Notes for sheet 12.

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a)

- Average $\boldsymbol{Q}$ and E:

$$\langle \boldsymbol{Q} \rangle = \begin{pmatrix} 1.38\,\text{Å}^{-1} \\ 1.38\,\text{Å}^{-1} \\ 0 \end{pmatrix}, \quad \langle E \rangle = 0.004\,\text{meV} \tag{1}$$

- Covariance matrix:

$$C = \frac{\sum_{j=1}^{N} p_j \left(\boldsymbol{Q_j} - \langle \boldsymbol{Q} \rangle\right) \otimes \left(\boldsymbol{Q_j} - \langle \boldsymbol{Q} \rangle\right)}{\sum_{j=1}^{N} p_j} = \begin{pmatrix} 0.00013 & -0.000097 & 0.000064 & -0.0010 \\ -0.000097 & 0.000081 & -0.000044 & 0.00075 \\ 0.000064 & -0.000044 & 0.00011 & -0.00056 \\ -0.0010 & 0.00075 & -0.00056 & 0.0080 \end{pmatrix} \tag{2}$$

- Transformation from the $\langle \boldsymbol{Q_x}, \boldsymbol{Q_y}, \boldsymbol{Q_z}, E \rangle$ system to the $\langle \boldsymbol{Q}_{||}, \boldsymbol{Q}_{\perp}, \boldsymbol{Q_z}, E \rangle$ system (with x along the average $\boldsymbol{Q}$):

$$\boldsymbol{Q}_{||} = \frac{\langle \boldsymbol{Q} \rangle}{\|\langle \boldsymbol{Q} \rangle\|} \tag{3}$$

$$\boldsymbol{Q}_{\perp} = \begin{pmatrix} -Q_{||}^{y} \\ Q_{||}^{x} \\ Q_{||}^{z} \end{pmatrix} \tag{4}$$

- Transformation matrix:

$$T = \begin{pmatrix} Q_{||}^{x} & Q_{\perp}^{x} & Q_{z}^{x} & 0 \\ Q_{||}^{y} & Q_{\perp}^{y} & Q_{z}^{y} & 0 \\ Q_{||}^{z} & Q_{\perp}^{z} & Q_{z}^{z} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0.71 & -0.71 & 0 & 0 \\ 0.71 & 0.71 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{5}$$

- Transformed covariance matrix:

$$C_T = TCT^t = \begin{pmatrix} 9.77 \cdot 10^{-6} & -2.60 \cdot 10^{-5} & 1.47 \cdot 10^{-5} & -0.00019 \\ -2.60 \cdot 10^{-5} & 0.00020 & -7.67 \cdot 10^{-5} & 0.0013 \\ 1.47 \cdot 10^{-5} & -7.67 \cdot 10^{-5} & 0.00011 & -0.00056 \\ -0.00019 & 0.0013 & -0.00056 & 0.0080 \end{pmatrix} \tag{6}$$

- Resolution matrix:

$$M = C_T^{-1} = \begin{pmatrix} 293000 & -172000 & 18100 & 35200 \\ -172000 & 281000 & -36600 & -50900 \\ 18000 & -36600 & 18400 & 7470 \\ 35200 & -50900 & 7470 & 9480 \end{pmatrix} \tag{7}$$

b)

- Eigenvectors $\boldsymbol{v}$ and -values λ of M:

$$\boldsymbol{v_1} = \begin{pmatrix} -0.022 \\ 0.156 \\ -0.068 \\ 0.99 \end{pmatrix}, \ \lambda_1 = 105 \tag{8}$$

$$\boldsymbol{v_2} = \begin{pmatrix} -0.031 \\ -0.16 \\ -0.99 \\ -0.043 \end{pmatrix}, \ \lambda_2 = 13300 \tag{9}$$

$$\boldsymbol{v_3} = \begin{pmatrix} -0.71 \\ -0.69 \\ 0.13 \\ 0.10 \end{pmatrix}, \ \lambda_3 = 118000 \tag{10}$$

$$\boldsymbol{v_4} = \begin{pmatrix} 0.70 \\ -0.69 \\ 0.086 \\ 0.13 \end{pmatrix}, \ \lambda_4 = 471000 \tag{11}$$

- HWHM of ellipse axes (the factor $\sqrt{2\ln 2}$ scales σ to HWHM):

$$r_1 = \sqrt{2\ln 2} \cdot \frac{1}{\sqrt{\lambda_1}} = 0.11 \tag{12}$$

$$r_2 = \sqrt{2\ln 2} \cdot \frac{1}{\sqrt{\lambda_2}} = 0.010 \tag{13}$$

$$r_3 = \sqrt{2\ln 2} \cdot \frac{1}{\sqrt{\lambda_3}} = 0.0034 \tag{14}$$

$$r_4 = \sqrt{2\ln 2} \cdot \frac{1}{\sqrt{\lambda_4}} = 0.0017 \tag{15}$$

- Plot of resolution function (blue: slices, green: projections):