

scatter
The Reference Manual
version 1.3.9

Diab Jerius
Smithsonian Astrophysical Observatory
Chandra X-ray Center

March 8, 2012

Copyright ©2006 by The Smithsonian Astrophysical Observatory All rights reserved.

This manual may be redistributed and/or modified under the terms of the GNU General Public License as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version.

This manual is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with this manual; if not, write to the Free Software Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307 USA

Contents

1	Scattering Geometry	1
1.1	General Definitions	1
1.2	ϕ in $(\hat{\mathbf{u}}, \hat{\mathbf{v}})$ plane	2
1.3	ϕ in $(\hat{\mathbf{s}}_\theta, \hat{\mathbf{u}})$ plane	3
1.4	ϕ in $(\hat{\mathbf{r}}, \hat{\mathbf{u}})$ plane	4
1.5	Summary	6
2	Layout and Use of Scattering Tables	7
2.1	Old (LVS) tables	7
2.2	New (PZ) tables	8

Chapter 1

Scattering Geometry

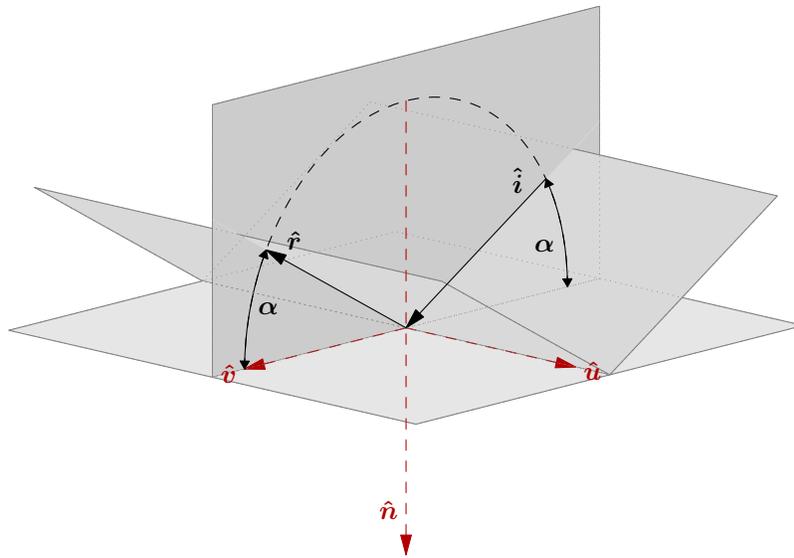


Figure 1.1: Incident and reflected rays and basis vectors for the reflecting surface

1.1 General Definitions

The incident (\hat{i}) and reflected (\hat{r}) rays are at the grazing angle α to the reflecting surface (plane), and the vector \hat{n} is normal to the reflecting plane and oriented such that

$$\begin{aligned}\hat{n} \cdot \hat{i} &= \sin \alpha \\ \hat{n} \cdot \hat{r} &= -\sin \alpha\end{aligned}$$

The reflecting plane is defined by the vectors

$$\begin{aligned}\hat{u} &= \hat{r} \times \hat{n} / \cos \alpha \\ \hat{v} &= \hat{n} \times \hat{u}\end{aligned}$$

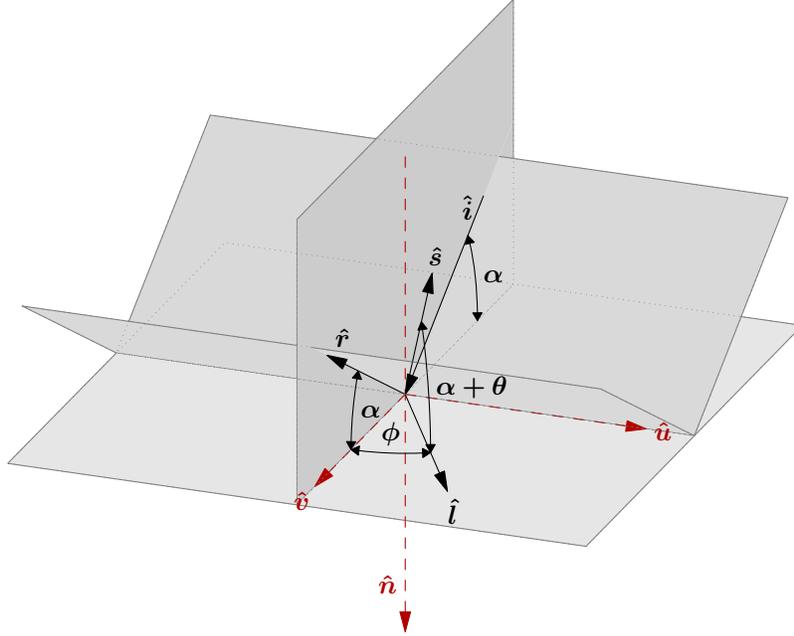


Figure 1.2: ϕ in (\hat{u}, \hat{v}) plane

\hat{v} may also be written in terms of \hat{r} and \hat{n} , to avoid computing an extra cross-product:

$$\begin{aligned}\hat{r} &= -\sin \alpha \hat{n} + \cos \alpha \hat{v} \\ \hat{v} &= \frac{\hat{r} + \sin \alpha \hat{n}}{\cos \alpha}\end{aligned}$$

The specular plane is that which contains both the incident and non-scattered reflected rays. The vectors (\hat{n}, \hat{v}) form basis vectors for it.

The ray is scattered through angle θ relative to \hat{r} , in the specular plane, and ϕ , relative to \hat{r} . Which plane is ϕ in? Therein lies the rub.

The following relationships are useful to improve computational efficiency:

$$\begin{aligned}\sin \alpha &= -\hat{n} \cdot \hat{r} \\ \cos \alpha &= \sqrt{1 - \sin^2 \alpha} \\ \cos(\alpha + \theta) &= \cos \alpha \cos \theta - \sin \alpha \sin \theta \\ \sin(\alpha + \theta) &= \sin \alpha \cos \theta + \cos \alpha \sin \theta\end{aligned}$$

1.2 ϕ in (\hat{u}, \hat{v}) plane

Let \hat{l} be a unit vector in the (\hat{u}, \hat{v}) plane at an angle ϕ to the specular plane (see Fig. 1.2).

$$\hat{l} = \cos \phi \hat{v} + \sin \phi \hat{u}$$

The scattered ray is then given by

$$\begin{aligned}
\hat{\mathbf{s}} &= -\sin(\alpha + \theta) \hat{\mathbf{n}} + \cos(\alpha + \theta) \hat{\mathbf{l}} \\
&= -\sin(\alpha + \theta) \hat{\mathbf{n}} + \cos(\alpha + \theta) [\cos \phi \hat{\mathbf{v}} + \sin \phi \hat{\mathbf{u}}] \\
&= -\sin(\alpha + \theta) \hat{\mathbf{n}} + \cos(\alpha + \theta) \cos \phi \hat{\mathbf{v}} + \cos(\alpha + \theta) \sin \phi \hat{\mathbf{u}} \\
&= -\sin(\alpha + \theta) \hat{\mathbf{n}} + \cos(\alpha + \theta) \cos \phi \left[\frac{\hat{\mathbf{r}} + \sin \alpha \hat{\mathbf{n}}}{\cos \alpha} \right] + \cos(\alpha + \theta) \sin \phi \hat{\mathbf{u}} \\
&= -\sin(\alpha + \theta) \hat{\mathbf{n}} + \frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha} \hat{\mathbf{r}} + \frac{\cos(\alpha + \theta) \sin \alpha \cos \phi}{\cos \alpha} \hat{\mathbf{n}} + \cos(\alpha + \theta) \sin \phi \hat{\mathbf{u}} \\
&= \left(\frac{\cos(\alpha + \theta) \sin \alpha \cos \phi}{\cos \alpha} - \sin(\alpha + \theta) \right) \hat{\mathbf{n}} + \frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha} \hat{\mathbf{r}} + \cos(\alpha + \theta) \sin \phi \hat{\mathbf{u}}
\end{aligned}$$

For computational efficiency, define

$$A = \frac{\cos(\alpha + \theta)}{\cos \alpha}$$

Then,

$$\hat{\mathbf{s}} = (A \sin \alpha \cos \phi - \sin(\alpha + \theta)) \hat{\mathbf{n}} + A (\cos \phi \hat{\mathbf{r}} + \sin \phi \hat{\mathbf{r}} \times \hat{\mathbf{n}})$$

The $\hat{\mathbf{n}}$ component may be re-written for easier comparison with the other approaches:

$$\begin{aligned}
&\frac{\cos(\alpha + \theta) \sin \alpha \cos \phi}{\cos \alpha} - \sin(\alpha + \theta) \\
&= \frac{\cos(\alpha + \theta) \sin \alpha \cos \phi - \sin(\alpha + \theta) \cos \alpha}{\cos \alpha} \\
&= \frac{(\cos(\alpha + \theta) \sin \alpha - \sin(\alpha + \theta) \cos \alpha) \cos \phi + \sin(\alpha + \theta) \cos \alpha \cos \phi - \sin(\alpha + \theta) \cos \alpha}{\cos \alpha} \\
&= \frac{-\sin \theta \cos \phi + \sin(\alpha + \theta) \cos \alpha (\cos \phi - 1)}{\cos \alpha} \\
&= -\frac{\sin \theta \cos \phi}{\cos \alpha} + \sin(\alpha + \theta) (\cos \phi - 1)
\end{aligned}$$

1.3 ϕ in $(\hat{\mathbf{s}}_\theta, \hat{\mathbf{u}})$ plane

$\hat{\mathbf{s}}_\theta$ is the scattered ray in the specular plane, i.e. $\phi = 0$ (see Fig. 1.3).

$$\hat{\mathbf{s}}_\theta = \cos(\alpha + \theta) \hat{\mathbf{v}} - \sin(\alpha + \theta) \hat{\mathbf{n}}$$

$\hat{\mathbf{s}}_\theta$ and $\hat{\mathbf{u}}$ serve as basis vectors for a plane perpendicular to the specular plane. The final scattered ray is given by

$$\begin{aligned}
\hat{\mathbf{s}} &= \cos \phi \hat{\mathbf{s}}_\theta + \sin \phi \hat{\mathbf{u}} \\
&= \cos \phi [\cos(\alpha + \theta) \hat{\mathbf{v}} - \sin(\alpha + \theta) \hat{\mathbf{n}}] + \sin \phi \hat{\mathbf{u}} \\
&= \cos(\alpha + \theta) \cos \phi \hat{\mathbf{v}} - \sin(\alpha + \theta) \cos \phi \hat{\mathbf{n}} + \sin \phi \hat{\mathbf{u}} \\
&= \cos(\alpha + \theta) \cos \phi \left[\frac{\hat{\mathbf{r}} + \sin \alpha \hat{\mathbf{n}}}{\cos \alpha} \right] - \sin(\alpha + \theta) \cos \phi \hat{\mathbf{n}} + \sin \phi \hat{\mathbf{u}} \\
&= \frac{\sin \alpha \cos(\alpha + \theta) \cos \phi}{\cos \alpha} \hat{\mathbf{n}} - \sin(\alpha + \theta) \cos \phi \hat{\mathbf{n}} + \frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha} \hat{\mathbf{r}} + \sin \phi \hat{\mathbf{u}}
\end{aligned}$$

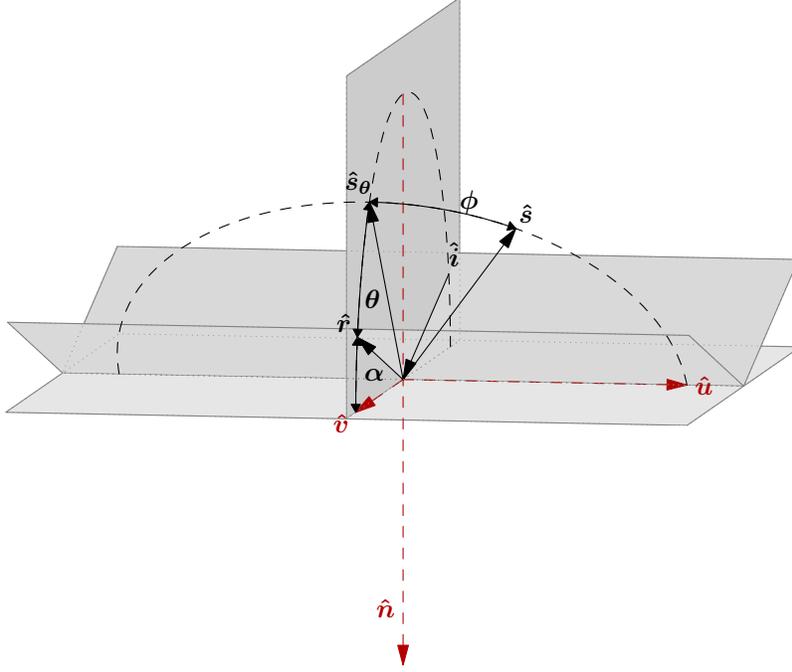


Figure 1.3: ϕ in $(\hat{s}_\theta, \hat{u})$ plane

$$\begin{aligned}
 &= \frac{\cos \phi}{\cos \alpha} (\sin \alpha \cos(\alpha + \theta) - \cos \alpha \sin(\alpha + \theta)) \hat{n} + \frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha} \hat{r} + \sin \phi \hat{u} \\
 &= -\frac{\sin \theta \cos \phi}{\cos \alpha} \hat{n} + \frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha} \hat{r} + \sin \phi \hat{u}
 \end{aligned}$$

1.4 ϕ in (\hat{r}, \hat{u}) plane

\hat{s}_ϕ is the scattered ray in the plane perpendicular to the specular plane containing the reflected ray, i.e. $\theta = 0$ (see Fig. 1.4).

$$\hat{s}_\phi = \cos \phi \hat{r} + \sin \phi \hat{u}$$

Let \hat{q} be the vector perpendicular to \hat{r} and the (\hat{r}, \hat{u}) plane.

$$\begin{aligned}
 \hat{q} &= \hat{r} \times \hat{u} \\
 &= -\sin \alpha \hat{v} - \cos \alpha \hat{n} \\
 &= -\sin \alpha \left[\frac{\hat{r} + \sin \alpha \hat{n}}{\cos \alpha} \right] - \cos \alpha \hat{n} \\
 &= -\frac{\sin \alpha}{\cos \alpha} \hat{r} - \left(\frac{\sin^2 \alpha}{\cos \alpha} + \cos \alpha \right) \hat{n} \\
 &= -\frac{\sin \alpha}{\cos \alpha} \hat{r} - \frac{\sin^2 \alpha + \cos^2 \alpha}{\cos \alpha} \hat{n} \\
 &= -\frac{\sin \alpha}{\cos \alpha} \hat{r} - \frac{1}{\cos \alpha} \hat{n}
 \end{aligned}$$

The final scattered ray is given by

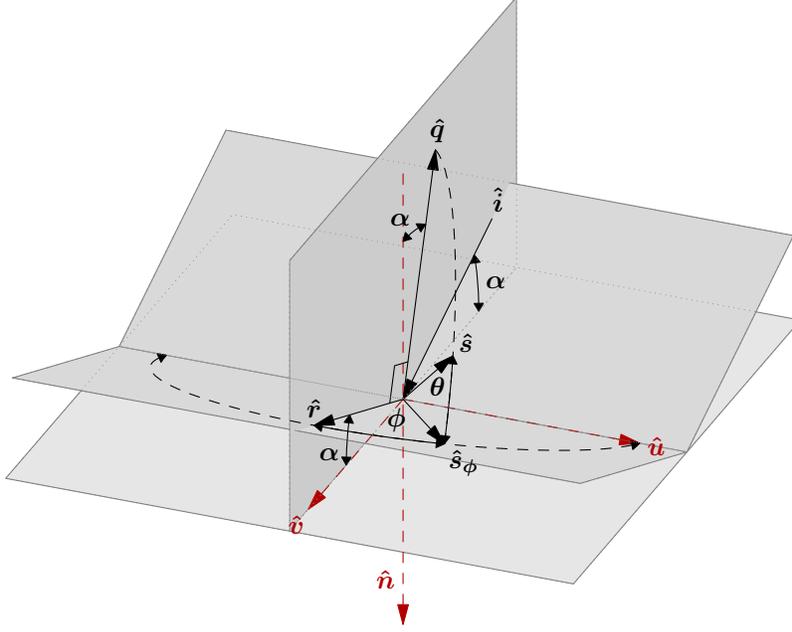


Figure 1.4: ϕ in (\hat{r}, \hat{u}) plane

$$\begin{aligned}
 \hat{s} &= \cos \theta \hat{s}_\phi + \sin \theta \hat{q} \\
 &= \cos \theta \cos \phi \hat{r} + \cos \theta \sin \phi \hat{u} + \sin \theta \left[-\frac{\sin \alpha}{\cos \alpha} \hat{r} - \frac{1}{\cos \alpha} \hat{n} \right] \\
 &= -\frac{\sin \theta}{\cos \alpha} \hat{n} + \cos \theta \cos \phi \hat{r} - \frac{\sin \alpha \sin \theta}{\cos \alpha} \hat{r} + \cos \theta \sin \phi \hat{u} \\
 &= -\frac{\sin \theta}{\cos \alpha} \hat{n} + \left(\cos \theta \cos \phi - \frac{\sin \alpha \sin \theta}{\cos \alpha} \right) \hat{r} + \cos \theta \sin \phi \hat{u}
 \end{aligned}$$

The \hat{r} component may be re-written for easier comparison with the other approaches:

$$\begin{aligned}
 \cos \theta \cos \phi - \frac{\sin \alpha \sin \theta}{\cos \alpha} &= \frac{1}{\cos \alpha} (\cos \alpha \cos \theta \cos \phi - \sin \alpha \sin \theta) \\
 &= \frac{1}{\cos \alpha} ([\cos \alpha \cos \theta - \sin \alpha \sin \theta] \cos \phi + \sin \alpha \sin \theta \cos \phi - \sin \alpha \sin \theta) \\
 &= \frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha} + \frac{\sin \alpha \sin \theta (\cos \phi - 1)}{\cos \alpha}
 \end{aligned}$$

1.5 Summary

ϕ plane	\hat{n}	\hat{r}	\hat{u}
(\hat{u}, \hat{v})	$-\frac{\sin \theta}{\cos \alpha} \cos \phi + \sin(\alpha + \theta) (\cos \phi - 1)$	$\frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha}$	$\cos(\alpha + \theta) \sin \phi$
$(\hat{s}_\theta, \hat{u})$	$-\frac{\sin \theta}{\cos \alpha} \cos \phi$	$\frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha}$	$\sin \phi$
(\hat{r}, \hat{u})	$-\frac{\sin \theta}{\cos \alpha}$	$\frac{\cos(\alpha + \theta) \cos \phi}{\cos \alpha} + \frac{\sin \alpha \sin \theta (\cos \phi - 1)}{\cos \alpha}$	$\cos \theta \sin \phi$

Or, in orthogonal coordinates,

ϕ plane	\hat{n}	\hat{u}	\hat{v}
(\hat{u}, \hat{v})	$-\sin(\alpha + \theta)$	$\cos(\alpha + \theta) \sin \phi$	$\cos(\alpha + \theta) \cos \phi$
$(\hat{s}_\theta, \hat{u})$	$-\sin(\alpha + \theta) \cos \phi$	$\sin \phi$	$\cos(\alpha + \theta) \cos \phi$
(\hat{r}, \hat{u})	$-\sin(\alpha + \theta) \cos \phi + \cos \alpha \sin \theta (\cos \phi - 1)$	$\cos \theta \sin \phi$	$\cos(\alpha + \theta) \cos \phi + \sin \alpha \sin \theta (\cos \phi - 1)$

Chapter 2

Layout and Use of Scattering Tables

Scattering angles which would lead to the ray being scattered into the optic ($\hat{\mathbf{s}} \cdot \hat{\mathbf{n}} > 0$) are rejected.

Scattering angles which result in backscattered rays ($\text{sgn}(\hat{\mathbf{s}} \cdot \hat{\mathbf{v}}) \neq \text{sgn}(\hat{\mathbf{r}} \cdot \hat{\mathbf{v}})$) are rejected.

2.1 Old (LVS) tables

The scattering distribution is split into three regimes

- specular reflection (i.e. no scattering);
- a look-up table; and
- an analytical power law

The distribution is one-sided, so must be reflected to achieve both forwards and backwards scattering. The data are parameterized as a function of $E \sin \alpha$. They are stored as a FITS binary table with columns:

ESA	$E \sin \alpha$
PDIST	vector of scattering angles θ , in radians
PO	largest probability such that the reflection is still specular
PTOP	upper bound probability for the table lookup
PDELTA	spacing in probability of values in PDIST
POWTOP	power law exponent
NORMTOP	power law normalization factor

The ESA column must be in ascending order.

The interpolated scattering angle is given by

$$\theta(E \sin \alpha, P) = \theta_i + (\theta_{i+1} - \theta_i) \frac{E \sin \alpha - \text{ESA}_i}{\text{ESA}_{i+1} - \text{ESA}_i}$$

where

$$\text{ESA}_i < E \sin \alpha < \text{ESA}_{i+1}$$

The scattering angle θ_m for a particular value of $E \sin \alpha$ (ESA_m) is determined as follows:

$$\theta_m = \begin{cases} 0 & P \leq \text{PO}_m \\ \theta_{m,\text{interp}} & \text{PO}_m < P \leq \text{PTOP}_m \\ (\text{NORMTOP}_m (1 - P))^{\text{POWTOP}_m} & \text{PTOP}_m < P < 0.99999 \\ (\text{NORMTOP}_m (1 - 0.99999))^{\text{POWTOP}_m} & 0.99999 \leq P \end{cases}$$

For each angle θ_n in PDIST_m ,

$$P_n = n \text{PDELTA}_m + \text{PO}_m$$

and for a given input value of P ,

$$\begin{array}{ccc} P_j & < & P < & P_{j+1} \\ j & < & j' < & j+1 \end{array}$$

where $j' = (P - \text{PO}_m)/\text{PDELTA}_m$. This leads to

$$\begin{aligned} \theta_{m,\text{interp}} &= \text{PDIST}_{m,j} + (\text{PDIST}_{m,j+1} - \text{PDIST}_{m,j}) \frac{P - P_j}{P_{j+1} - P_j} \\ &= \text{PDIST}_{m,j} + (\text{PDIST}_{m,j+1} - \text{PDIST}_{m,j})(j' - j) \\ &= \text{PDIST}_{m,j}(1 - (j' - j)) + \text{PDIST}_{m,j+1}(j' - j) \end{aligned}$$

The out-of-plane scattering angle is determined via.

$$\phi = \sin \alpha \theta(E \sin \alpha, P')$$

2.2 New (PZ) tables

The scattering distribution is parameterized as a function of $E \sin \alpha$, and is composed of tables of scattering angles. Each table has the same number of angles, each of which have equal probability. The direction of the scattering is such that

$$\theta = \alpha_i - \alpha_s$$

where α_i and α_s are the incident and scattered grazing angles, respectively. θ is thus positive in the forward scattering direction.

The distribution is stored as a FITS binary table with columns

ESA	$E \sin \alpha$
THETA	vector of scattering angles θ , in seconds of arc

The **ESA** column must be in ascending order.

The interpolated scattering angle is given by

$$\theta(E \sin \alpha, P) = \theta_i + (\theta_{i+1} - \theta_i) \frac{E \sin \alpha - \text{ESA}_i}{\text{ESA}_{i+1} - \text{ESA}_i}$$

where

$$\text{ESA}_i < E \sin \alpha < \text{ESA}_{i+1}$$

and, given $P_n = n/N$ (where N is the number of elements in the table), and,

$$\begin{array}{ccc} P_j & < & P < & P_{j+1} \\ j & < & j' < & j+1 \end{array}$$

where $j' = PN$. This leads to

$$\begin{aligned} \theta_m &= \text{THETA}_{m,j} + (\text{THETA}_{m,j+1} - \text{THETA}_{m,j}) \frac{P - P_j}{P_{j+1} - P_j} \\ &= \text{THETA}_{m,j} + (\text{THETA}_{m,j+1} - \text{THETA}_{m,j})(j' - j) \\ &= \text{THETA}_{m,j}(1 - (j' - j)) + \text{THETA}_{m,j+1}(j' - j) \end{aligned}$$

The out-of-plane scattering angle is determined via.

$$\phi = \sin \alpha \times \theta(E \sin \alpha, P') \times \text{sgn}(0.5 - P'')$$