Instrumental Resolution

MLZ Triple-Axis Workshop

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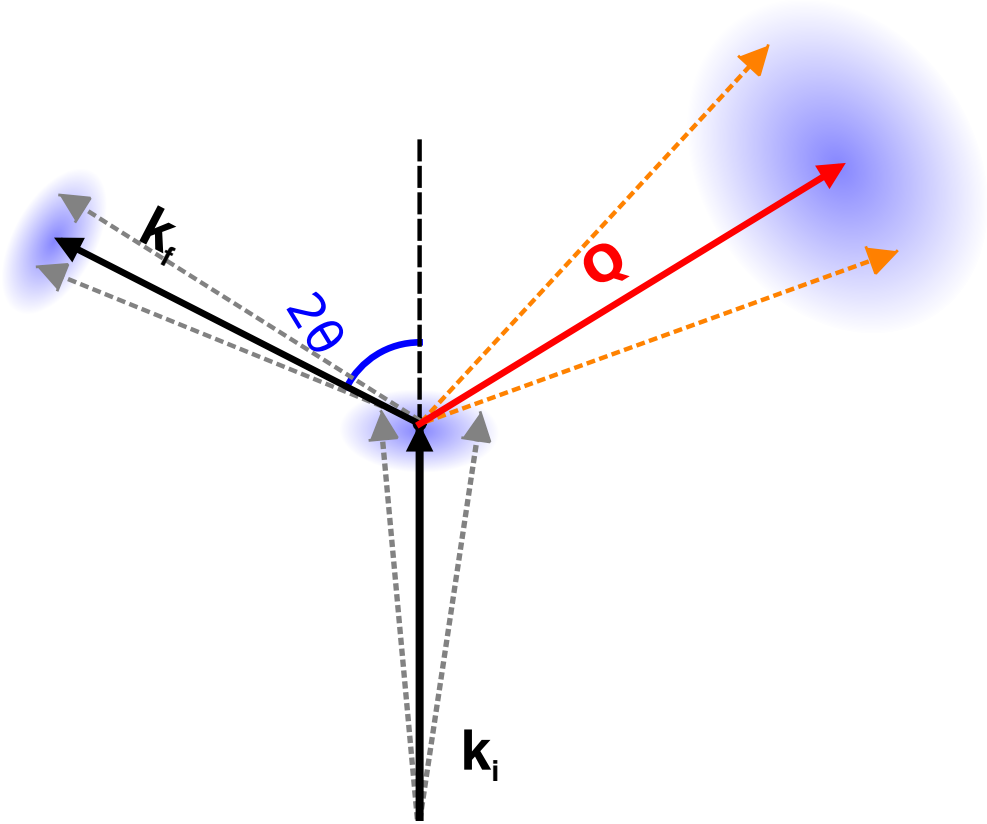
Introduction to resolution calculation

- Scattering triangle: $\boldsymbol{k}_i - \boldsymbol{k}_f = \boldsymbol{Q}$ and $\hbar^2/(2m_n) \cdot k_i^2 - \hbar^2/(2m_n) \cdot k_f^2 = E$
- Variances in $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ add up to a variance in $\boldsymbol{Q}$ and E.



General formalism – Overview

- General formalism presented here is based on Violini [1] and Eckold [2] papers.
- Assume Gaussian transmissions
- Starting with known variances of components
- Need result in a $(\delta \boldsymbol{Q}, \delta E)$ coordinate system:

$$R(\delta \boldsymbol{Q}, \delta E) = R_0 \exp\left(-\frac{1}{2}\begin{pmatrix} \delta \boldsymbol{Q} \\ \delta E \end{pmatrix}^t \cdot R \cdot \begin{pmatrix} \delta \boldsymbol{Q} \\ \delta E \end{pmatrix} - \boldsymbol{r} \cdot \begin{pmatrix} \delta \boldsymbol{Q} \\ \delta E \end{pmatrix} - c\right).$$

- With $\delta \boldsymbol{Q} = \boldsymbol{Q} - \boldsymbol{Q}_0$ and $\delta E = E - E_0$.

General formalism – Important quantities

$$R(\delta\boldsymbol{Q}, \delta E) = R_0 \exp\left(-\frac{1}{2}\begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix}^t \cdot R \cdot \begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix} - \boldsymbol{r}\cdot\begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix} - c\right)$$

- R is called the "resolution matrix".
- $\boldsymbol{r}$ is a vector shifting the mean positions $\boldsymbol{Q}_0$ and E_0.
- R_0 is often called the "resolution volume".
- c is a factor diminishing the scattering intensity.

General formalism – Covariance

- R is the inverse covariance matrix:

$$R = C^{-1}.$$

- Reminder: The covariance of two random variables X and Y is defined as:

$$\mathrm{cov}(X, Y) = \langle (X - \langle X \rangle)(Y - \langle Y \rangle) \rangle .$$

- It is a measure of the correlation between X and Y.

General formalism – Instrument parameters

- Start with known variances σ_i^2 of instrument parameters p_i:

$$C_{\text{instr}} = \text{diag}\left(\sigma_1^2, \sigma_2^2, ..., \sigma_N^2\right)$$

- Assuming no correlation: C_{instr} is diagonal.
- The parameters p_i are defined in terms of $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$.

General formalism – Jacobian

- Transform the instrument parameters to a system given by $\boldsymbol{Q}$ and E:

$$\langle p_1, p_2, ..., p_N \rangle \quad \longmapsto \quad \langle Q_x, Q_y, Q_z, E \rangle$$

- Covariance matrix C' in new $\langle Q_x, Q_y, Q_z, E \rangle$ system with x along $\boldsymbol{k}_i$ and y perpendicular to $\boldsymbol{k}_i$:

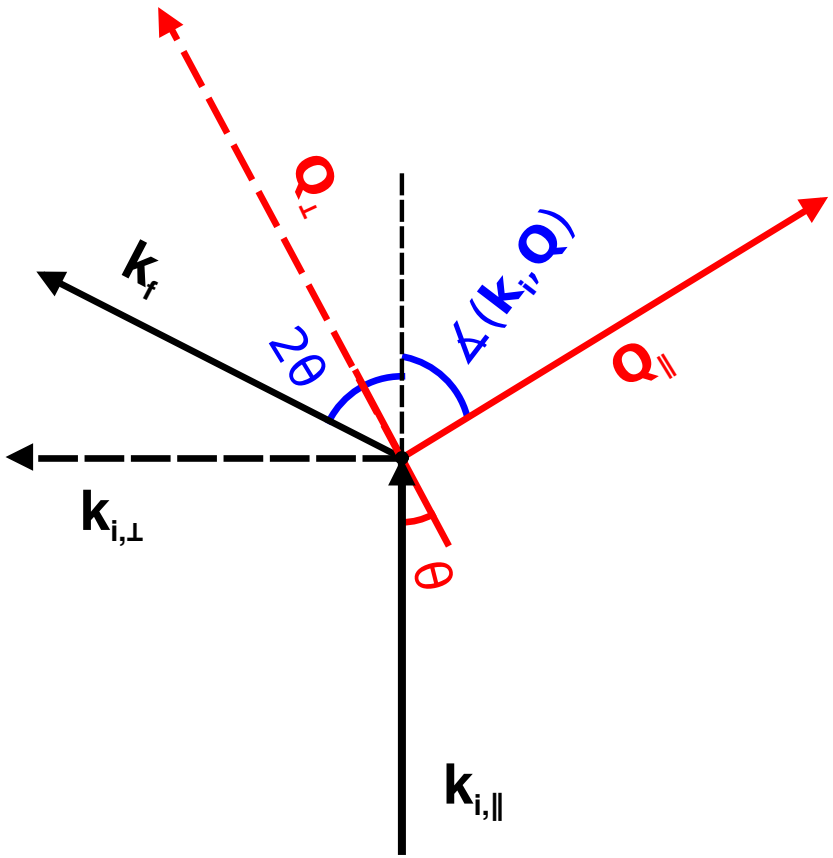
$$C' = T \cdot C_{\text{instr}} \cdot T^t.$$

- With the Jacobian:

$$T = \begin{pmatrix} \frac{\partial Q_x}{\partial p_1} & \frac{\partial Q_x}{\partial p_2} & \cdots & \frac{\partial Q_x}{\partial p_N} \\ \frac{\partial Q_y}{\partial p_1} & \frac{\partial Q_y}{\partial p_2} & \cdots & \frac{\partial Q_y}{\partial p_N} \\ \frac{\partial Q_z}{\partial p_1} & \frac{\partial Q_z}{\partial p_2} & \cdots & \frac{\partial Q_z}{\partial p_N} \\ \frac{\partial E}{\partial p_1} & \frac{\partial E}{\partial p_2} & \cdots & \frac{\partial E}{\partial p_N} \end{pmatrix}$$

General formalism – Rotation

- We could stick with the absolute $\langle Q_x, Q_y, Q_z, E \rangle$ system (in fact, Violini [1] does).
- A more convenient system is the local $\langle \boldsymbol{Q}_\parallel, \boldsymbol{Q}_\perp, Q_z, E \rangle$ system with x along $\langle \boldsymbol{Q} \rangle$:



General formalism – Rotation

- The coordinate systems are rotated by the angle between $\boldsymbol{k}_i$ and $\boldsymbol{Q}$:

$$\langle Q_x, Q_y, Q_z, E \rangle \quad \longmapsto \quad \left\langle \boldsymbol{Q}_{\parallel}, \boldsymbol{Q}_{\perp}, Q_z, E \right\rangle .$$

- The final covariance matrix is:

$$C = S \cdot C' \cdot S^t = S \cdot T \cdot C_{\text{instr}} \cdot T^t \cdot S^t .$$

- With the rotation matrix:

$$S = \begin{pmatrix} \cos\angle(\boldsymbol{k}_i, \boldsymbol{Q}) & \sin\angle(\boldsymbol{k}_i, \boldsymbol{Q}) & 0 & 0 \\ -\sin\angle(\boldsymbol{k}_i, \boldsymbol{Q}) & \cos\angle(\boldsymbol{k}_i, \boldsymbol{Q}) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} .$$

General formalism – Contour line

- We set the general expression equal to 0.5 to get the HWHM contour of the Gaussian ($c = 0$):

$$R(\delta\boldsymbol{Q}, \delta E) \propto \exp\left(-\frac{1}{2}\begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix}^{t} \cdot R \cdot \begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix}\right) \cdot$$

$$\cdot \exp\left(-\boldsymbol{r} \cdot \begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix}\right) \equiv \frac{1}{2}$$

$$\begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix}^{t} \cdot R \cdot \begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix} + 2\boldsymbol{r} \cdot \begin{pmatrix}\delta\boldsymbol{Q}\\ \delta E\end{pmatrix} = 2\ln 2$$

General formalism – Quadric

- This contour outlines a four-dimensional quadric, namely an ellipsoid:

$$\underbrace{\begin{pmatrix} \delta \boldsymbol{Q} \\ \delta E \end{pmatrix}^t \cdot R \cdot \begin{pmatrix} \delta \boldsymbol{Q} \\ \delta E \end{pmatrix}}_{\text{orientation}} + \underbrace{2\boldsymbol{r} \cdot \begin{pmatrix} \delta \boldsymbol{Q} \\ \delta E \end{pmatrix}}_{\text{translation}} = 2\ln 2.$$

- The lengths and the orientation of the ellipsoid axes are obtained via the principal axis theorem, i.e. calculating the eigenvectors and -values of R.

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Minimal example – Definitions

- Assume the variances of $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ are known and are the only parameters, the Jacobian is:

$$T = \begin{pmatrix} \frac{\partial Q_x}{\partial k_{i,x}} & \frac{\partial Q_x}{\partial k_{i,y}} & \frac{\partial Q_x}{\partial k_{i,z}} & \frac{\partial Q_x}{\partial k_{f,x}} & \frac{\partial Q_x}{\partial k_{f,y}} & \frac{\partial Q_x}{\partial k_{f,z}} \\ \frac{\partial Q_y}{\partial k_{i,x}} & \frac{\partial Q_y}{\partial k_{i,y}} & \frac{\partial Q_y}{\partial k_{i,z}} & \frac{\partial Q_y}{\partial k_{f,x}} & \frac{\partial Q_y}{\partial k_{f,y}} & \frac{\partial Q_y}{\partial k_{f,z}} \\ \frac{\partial Q_z}{\partial k_{i,x}} & \frac{\partial Q_z}{\partial k_{i,y}} & \frac{\partial Q_z}{\partial k_{i,z}} & \frac{\partial Q_z}{\partial k_{f,x}} & \frac{\partial Q_z}{\partial k_{f,y}} & \frac{\partial Q_z}{\partial k_{f,z}} \\ \frac{\partial E}{\partial k_{i,x}} & \frac{\partial E}{\partial k_{i,y}} & \frac{\partial E}{\partial k_{i,z}} & \frac{\partial E}{\partial k_{f,x}} & \frac{\partial E}{\partial k_{f,y}} & \frac{\partial E}{\partial k_{f,z}} \end{pmatrix}.$$

Minimal example – Jacobian

- Using $\boldsymbol{Q} = \boldsymbol{k}_i - \boldsymbol{k}_f$ and $E = \frac{\hbar^2}{2m_n}\left(\boldsymbol{k}_i^2 - \boldsymbol{k}_f^2\right)$:

$$T = \begin{pmatrix} 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ \frac{\hbar^2}{m_n} k_{i,x} & \frac{\hbar^2}{m_n} k_{i,y} & \frac{\hbar^2}{m_n} k_{i,z} & \frac{-\hbar^2}{m_n} k_{f,x} & \frac{-\hbar^2}{m_n} k_{f,y} & \frac{-\hbar^2}{m_n} k_{f,z} \end{pmatrix}.$$

Minimal example – Covariance

- The covariance matrix then reads:

$$C = T \cdot \mathrm{diag}\left(\sigma^2_{k_i,x}, \sigma^2_{k_i,y}, \sigma^2_{k_i,z}, \sigma^2_{k_f,x}, \sigma^2_{k_f,y}, \sigma^2_{k_f,z}\right) \cdot T^t.$$

$$C = \begin{pmatrix} C_{xx} & 0 & 0 & C_{xE} \\ 0 & C_{yy} & 0 & C_{yE} \\ 0 & 0 & C_{zz} & C_{zE} \\ C_{xE} & C_{yE} & C_{zE} & C_{EE} \end{pmatrix}, \text{ with}$$

$$C_{qq} = \sigma^2_{k_i,q} + \sigma^2_{k_f,q},$$

$$C_{EE} = \frac{\hbar^4}{m_n^2}\left(k^2_{i,x} \cdot \sigma^2_{k_i,x} + \ldots + k^2_{f,x} \cdot \sigma^2_{k_f,x} + \ldots\right),$$

$$C_{qE} = \frac{\hbar^2}{m_n}\left(k_{i,q} \cdot \sigma^2_{k_i,q} + k_{f,q} \cdot \sigma^2_{k_f,q}\right).$$

Minimal example – Correlation

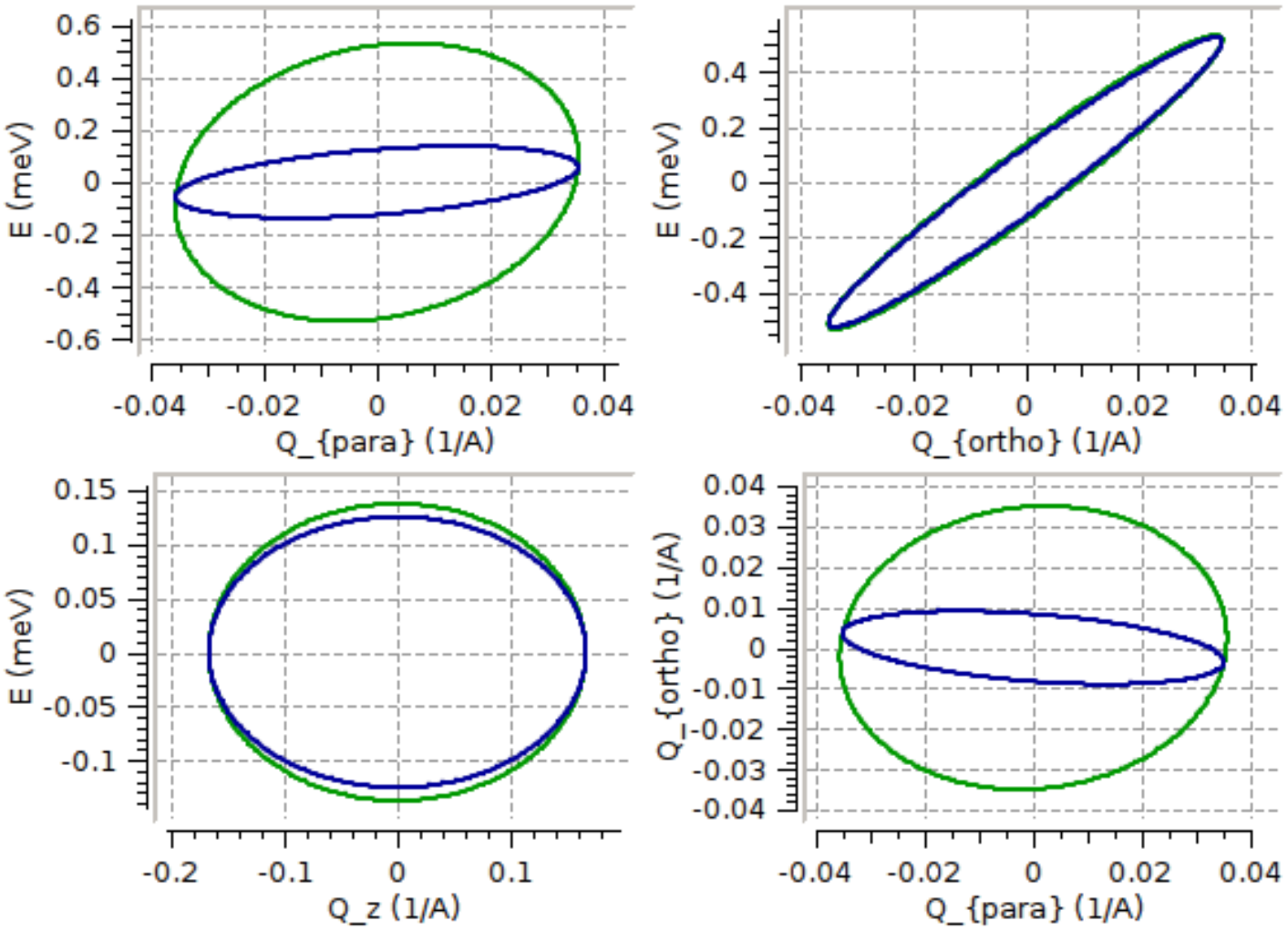
- The covariance matrix is not diagonal, there are q, E correlation terms:

$$C_{qE} = \underbrace{\frac{\hbar^2}{m_n}}_{\approx 4.1\,\mathrm{meV\AA^2}} \left(k_{i,q} \cdot \sigma^2_{k_i,q} + k_{f,q} \cdot \sigma^2_{k_f,q}\right).$$

- In the standard $\langle \boldsymbol{Q}_{\parallel}, \boldsymbol{Q}_{\perp}, Q_z \rangle$ coordinate system (we're still in $\langle Q_x, Q_y, Q_z, E \rangle$) this leads to the important focusing formula for transverse scans:

$$\frac{\delta E\,[\mathrm{meV}]}{\delta Q_{\perp}\left[\mathrm{\AA}^{-1}\right]} \approx 4 \cdot k_{fix}\left[\mathrm{\AA}^{-1}\right].$$

Minimal example – Correlation



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Monte-Carlo method

- In Monte-Carlo simulations (e.g. McStas [3]) we can directly obtain $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ for each neutron and immediately get the covariance matrix:

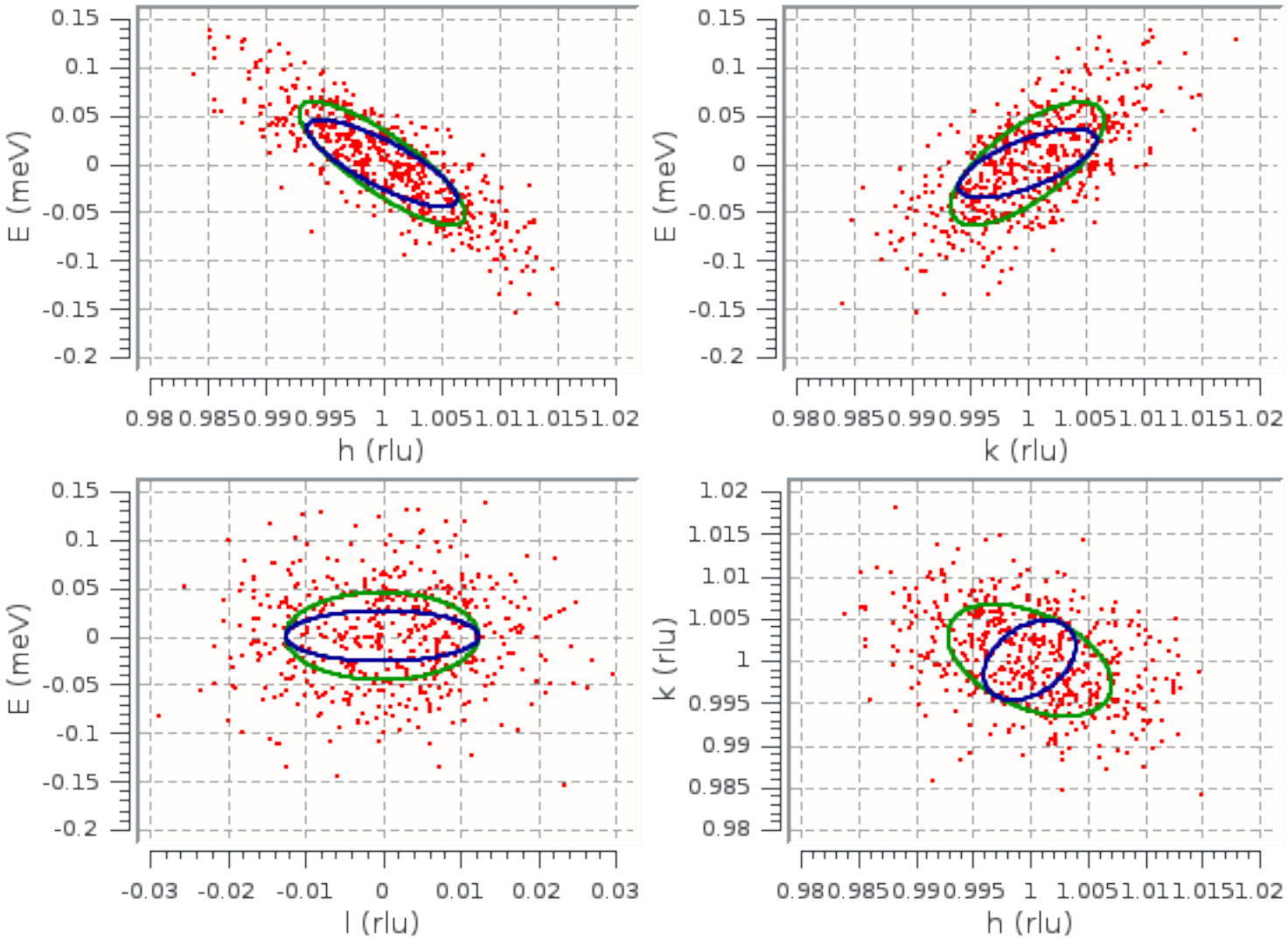
$$C = \frac{\sum_{j=1}^{N} p_j \left(\boldsymbol{Q}_j - \langle \boldsymbol{Q} \rangle\right) \otimes \left(\boldsymbol{Q}_j - \langle \boldsymbol{Q} \rangle\right)}{\sum_{j=1}^{N} p_j}$$

  where j numbers the N Monte-Carlo events.

- The $\boldsymbol{Q}_j$ are the four-vectors:

$$\boldsymbol{Q}_j = \begin{pmatrix} \boldsymbol{k}_{i,j} - \boldsymbol{k}_{f,j} \\ \frac{\hbar^2}{2m_n}\left[\boldsymbol{k}_{i,j}^2 - \boldsymbol{k}_{f,j}^2\right] \end{pmatrix}.$$

Monte-Carlo method



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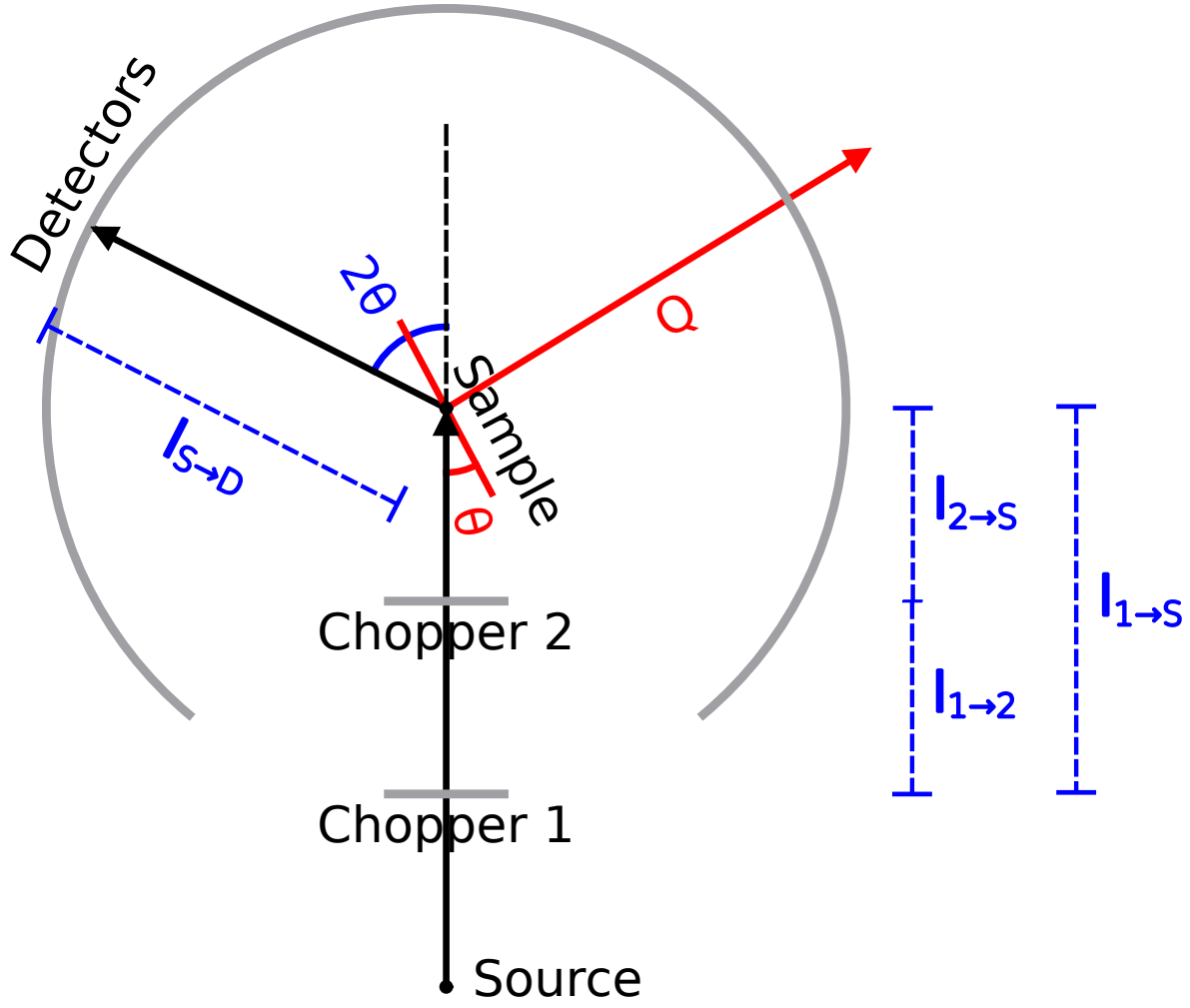
Time-of-flight spectrometers



Time-of-flight spectrometers – Energy expression

- TOF resolution: Violini method [1]:

$$
\begin{aligned}
E &= \frac{\hbar^2}{2m_n}\left(\boldsymbol{k}_i^2 - \boldsymbol{k}_f^2\right) = \frac{m_n}{2}\left(\boldsymbol{v}_i^2 - \boldsymbol{v}_f^2\right) \\
&= \frac{m_n}{2}\left[\left(\frac{l_{1\to 2}}{t_i}\right)^2 - \left(\underbrace{\frac{l_{S\to D}}{t_f}}_{=t_{S\to D}}\right)^2\right] \\
&= \frac{m_n}{2}\left[\left(\frac{l_{1\to 2}}{t_i}\right)^2 - \left(\frac{l_{S\to D}}{t_{2\to D} - \underbrace{t_{2\to S}}_{=l_{2\to S}/v_i}}\right)^2\right].
\end{aligned}
$$

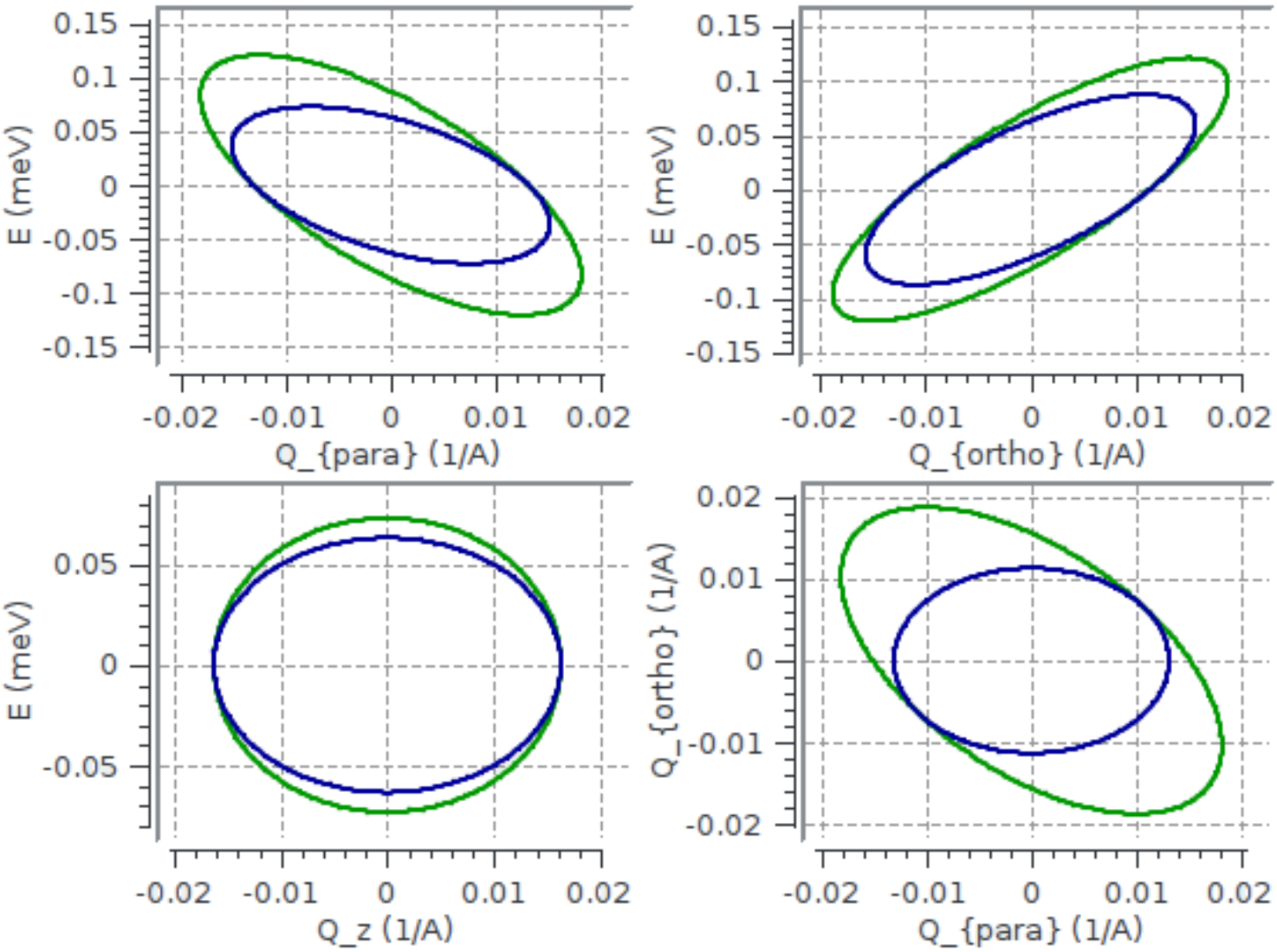
Time-of-flight spectrometers – Momentum expression

- TOF resolution: Violini method [1]:

$$
\begin{aligned}
\boldsymbol{Q} &= \boldsymbol{k}_i - \boldsymbol{k}_f \\
&= \frac{m_n}{\hbar}\left(\boldsymbol{v}_i - \boldsymbol{v}_f\right) \\
&= \frac{m_n}{\hbar}\left[\frac{l_{1\to 2}}{t_i}\begin{pmatrix}1\\0\\0\end{pmatrix} - \frac{l_{S\to D}}{t_f}\begin{pmatrix}\cos 2\vartheta\cdot\cos 2\phi\\ \sin 2\vartheta\cdot\cos 2\phi\\ \sin 2\phi\end{pmatrix}\right].
\end{aligned}
$$

- 2ϑ is the in-plane and 2ϕ the out-of-plane scattering angle.

Time-of-flight spectrometers



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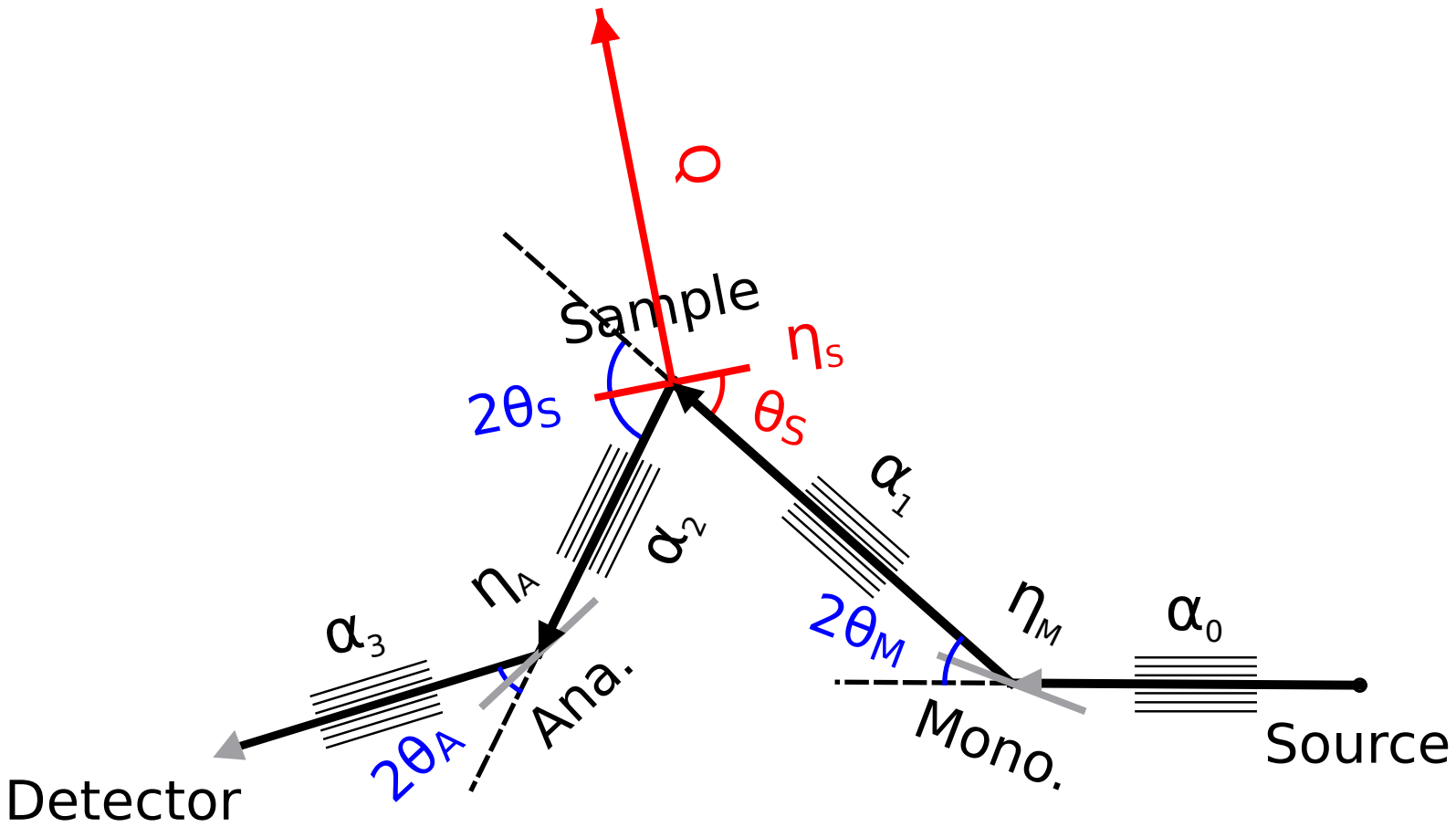
Triple-Axis spectrometers



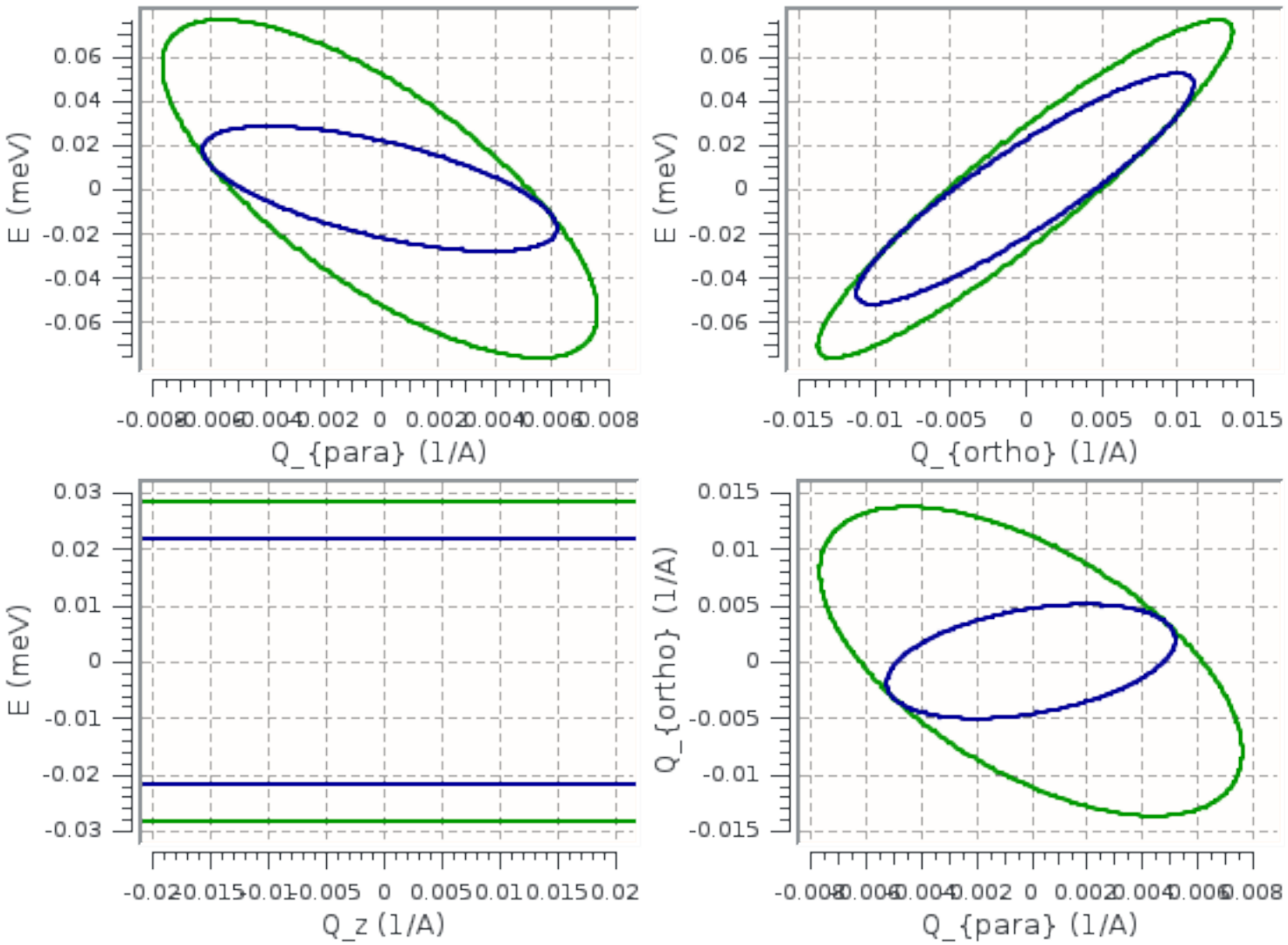
Triple-Axis spectrometers – Algorithms

- Comparison of TAS resolution algorithms:

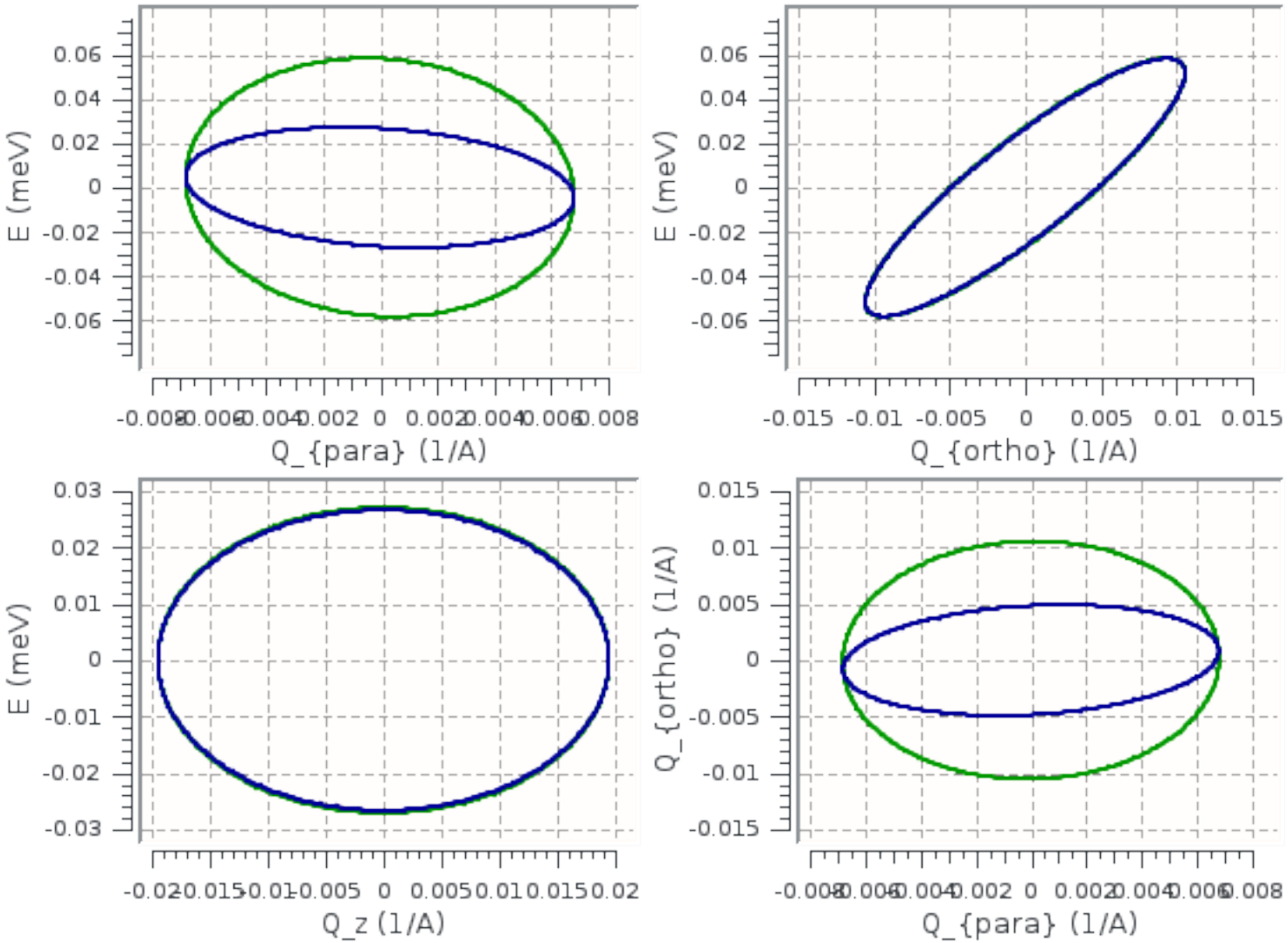
Method	**Description**
Cooper-Nathans [4, 5]	only considers collimators, no geometry
Popovici [6]	collimators + instrument geometry
Eckold-Sobolev [2]	collimators + geometry + + non-centered beams

- The Eckold-Sobolev algorithm is the only TAS algorithm considering the linear part of the quadric.
- It thus allows to calculate the resolution for off-centre neutron paths, non-centered samples and for monochromator and analyser focusing.

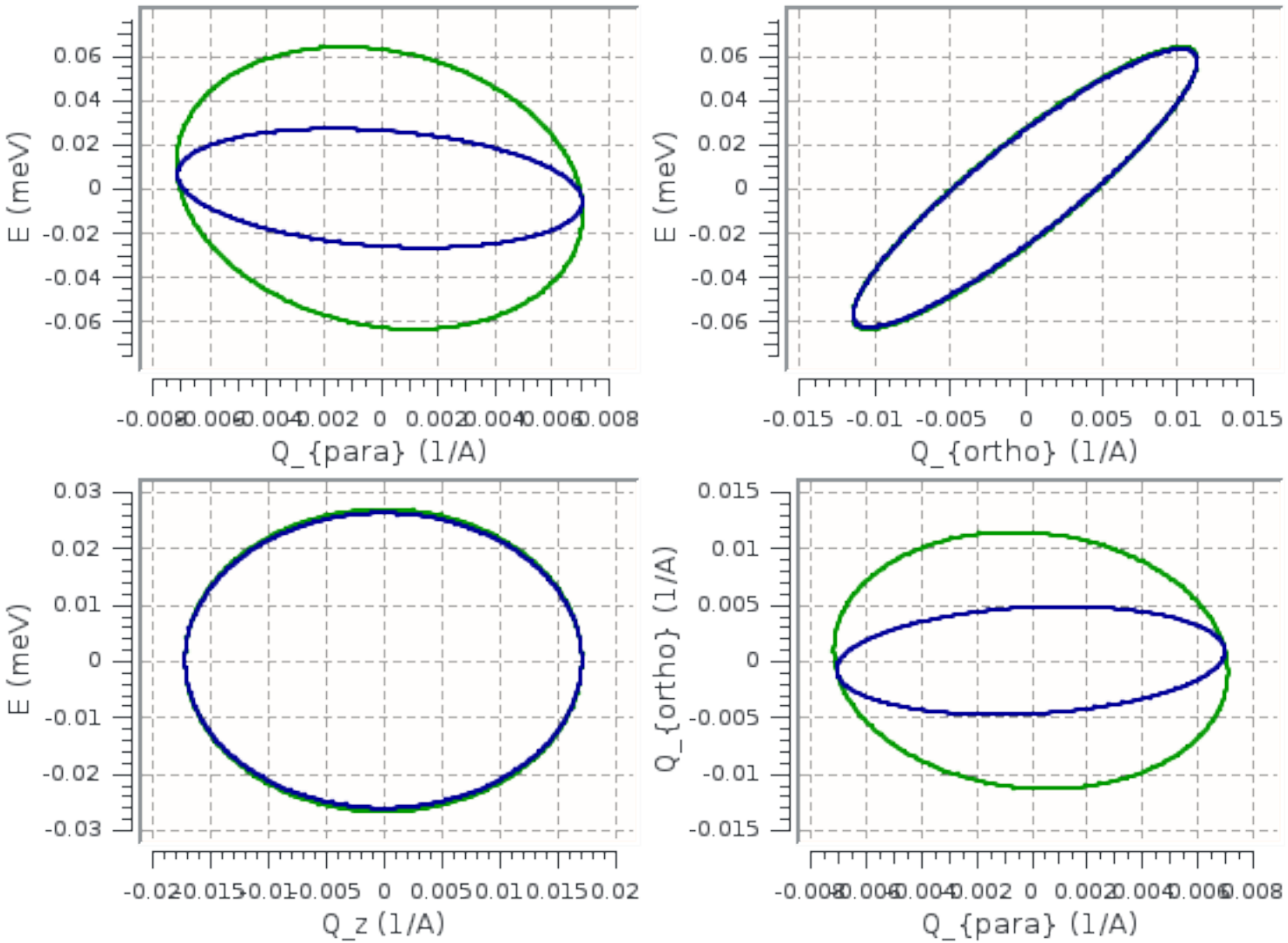
Triple-Axis spectrometers – Cooper-Nathans



Triple-Axis spectrometers – Popovici



Triple-Axis spectrometers – Eckold-Sobolev



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Triple-Axis spectrometers – Cooper-Nathans method

- Cooper-Nathans [5] resolution matrix in $(\delta \boldsymbol{k}_i, \delta \boldsymbol{k}_f)$ frame:

$$R = \begin{pmatrix} R_M & \\ & R_A \end{pmatrix}, \text{ with } R_M = \begin{pmatrix} R_{M,h} & \\ & R_{M,v} \end{pmatrix} \text{ and } R_A \text{ similarly}$$

$$R_{M,h} = \begin{pmatrix} \frac{4\tan^2\vartheta_M}{k_i^2}\left(\frac{1}{\alpha_0^2} + \frac{1}{(2\eta_M)^2}\right) & \frac{-2\varepsilon_M \tan\vartheta_M}{k_i^2}\left(\frac{1}{\alpha_0^2} + \frac{1}{2\eta_M^2}\right) \\ \frac{-2\varepsilon_M \tan\vartheta_M}{k_i^2}\left(\frac{1}{\alpha_0^2} + \frac{1}{2\eta_M^2}\right) & \frac{1}{k_i^2}\left(\frac{1}{\alpha_0^2} + \frac{1}{\alpha_1^2} + \frac{1}{\eta_M^2}\right) \end{pmatrix}$$

Triple-Axis spectrometers – Cooper-Nathans method

- Transformation of resolution matrix from $(\delta \boldsymbol{k}_i, \delta \boldsymbol{k}_f)$ to $(\delta \boldsymbol{Q}, \delta E)$ frame:

$$\begin{pmatrix} \delta Q_x \\ \delta Q_y \\ \delta Q_z \\ \delta E \\ \delta k_{ix} \\ \delta k_{iz} \end{pmatrix} = \begin{pmatrix} \cos\varphi_i & -\sin\varphi_i & 0 & -\cos\varphi_f & \sin\varphi_f & 0 \\ \sin\varphi_i & \cos\varphi_i & 0 & -\sin\varphi_f & -\cos\varphi_f & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ 2k_i \cdot c & 0 & 0 & -2k_f \cdot c & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} \delta k_{ix} \\ \delta k_{iy} \\ \delta k_{iz} \\ \delta k_{fx} \\ \delta k_{fy} \\ \delta k_{fz} \end{pmatrix}$$

using $\varphi_i = \angle(\boldsymbol{k}_i, \boldsymbol{Q})$, $\varphi_f = \angle(\boldsymbol{k}_f, \boldsymbol{Q})$, and $c = \hbar^2/(2m_n)$.

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Triple-Axis spectrometers – Popovici method

- Popovici [6] resolution matrix in $(\delta \boldsymbol{k}_i, \delta \boldsymbol{k}_f)$ frame:

$$R = A \left\{ \left[D \left(S + T^T F T \right)^{-1} D^T \right]^{-1} + G \right\}^{-1} A^T$$

- S: Covariance matrix of source, monochromator, sample, analyser, and detector sizes.
  F: Covariance matrix of crystal mosaics.
  G: Covariance matrix of collimators.
  D: Matrix of instrumental lengths.
- Transformation from $(\delta \boldsymbol{k}_i, \delta \boldsymbol{k}_f)$ to $(\delta \boldsymbol{Q}, \delta E)$ frame as before in Cooper-Nathans.

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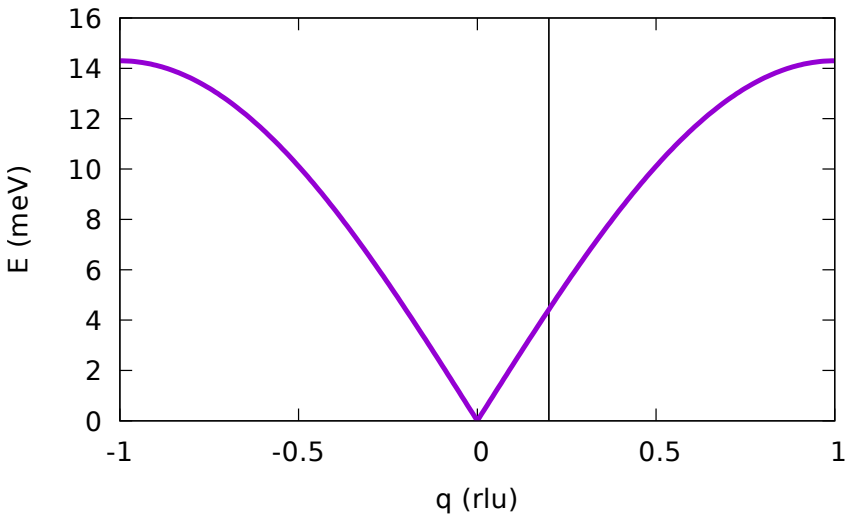
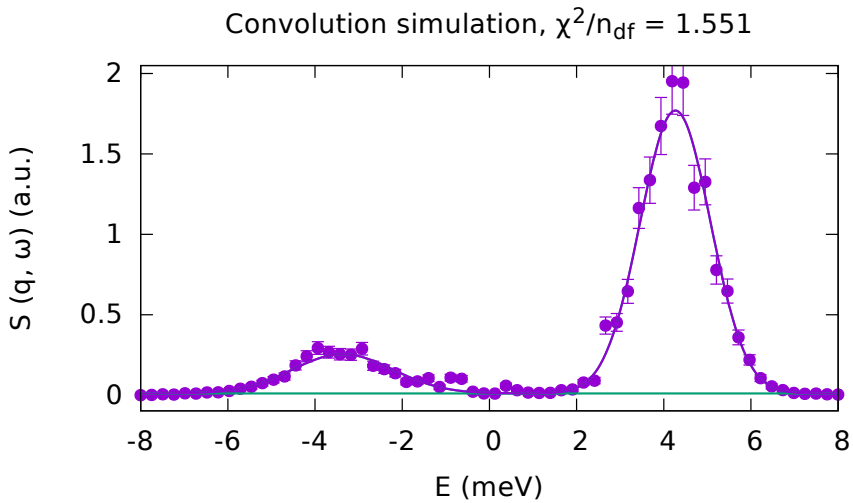
Convolution

- The measured intensity is the convolution of the dynamical structure factor S with the instrumental resolution function R:

$$I(\boldsymbol{Q}, E) = \int d(\delta\boldsymbol{Q})\, d(\delta E)\; S(\boldsymbol{Q} + \delta\boldsymbol{Q}, E + \delta E) \cdot R(\delta\boldsymbol{Q}, \delta E).$$

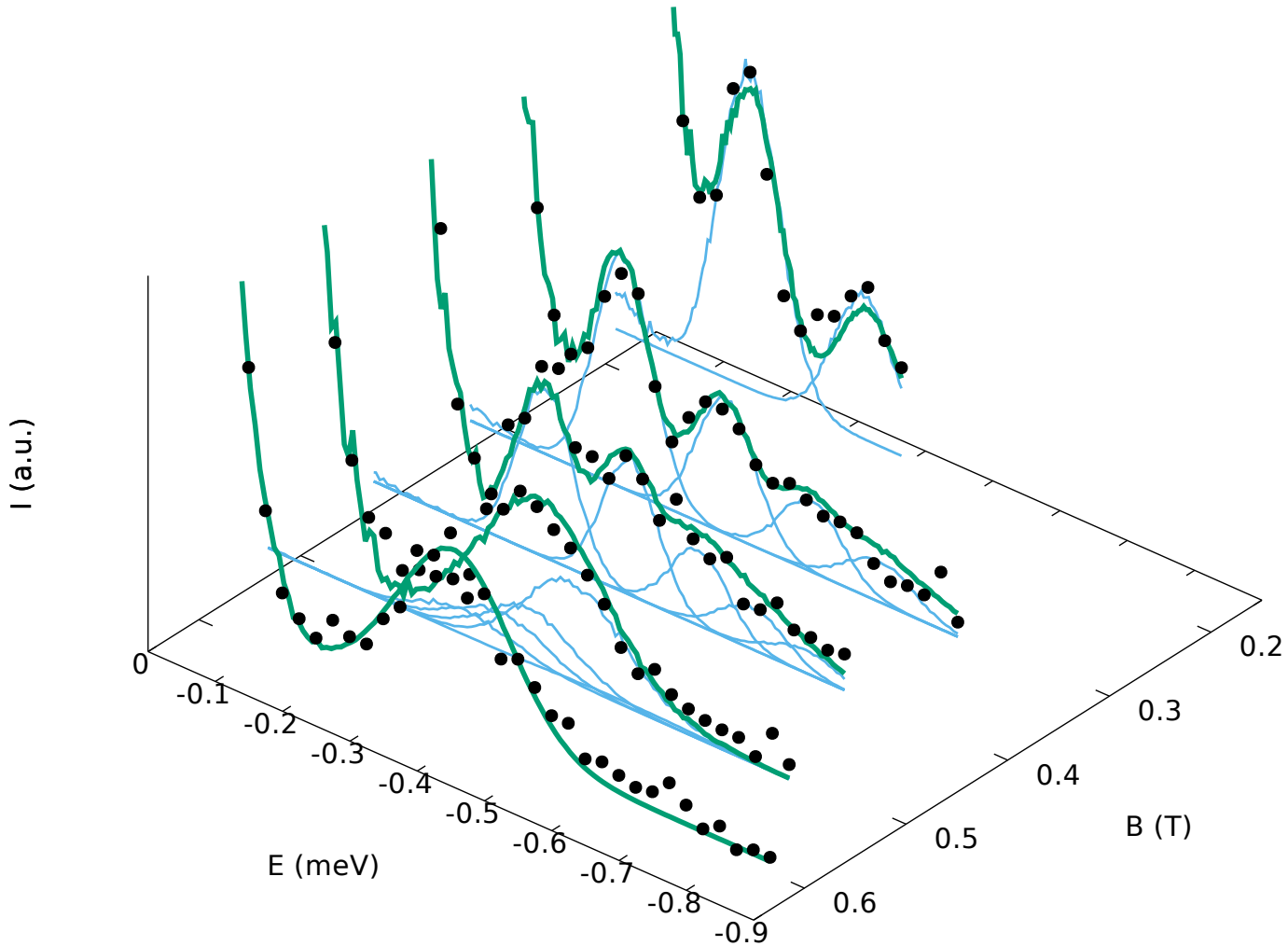
- Convolution of a simple transverse-acoustic phonon branch:





Convolution Fitting

- Change model parameters and minimise χ^2.



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Summary

- General formalism: Resolution = Covariance^{-1}
- For Monte-Carlo simulations the resolution can be directly obtained.
- Several different methods of increasing complexity available for triple-axis resolution calculation.
- Important instrument-independent rule of thumb:
  $E\,[\mathrm{meV}]\,/\,q_{\perp}\left[\mathrm{\AA}^{-1}\right] \approx 4 \cdot k_{fix}\left[\mathrm{\AA}^{-1}\right]$.
  Also valid for TOF!

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