polarization and magnetic scattering is under development. The name, `BornAgain`, alludes to the central role of the distorted-wave Born approximation (DWBA) in the physical description of the scattering process.

`BornAgain` is being developed by the Scientific Computing Group of the Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ) Garching, Germany. It is intended to serve experimentalists in analysing all kinds of reflectometry data. It is equally aimed at users of MLZ reflectometers [1, 2, 3], at JCNS in-house researchers, and at the reflectometry and GISAS community at large. It is the main contribution of JCNS to national [4] and international [5] collaborations of large-scale facilities for the development of better user software.

`BornAgain` is released as free and open source software under the GNU General Public License (GPL, version 3 or higher). This documentation comes under the Creative Commons license CC-BY-SA.

The converse of this liberal policy is that we cannot guarantee correctness and accuracy of the code. It is entirely in the responsibility of users to convince themselves that their data interpretation is physically meaningful and plausible.

`BornAgain` is still under intense development. New major versions are released about every two months. When need arises, bugfix versions are released in between. It is strongly recommended that users regularly update their installations.

The software `BornAgain` embodies nontrivial scientific ideas. Therefore when `BornAgain` is used in preparing scientific papers, it is mandatory to cite the software:

> C. Durniak, M. Ganeva, G. Pospelov, W. Van Herck, J. Wuttke (2015),
> BornAgain — Software for simulating and fitting X-ray and neutron small-angle scattering at grazing incidence, version [...],
> http://www.bornagainproject.org

The initial design of BornAgain owes much to the widely used program IsGISAXS by Rémi Lazzari [6, 7]. Therefore when using BornAgain in scientific work, it might be appropriate to also cite the pioneering papers by Lazzari *et al.* [6, 8].

Since version 1.0, BornAgain almost completely reproduces the functionality of IsGISAXS. About 20 exemplary simulations have been tested against IsGISAXS, and found to agree up to almost the last floating-point digit. BornAgain goes beyond IsGISAXS in supporting an unrestricted number of layers and particles, diffuse reflection from rough layer interfaces and particles with inner structures. Support for neutron polarization and magnetic scattering is under development. Adhering to a strict object-oriented design, BornAgain provides a solid base for future extensions in response to specific user needs.

About this Manual

This user manual is complementary to the online documentation at http://www.bornagainproject.org. It does not duplicate information that is more conveniently read online. Therefore, Sec. 1 just contains a few pointers to the web site. The remainder of this manual mostly contains background on the scattering theory and on the sample models implemented in BornAgain, and some documentation of the corresponding Python functions.

This manual is incomplete. Several important chapters are still missing.

Specifically, we plan to provide documentation on

- X-ray propagation and scattering,
- polarized neutron propagation and magnetic scattering,
- mapping of $\partial\sigma/\partial\Omega$ onto flat detectors,
- scattering by rough interfaces,
- scattering by particle assemblies.

We intend to publish these chapters successively, along with new software release. To avoid confusion, starting with release 1.2 the manual carries the same version number as the software, even though it is in a less mature state.

We urge users to subscribe to our newsletter (see Sec. 1.3), and to contact us for any question not answered here or in the online documentation.

We are grateful for all kind of feedback: criticism, praise, bug reports, feature requests or contributed modules. If questions go beyond normal user support, we will be glad to discuss a scientific collaboration.

Typesetting conventions

In this manual, we use the following colored boxes to highlight certain information:

Such a box contains a **warning** about potential problems with the software or the documentation.

This road sign in the margin indicates **work in progress**.

Such a box contains an **important fact**, for instance an equation that has a central role in the further development of the theory.

Such a box contains an **implementation note** that explains how the theory exposed in this manual is actually used in `BornAgain`.

Such a box provides one or several links to a usages examples in the online tutorial, like the basic script cylinders in distorted wave Born approximation or the long list of all available form factors.

Variations of the equation sign (as $\equiv$, $:=$, $\doteq$) are explained in the symbol index, page 77. See there as well for less common mathematical functions like the cardinal sine function "sinc".

Chapter 1

Online documentation

This User Manual is complementary to the online documentation at the project web site http://www.bornagainproject.org. It does not duplicate information that is more conveniently read online. This brief chapter contains no more than a few pointers to the web site.

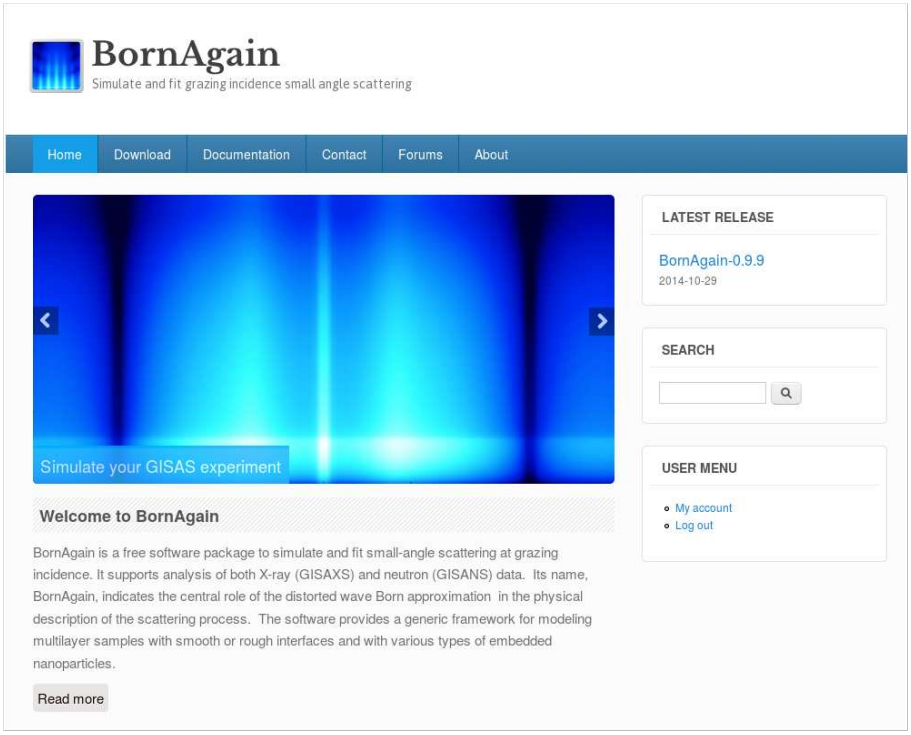

Figure 1.1: A screenshot of the home page http://www.bornagainproject.org.

1.1 Download and installation

`BornAgain` is a multi-platform software. We actively support the operating systems Linux, MacOS and Microsoft Windows. The DOWNLOAD section on the `BornAgain`

web site points to the download location for binary and source packages. It also provides a link to our `git` server where the unstable development trunk is available for contributors or for users who want to live on the edge.

The DOCUMENTATION section contains pages with *Installation instructions*.

1.2 Further online information

The DOCUMENTATION section of the project web site contains in particular

- an overview of the software architecture,
- a list of implemented functionality,
- tutorials for "Working with `BornAgain`", using either the Graphical User Interface or `Python` scripts,
- a comprehensive collection of tutorial examples that demonstrate how to use `BornAgain` for modeling various sample structures and different experimental conditions,
- a link to the API reference for using `BornAgain` through `Python` scripts or C++ programs.

1.3 Registration, contact, discussion forum

To stay informed about the ongoing development of `BornAgain`, register on the project homepage `http://www.bornagainproject.org` ("Create new account"). You will then receive our occasional newsletters, and be authorized to post to the discussion forum.

To contact the `BornAgain` development and maintenance team in the Scientific Computing Group of Heinz Maier-Leibnitz Zentrum (MLZ) Garching, write a mail to `contact@bornagainproject.org`, or fill the form in the CONTACT section of the project web site.

For questions that might be of wider interest, please consider posting to the discussion forum, accessible through the FORUMS tab of the project web site.

Chapter 2

Small-angle scattering and the Born approximation

This chapter introduces the basic theory of small-angle scattering (SAS). We specifically consider scalar neutron propagation, adjourning the notationally more involved vectorial theory of X-rays and polarized neutrons a later edition. Our exposition is self-contained, except for the initial passage from the microscopic to the macroscopic Schrödinger equation, which we outline only briefly (Sec. 2.1). The standard description of scattering in first order Born approximation is introduced in a way that is suitable subsequent modification into the distorted wave Born approximation needed for grazing-incidence small-angle scattering (Sec.2.2).

2.1 Coherent neutron propagation

The scalar wavefunction $\psi(\boldsymbol{r}, t)$ of a free neutron is governed by the microscopic Schrödinger equation

$$i\hbar\partial_t\psi(\boldsymbol{r}, t) = \left\{-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{r})\right\}\psi(\boldsymbol{r}, t). \tag{2.1}$$

By assuming a time-independent potential $V(\boldsymbol{r})$, we have excluded inelastic scattering. Therefore we only need to consider monochromatic waves with given frequency ω. In consequence, we have a stationary wavefunction

$$\psi(\boldsymbol{r}, t) = \psi(\boldsymbol{r})\mathrm{e}^{-i\omega t}. \tag{2.2}$$

The minus sign in the exponent of the phase factor is an inevitable consequence of the standard form of the Schrödinger equation, and is therefore called the *quantum-mechanical sign convention*. For electromagnetic radiation usage is less uniform. While most optics textbooks have adopted the quantum-mechanical convention (2.2), in X-ray crystallography the conjugate phase factor $\mathrm{e}^{+i\omega t}$ is prefered. This *crystallographic sign convention* has also been chosen in influential texts on GISAXS (e.g. [8]). Here, however, we are concerned not only with X-rays, but also with neutrons, and therefore we need to leave the Schrödinger equation (2.1) intact. Thence:

In this manual, and in the program code of `BornAgain`, the quantum-mechanical sign convention (2.2) is chosen. This has implications for the sign of the imaginary part of the refractive index, as explained in Sec. 3.1.2.

Inserting (2.2) in (2.1), we obtain the stationary Schrödinger equation

$$\left\{-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{r}) - \hbar\omega\right\}\psi(\boldsymbol{r}) = 0. \tag{2.3}$$

The *nuclear* (or *microscopic*) *optical potential* $V(\boldsymbol{r})$, in a somewhat "naive conception" [9, p. 7], consists of a sum of delta functions, representing Fermi's "pseudopotential". The superposition of the incident wave with the scattered waves originating from each illuminated nucleus results in *coherent forward scattering*, in line with Huygens' principle.

Coherent superposition also leads to *Bragg scattering*. However, Bragg scattering by atomic lattices only occurs at angles far above the small-angle range covered in GISAS experiments. Accordingly, it can be neglected in the analysis of GISAS data, or at most, is taken into account as a loss channel.

Therefore, we can neglect the atomic structure of $V(\boldsymbol{r})$, and perform some coarse graining to arrive at a *continuum approximation*. This is similar to the passage from the microscopic to the macroscopic Maxwell equations. The details are intricate [9, 10], but the result [9, eq. 2.8.32] looks very simple: The macroscopic field equation has still the form of a stationary Schrödinger equation,

$$\left\{-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + v(\boldsymbol{r}) - \hbar\omega\right\}\psi(\boldsymbol{r}) = 0, \tag{2.4}$$

where ψ now stands for the *coherent wavefunction* obtained by superposition of incident and forward scattered states, and $v(\boldsymbol{r})$ is the *macroscopic optical potential*. This potential is weak, and slowly varying compared to atomic length scales. It can be rewritten in a number of ways, especially in terms of a *bound scattering length density* $\rho_s(\boldsymbol{r})$ [9, eq. 2.8.37],

$$v(\boldsymbol{r}) = \frac{2\pi\hbar^2}{m}\rho_s(\boldsymbol{r}), \tag{2.5}$$

or of a *refractive index* $n(\boldsymbol{r})$ defined by

$$n(\boldsymbol{r})^2 := 1 - \frac{4\pi}{K^2}\rho_s(\boldsymbol{r}) = 1 - \frac{2m}{\hbar^2K^2}v(\boldsymbol{r}). \tag{2.6}$$

In the latter expression, we introduced the *vacuum wavenumber* K, which is connected with the frequency ω through the *dispersion relation*

$$\frac{\hbar^2K^2}{2m} = \hbar\omega. \tag{2.7}$$

Since we only consider stationary solutions (2.2), ω will not appear any further in our derivations. Instead, we use K as the given parameter that characterizes the incoming radiation. In terms of K and n, the macroscopic Schrödinger equation (2.4) can be rewritten as

$$\left\{\boldsymbol{\nabla}^2 + K^2 n(\boldsymbol{r})^2\right\}\psi(\boldsymbol{r}) = 0. \tag{2.8}$$

This equation is the starting point for the analysis of all small-angle scattering experiments, whether under grazing incidence (GISAS) or not (regular SAS).

2.2 Neutron scattering in Born approximation

2.2.1 The Born expansion

To describe an elastic scattering experiment, we need to solve the Schrödinger equation (2.8) under the asymptotic boundary condition

$$\psi(\boldsymbol{r}) \simeq \psi_{\mathrm{i}}(\boldsymbol{r}) + f(\vartheta,\varphi)\frac{\mathrm{e}^{iKr}}{4\pi r} \text{ for } r \to \infty, \tag{2.9}$$

where $\psi_{\mathrm{i}}(\boldsymbol{r})$ is the incident wave as prepared by the experimental apparatus, and the second term on the right-hand side is the outgoing scattered wave that carries information in form of the angular distribution $f(\vartheta,\varphi)$.

For thermal or cold neutrons, as for X-rays, the refractive index n is almost always very close to 1. This suggests a solution of the Schrödinger equation by means of a perturbation expansion in powers of $n^2 - 1$. This expansion is named after Max Born who introduced it in quantum mechanics.[1]

To carry out this idea, we rewrite the Schrödinger equation once more so that it takes the form of a Helmholtz equation with a perturbation term on the right side:

$$\left(\boldsymbol{\nabla}^2 + K^2\right)\psi(\boldsymbol{r}) = 4\pi\chi(\boldsymbol{r})\psi(\boldsymbol{r}) \tag{2.10}$$

with

$$\chi(\boldsymbol{r}) := \frac{K^2}{4\pi}\left(1 - n^2(\boldsymbol{r})\right). \tag{2.11}$$

This definition just compensates (2.6) so that $\chi = \rho_s$. In the following, we prefer the notation χ and the appellation *perturbative potential* over the scattering length density ρ_s to prepare for the generalization to the electromagnetic case.

Equation (2.10) looks like an inhomogeneous differential equation — provided we neglect for a moment that the unknown function ψ reappears on the right side. The homogeneous equation

$$\left(\boldsymbol{\nabla}^2 + K^2\right)\psi(\boldsymbol{r}) = 0 \tag{2.12}$$

is solved by plane waves and superpositions thereof. It applies in particular to the incident wave ψ_{i}.

[1] It goes back to Lord Rayleigh who devised it for sound, and later also applied it to electromagnetic waves, which resulted in his famous explanation of the blue sky.

For an isolated inhomogeneity,

$$(\boldsymbol{\nabla}^2 + K^2)\, G(\boldsymbol{r}, \boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{2.13}$$

is solved by the Green function[2]

$$G(\boldsymbol{r}, \boldsymbol{r}') = \frac{\mathrm{e}^{iK|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r} - \boldsymbol{r}'|}, \tag{2.14}$$

which is an outgoing spherical wave centered at $\boldsymbol{r}'$. Convoluting this function with the given inhomogeneity $4\pi\chi\psi$, we obtain what is known as the Lippmann-Schwinger equation,

$$\psi(\boldsymbol{r}) = \psi_\mathrm{i}(\boldsymbol{r}) + \int \mathrm{d}^3 r'\, G(\boldsymbol{r}, \boldsymbol{r}') 4\pi\chi(\boldsymbol{r}')\psi(\boldsymbol{r}'). \tag{2.15}$$

This integral equation for $\psi(\boldsymbol{r})$ improves upon the original stationary Schrödinger equation (2.10) in that it ensures the boundary condition (2.9). It can be resolved into an infinite series by iteratively substituting the full right-hand side of (2.15) into the integrand. Successive terms in this series contain rising powers of χ. Since χ is assumed to be small, the series is likely to converge. In *first-order Born approximation*, only the linear order in χ is retained,

$$\psi(\boldsymbol{r}) \doteq \psi_\mathrm{i}(\boldsymbol{r}) + 4\pi \int \mathrm{d}^3 r'\, G(\boldsymbol{r}, \boldsymbol{r}')\chi(\boldsymbol{r}')\psi_\mathrm{i}(\boldsymbol{r}'). \tag{2.16}$$

This is practically always adequate for material investigations with X-rays or neutrons, where the aim is to deduce $\chi(\boldsymbol{r}')$ from the scattered intensity $|\psi(\boldsymbol{r})|^2$. Since detectors are always placed at positions $\boldsymbol{r}$ that are not illuminated by the incident beam, we are only interested in the scattered wave field

$$\psi_\mathrm{s}(\boldsymbol{r}) := 4\pi \int \mathrm{d}^3 r'\, G(\boldsymbol{r}, \boldsymbol{r}')\chi(\boldsymbol{r}')\psi_\mathrm{i}(\boldsymbol{r}'). \tag{2.17}$$

2.2.2 Far-field approximation

We can further simplify (2.17) under the conditions of Fraunhofer diffraction: the distance from the sample to the detector location $\boldsymbol{r}$ must be much larger than the size of the sample. Since the scattered wave $\psi_\mathrm{s}(\boldsymbol{r})$ only depends on $\boldsymbol{r}$ through the Green function $G(\boldsymbol{r}, \boldsymbol{r}')$, we shall derive a far-field approximation for the latter.

We choose the origin within the sample so that the integral in (2.17) runs over $\boldsymbol{r}'$ with $r' \ll r$. This allows us to expand

$$\left|\boldsymbol{r} - \boldsymbol{r}'\right| \doteq \sqrt{r^2 - 2\boldsymbol{r}\,\boldsymbol{r}'} \doteq r - \frac{\boldsymbol{r}\,\boldsymbol{r}'}{r} \equiv r - \frac{\boldsymbol{k}_\mathrm{f}\boldsymbol{r}'}{K}, \tag{2.18}$$

[2]Verification under the condition $\boldsymbol{r} \neq 0$ is a straightforward exercise in vector analysis. For the special case $\boldsymbol{r} = 0$, one encloses the origin in a small sphere and integrates by means of the Gauss-Ostrogadsky divergence theorem. This explains the appearance of the factor 4π.

where we have introduced the outgoing wavevector

$$\boldsymbol{k}_\mathrm{f} := K\frac{\boldsymbol{r}}{r}. \tag{2.19}$$

We apply this to (2.14), and obtain in leading order the far-field Green function

$$G_\mathrm{far}(\boldsymbol{r},\boldsymbol{r'}) = \frac{\mathrm{e}^{iKr}}{4\pi r}\psi_\mathrm{f}^*(\boldsymbol{r'}) \tag{2.20}$$

where

$$\psi_\mathrm{f}(\boldsymbol{r}) := \mathrm{e}^{i\boldsymbol{k}_\mathrm{f}\boldsymbol{r}} \tag{2.21}$$

is a plane wave propagating towards the detector, and ψ^* designates the complex conjugate of ψ. With respect to $\boldsymbol{r}$, G_far is an outgoing spherical wave.

The scattered wave (2.17) becomes in the far-field approximation

$$\psi_\mathrm{s,far}(\boldsymbol{r}) = \frac{\mathrm{e}^{iKr}}{r}\langle\psi_\mathrm{f}|\chi|\psi_\mathrm{i}\rangle\,, \tag{2.22}$$

where we used Dirac notation for the transition matrix element

$$\langle\psi_\mathrm{f}|\chi|\psi_\mathrm{i}\rangle := \int \mathrm{d}^3r\,\psi_\mathrm{f}^*(\boldsymbol{r})\chi(\boldsymbol{r})\psi_\mathrm{i}(\boldsymbol{r}). \tag{2.23}$$

In order to reconcile conflicting sign conventions, we will in the following rather use its complex conjugate $\langle\psi_\mathrm{i}|\chi|\psi_\mathrm{f}\rangle = \langle\psi_\mathrm{f}|\chi|\psi_\mathrm{i}\rangle^*$. Under the standard assumption that the incident radiation is a plane wave

$$\psi_\mathrm{i}(\boldsymbol{r}) = \mathrm{e}^{i\boldsymbol{k}_\mathrm{i}\boldsymbol{r}} \tag{2.24}$$

with $k_\mathrm{i} = K$, the matrix element takes the form

$$\langle\psi_\mathrm{i}|\chi|\psi_\mathrm{f}\rangle = \int \mathrm{d}^3r\,e^{-i\boldsymbol{k}_\mathrm{i}\boldsymbol{r}}\chi(\boldsymbol{r})e^{i\boldsymbol{k}_\mathrm{f}\boldsymbol{r}} = \int \mathrm{d}^3r\,e^{i\boldsymbol{q}\boldsymbol{r}}\chi(\boldsymbol{r}) =: \chi(\boldsymbol{q}), \tag{2.25}$$

where we have introduced the *scattering vector*[3]

$$\boldsymbol{q} := \boldsymbol{k}_\mathrm{f} - \boldsymbol{k}_\mathrm{i} \tag{2.26}$$

and the notation $\chi(\boldsymbol{q})$ for the Fourier transform of the perturbative potential, which is what small-angle neutron scattering basically measures.

[3]With this choice of sign, $\hbar\boldsymbol{q}$ is the momentum *gained* by the scattered neutron, and *lost* by the sample. In much of the literature the opposite convention is prefered, since it emphasizes the sample physics over the scattering experiment. However, when working with twodimensional detectors it is highly desirable to express pixel coordinates and scattering vector components with respect to equally oriented coordinate axes, which can only be achieved by the convention (2.26).

2.2.3 Differential cross section

In connection with (2.16) we mentioned that a scattering experiment measures intensities $|\psi(\boldsymbol{r})|^2$. We shall now restate this in a more rigorous way. In the case of neutron scattering, one actually measures a *probability flux*. We define it in arbitrary relative units as

$$\boldsymbol{J}(\boldsymbol{r}) := \psi^* \frac{\boldsymbol{\nabla}}{2i}\psi - \psi \frac{\boldsymbol{\nabla}}{2i}\psi^*. \tag{2.27}$$

The ratio of the scattered flux hitting an infinitesimal detector area $r^2 \mathrm{d}\Omega$ to the incident flux is expressed as a *differential cross section*

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} := \frac{r^2 J(\boldsymbol{r})}{J_\mathrm{i}}. \tag{2.28}$$

With (2.24), the incident flux is

$$\boldsymbol{J}_\mathrm{i} = \boldsymbol{k}_\mathrm{i}. \tag{2.29}$$

With (2.22), the scattered flux at the detector is

$$\boldsymbol{J}(\boldsymbol{r}) = \hat{\boldsymbol{r}} \frac{K}{r^2} |\langle \psi_\mathrm{i} | \chi | \psi_\mathrm{f} \rangle|^2. \tag{2.30}$$

From (2.28) we obtain the generic differential cross section of elastic scattering in first order Born approximation,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |\langle \psi_\mathrm{i} | \chi | \psi_\mathrm{f} \rangle|^2. \tag{2.31}$$

As we shall see below, it holds not only for plane waves governed by the vacuum Helmholtz equation (2.12), but also for distorted waves.

In the plane-wave case (2.25) considered here, the differential cross section is just the squared modulus of the Fourier transform of the perturbative potential,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |\chi(\boldsymbol{q})|^2. \tag{2.32}$$

Chapter 3

Grazing-incidence scattering and the distorted wave Born approximation

Wave propagation through thin layers requires a special formalism that accounts for refraction and reflection (Sec. 3.1.1). Radiation impinging under grazing incidence has long trajectories so that absorption is often considerable (Sec. 3.1.2). The so obtained distorted plane waves are the base for the reformulation of Born's scattering theory in the distorted wave Born approximation (Sec. 3.2).

3.1 Wave propagation in $2+1$ dimensions

3.1.1 Factorization ansatz

Reflectometry and grazing-incidence scattering are designed for the investigation of surfaces, interfaces, and thin layers, or most generically: samples with a $2+1$ dimensional structure that are on average translationally invariant in x and y direction, but structured in z direction. By convention, we designate the *sample plane* (xy) as *horizontal*, and the *sample normal* (z) as *vertical*, even if this does not correspond to the actual experimental geometry.[1] The z axis points upwards, hence out of the sample towards the vacuum (or air) halfspace where the incident radiation comes from, as illustrated in Fig. 3.1.

Vertical modulations of the refractive index $n(\boldsymbol{r})$ cause refraction and reflection of an incident plane wave. For small glancing angles, these distortions can be arbitrary large, up to the limiting case of total reflection, even though $1-n$ is only of the order 10^{-5} or smaller. Such zeroth-order effects cannot be accounted for by perturbative scattering theory. Instead, we need to deal with refraction and reflection at the level of the wave propagation equation. We move the vertical variations of the squared refractive index to the left-hand side of the Schrödinger equation (2.8),

$$\left\{\boldsymbol{\nabla}^2 + K^2\overline{n^2}(z)\right\}\psi(\boldsymbol{r}) = 4\pi\chi(\boldsymbol{r})\psi(\boldsymbol{r}), \tag{3.1}$$

[1] In many reflectometers, the scattering plane and the sample normal are horizontal in laboratory space.

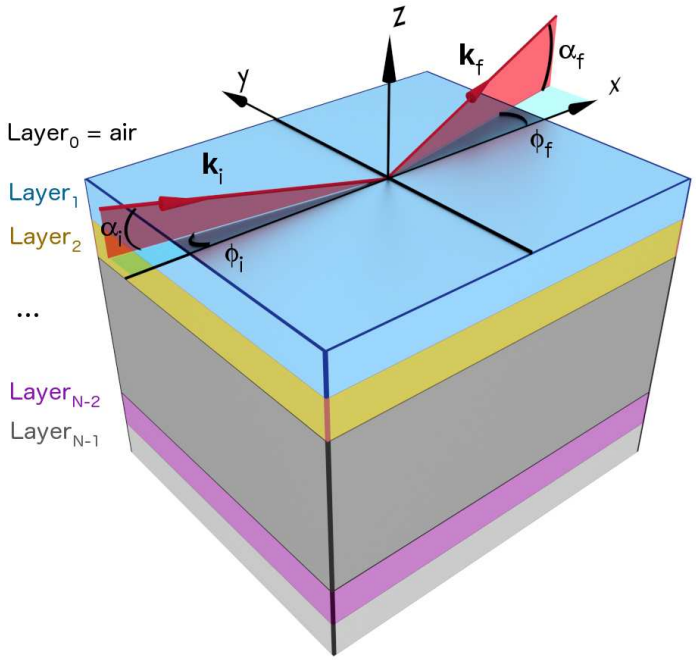

Figure 3.1: Geometric conventions in GISAS scattering comprise a Cartesian coordinate system and a set of angles. The coordinate system has a z axis normal to the sample plane, and pointing into the halfspace where the beam comes from. The x axis usually points along the incident beam, projected onto the sample plane. Incident and final plane waves are characterized by wavevectors $\boldsymbol{k}_\mathrm{i}$, $\boldsymbol{k}_\mathrm{f}$; the angle α_i is the incident glancing angle; ϕ_i is usually zero, unless used to describe a sample rotation; α_f is the exit angle with respect to the sample's surface; and ϕ_f is the scattering angle with respect to the scattering plane. The numbered layers illustrate a multilayer system as dicussed in Sec. 4.

where the overline indicates an horizontal average. Deviating from (2.11), the perturbation has been redefined as

$$\chi(\boldsymbol{r}) := \frac{K^2}{4\pi}\left(\overline{n^2}(z) - n^2(\boldsymbol{r})\right), \tag{3.2}$$

which only accounts for horizontal fluctuations of the refractive index. Wave propagation, unperturbed by χ, but including refraction and reflection effects, obeys the homogeneous equation

$$\left\{\boldsymbol{\nabla}^2 + K^2\overline{n^2}(z)\right\}\psi(\boldsymbol{r}) = 0. \tag{3.3}$$

It is solved for the horizontal coordinate $\boldsymbol{r}_\parallel$ by the factorization ansatz

$$\psi(\boldsymbol{r}) = \mathrm{e}^{i\boldsymbol{k}_\parallel \boldsymbol{r}_\parallel}\phi(z). \tag{3.4}$$

The horizontal wavevector $\boldsymbol{k}_\parallel$ remains constant as initialized by the incoming beam. The vertical wavefunction must fulfill

$$\left\{\partial_z^2 + K^2\overline{n^2}(z) - k_\parallel^2\right\}\phi(z) = 0. \tag{3.5}$$

When an incident plane wave, travelling downwards with $\phi(z) = \mathrm{e}^{-ik_\perp z}$, impinges on a sample with $\overline{n^2}(z) \neq 1$, then the wave is partly reflected ($-k_\perp$ reversed into $+k_\perp$) and partly refracted ($k_\perp$ changing while $\boldsymbol{k}_\parallel$ stays constant, resulting in a change of glancing angle). Similarly, reflection and refraction occur whenever $\overline{n^2}(z)$ varies within the sample. As a result, at any z within the zone where $\overline{n^2}(z)$ varies, the vertical wavefunction $\phi(z)$ is composed of a downward travelling component $\phi^-(z)$ and an upward travelling component $\phi^+(z)$.

For a graded refractive index $\overline{n^2}$ that is a smooth function of z, the differential equation (3.5) is best solved using the WKB method.[2] If otherwise $\overline{n^2}(z)$ is discontinuous at some interface $z = z_j$, then the limiting values of $\phi^-(z)$ and $\phi^+(z)$ on approaching z_j from above or below are connected to each other through Fresnel's transmission and reflection coefficients. This applies in particular to multilayer systems, discussed in chapter 4.

3.1.2 How to describe absorption

The complex refractive index of a given material shall be written as

$$n \doteq 1 - \delta + i\beta, \tag{3.6}$$

introducing two small real, nonnegative parameters δ, β. While a vertical gradation of δ causes refraction and reflection, a nonzero β describes absorption and leads to a damping of propagating waves. The plus sign in front of the imaginary part is a consequence of the quantum-mechanical sign convention; in the X-ray crystallography convention it would be a minus sign.

The factorization ansatz (3.4) leaves us some freedom how to deal with an imaginary part of n. We *choose* that horizontal wavevectors $\boldsymbol{k}_\parallel$ shall always be real. The damping then appears in the vertical wavefunction $\phi(z)$ that is governed by the complex wave equation (3.5).

3.2 Distorted-wave Born approximation (DWBA)

The standard form of the Born approximation, as presented in Sec. 2.2, combines an approximation scheme (computing (2.15) by iteration) with an assumption (the incident field is a plane wave) and an analytic result (in far-field approximation, the Green function of the Helmholtz equation is a plane wave with respect to the locus of scattering). These three elements must not necessarily go together. We can apply the very same approximation scheme, even if the incident field is not a plane wave, but a *distorted wave*, namely a superposition of downwards and upwards travelling plane

[2] Also called *semiclassical approximation* or *phase integral method*, named after Wentzel (1926), Kramers (1926), Brillouin (1926). See any textbook on quantum mechanics.

waves, as derived in the previous section. This is the core idea of the *distorted-wave Born approximation* (DWBA).[3]

To carry out this idea, we need to determine the Green function G. In Sec. 2.2.1 we did so quite specifically for a homogeneous material. Computing G in closed form for a more generic wave equation like (3.3) is far more difficult, if not outright impossible. Fortunately, this computation is not necessary, and would be but wasted effort: We do not need the full solution $G(\boldsymbol{r}, \boldsymbol{r}')$, but only its asymptotic far-field value $G(\boldsymbol{r}_\mathrm{D}, \boldsymbol{r}')$ at a detector position $\boldsymbol{r}_\mathrm{D}$. Thanks to a *source-detector reciprocity theorem* (A.10) proven in Appendix A.1, we can compute this value as

$$G(\boldsymbol{r}_\mathrm{D}, \boldsymbol{r}) = B(\boldsymbol{r}, \boldsymbol{r}_\mathrm{D}), \tag{3.7}$$

where B is the *adjoint Green function* that describes backward propagation from $\boldsymbol{r}_\mathrm{D}$ into the sample.

Outside the sample, B obeys the Helmholtz equation with isolated inhomogeneity (2.13), and therefore has the far-field expansion (2.20),

$$B_\mathrm{far}(\boldsymbol{r}, \boldsymbol{r}_\mathrm{D}) = \frac{\mathrm{e}^{iKr_\mathrm{D}}}{4\pi r_\mathrm{D}} \mathrm{e}^{-i\boldsymbol{k}_\mathrm{f}\boldsymbol{r}}. \tag{3.8}$$

When this backward propagating plane waves impinges on the sample, it undergoes reflection and refraction in exactly the same way as the incident plane wave $\mathrm{e}^{i\boldsymbol{k}_\mathrm{i}\boldsymbol{r}}$. Therefore, (3.8) admits a generalization that also holds inside the sample:

$$B_\mathrm{far}(\boldsymbol{r}, \boldsymbol{r}_\mathrm{D}) = \frac{\mathrm{e}^{iKr_\mathrm{D}}}{4\pi r_\mathrm{D}} \psi_\mathrm{f}^*(\boldsymbol{r}). \tag{3.9}$$

Applying now the reciprocity theorem (3.7), we obtain

$$G_\mathrm{far}(\boldsymbol{r}, \boldsymbol{r}') = \frac{\mathrm{e}^{iKr}}{4\pi r} \psi_\mathrm{f}^*(\boldsymbol{r}') \tag{3.10}$$

which agrees literally with (2.20), though ψ_f is not any longer a plane wave. Accordingly, the scattered far-field is still given by (2.22), and the differential cross section by (2.31). We only need to redetermine the matrix element $\langle\psi_\mathrm{i}|\chi|\psi_\mathrm{f}\rangle$, which no longer has the plane-wave form (2.25).

Since both the incident and the scattered distorted wavefunction are composed of downward and upward propagating waves,

$$\psi_w(\boldsymbol{r}) = \psi_w^-(\boldsymbol{r}) + \psi_w^+(\boldsymbol{r}) \quad \text{with} \quad w = \mathrm{i}, \mathrm{f}, \tag{3.11}$$

the matrix element can be expanded into four terms,

$$\langle\psi_\mathrm{i}|\chi|\psi_\mathrm{f}\rangle = \langle\psi_\mathrm{i}^-|\chi|\psi_\mathrm{f}^-\rangle + \langle\psi_\mathrm{i}^-|\chi|\psi_\mathrm{f}^+\rangle + \langle\psi_\mathrm{i}^+|\chi|\psi_\mathrm{f}^-\rangle + \langle\psi_\mathrm{i}^+|\chi|\psi_\mathrm{f}^+\rangle\,, \tag{3.12}$$

or in an obvious shorthand notation

[3] The distorted-wave Born approximation was originally devised by Massey and Mott (ca 1933) for collisions of charged particles.

$$\langle\psi_\mathrm{i}|\chi|\psi_\mathrm{f}\rangle = \sum_{\pm_\mathrm{i}}\sum_{\pm_\mathrm{f}} \langle\psi_\mathrm{i}^{\pm}|\chi|\psi_\mathrm{f}^{\pm}\rangle\,. \tag{3.13}$$

This equation contains the essence of the distorted-wave Born approximation for small-angle scattering under grazing incidence, and is the base for all scattering models implemented in `BornAgain`. Since $\langle\psi_\mathrm{i}|\chi|\psi_\mathrm{f}\rangle$ appears as a squared modulus in the differential cross section (2.31), the four terms of (3.13) can interfere with each other, which adds to the complexity of GISAS patterns.