

# Fourierova transformace

Rentgenová strukturní analýza



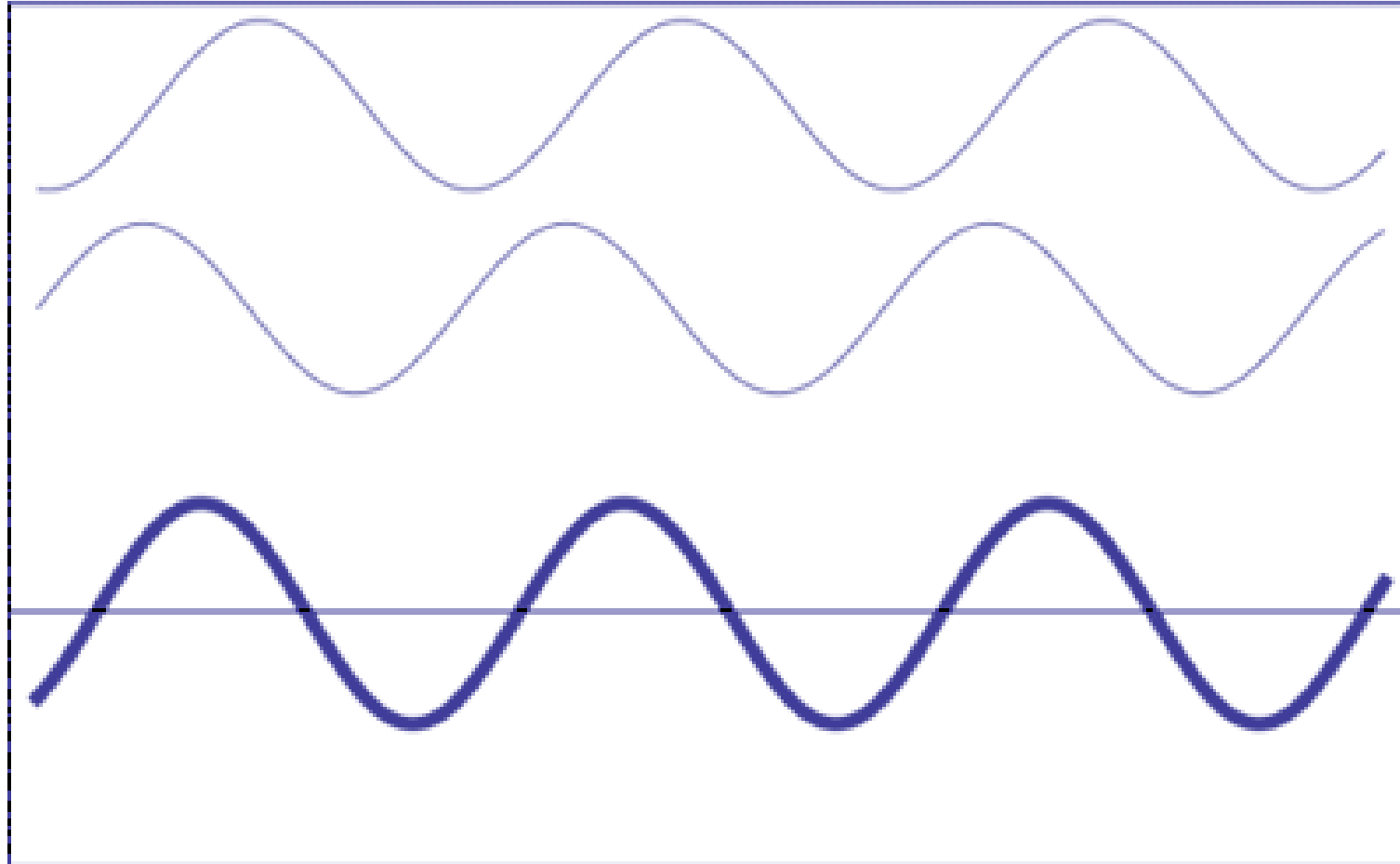
Napište jednu věc, kterou si pamatujete z videa.

Wordcloud Poll 23 responses 18 participants



slido

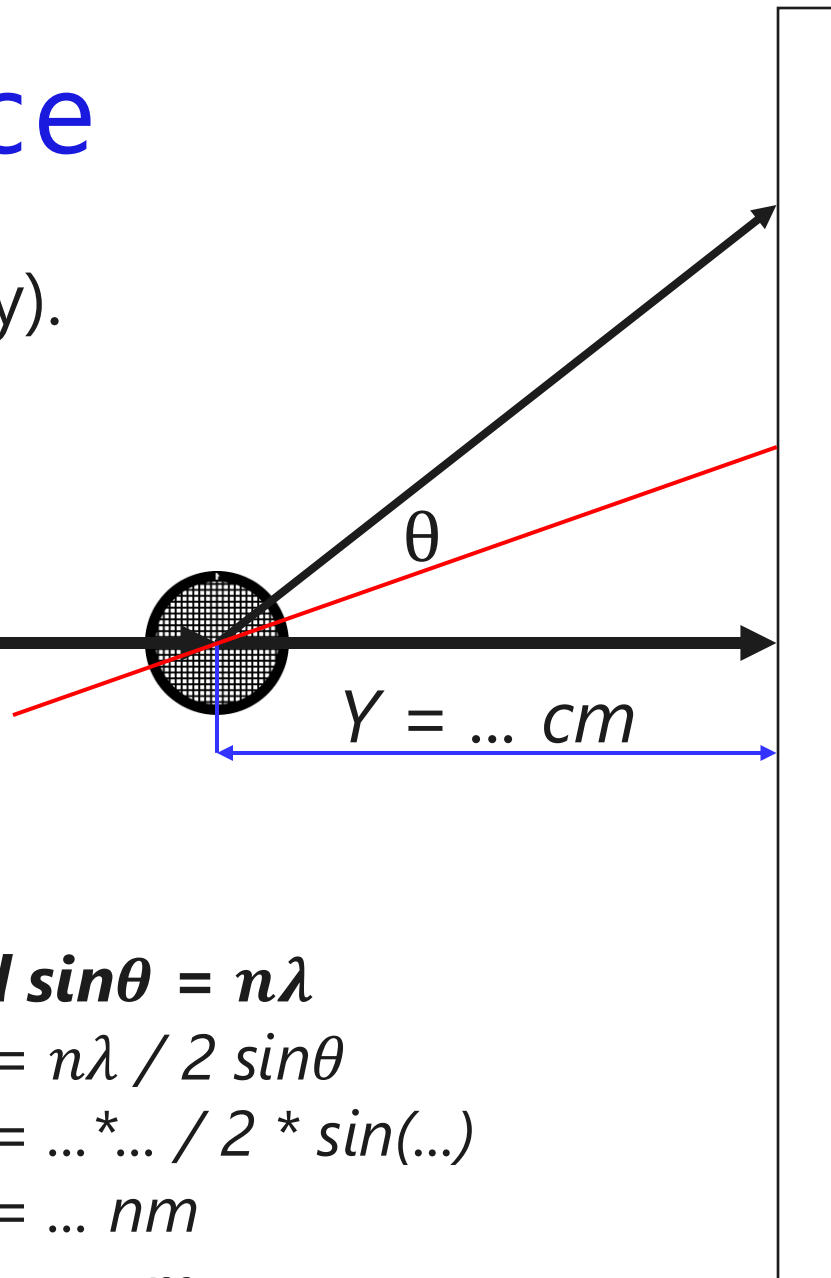
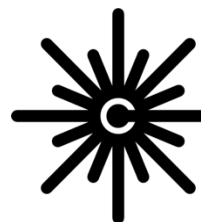
# Opakování



# Difrakce na mřížce

Vypočítejte **d** (parametr mřížky).

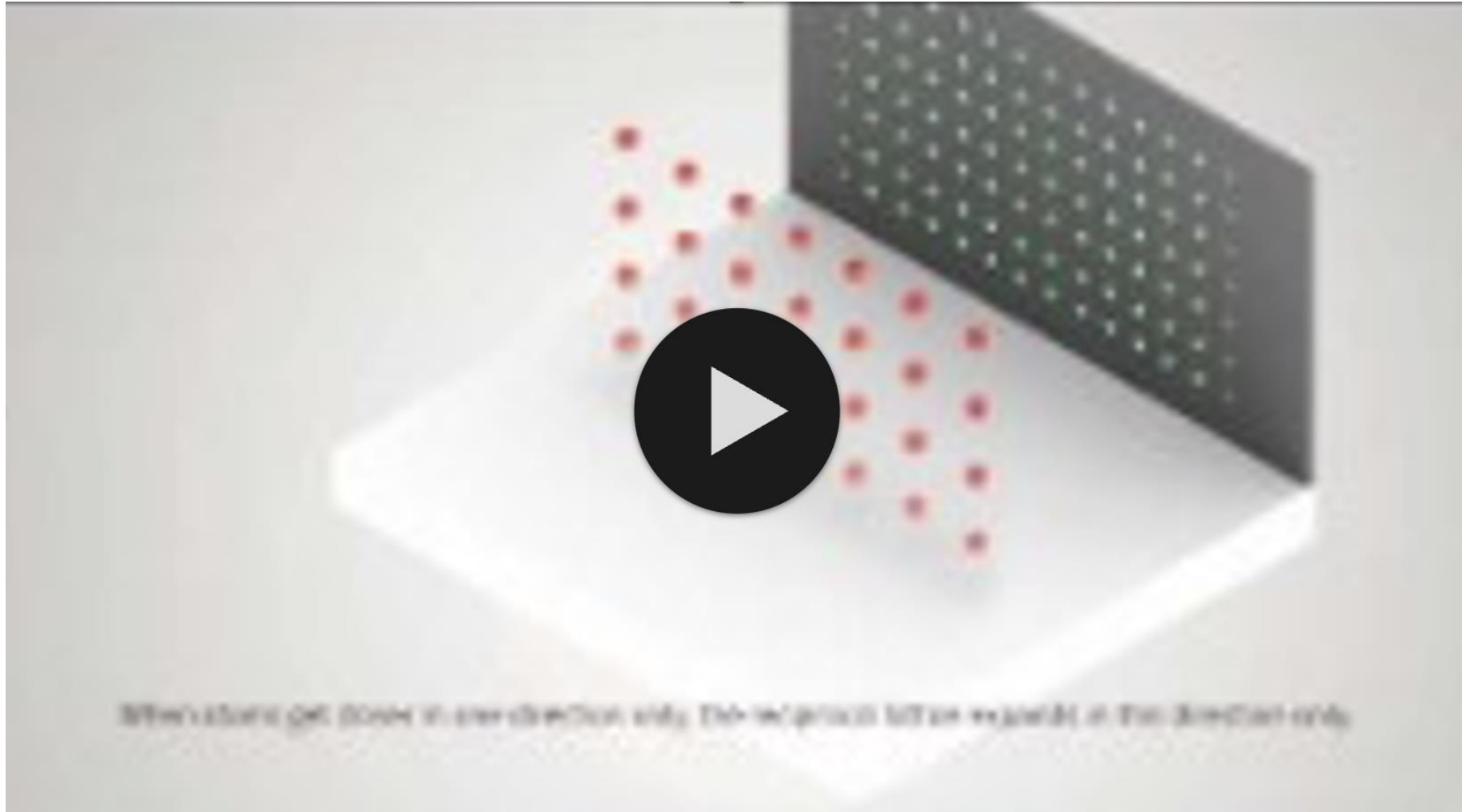
$$\lambda = 532\text{nm}$$



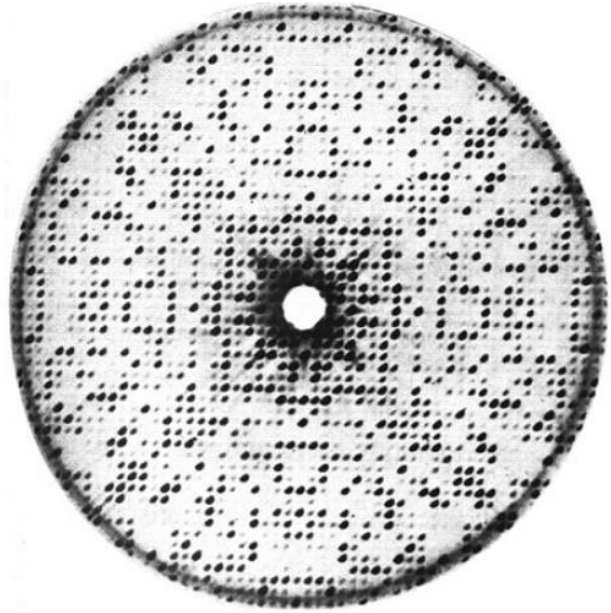
$$\begin{aligned} \text{tg}(2\theta) &= X1/Y \\ 2\theta &= \text{tg}^{-1}(X1/Y) \\ 2\theta &= \dots^\circ \\ \theta &= \dots^\circ \end{aligned}$$

$$\begin{aligned} 2d \sin\theta &= n\lambda \\ d &= n\lambda / 2 \sin\theta \\ d &= \dots * \dots / 2 * \sin(\dots) \\ d &= \dots \text{nm} \\ d &= \dots \mu\text{m} \end{aligned}$$

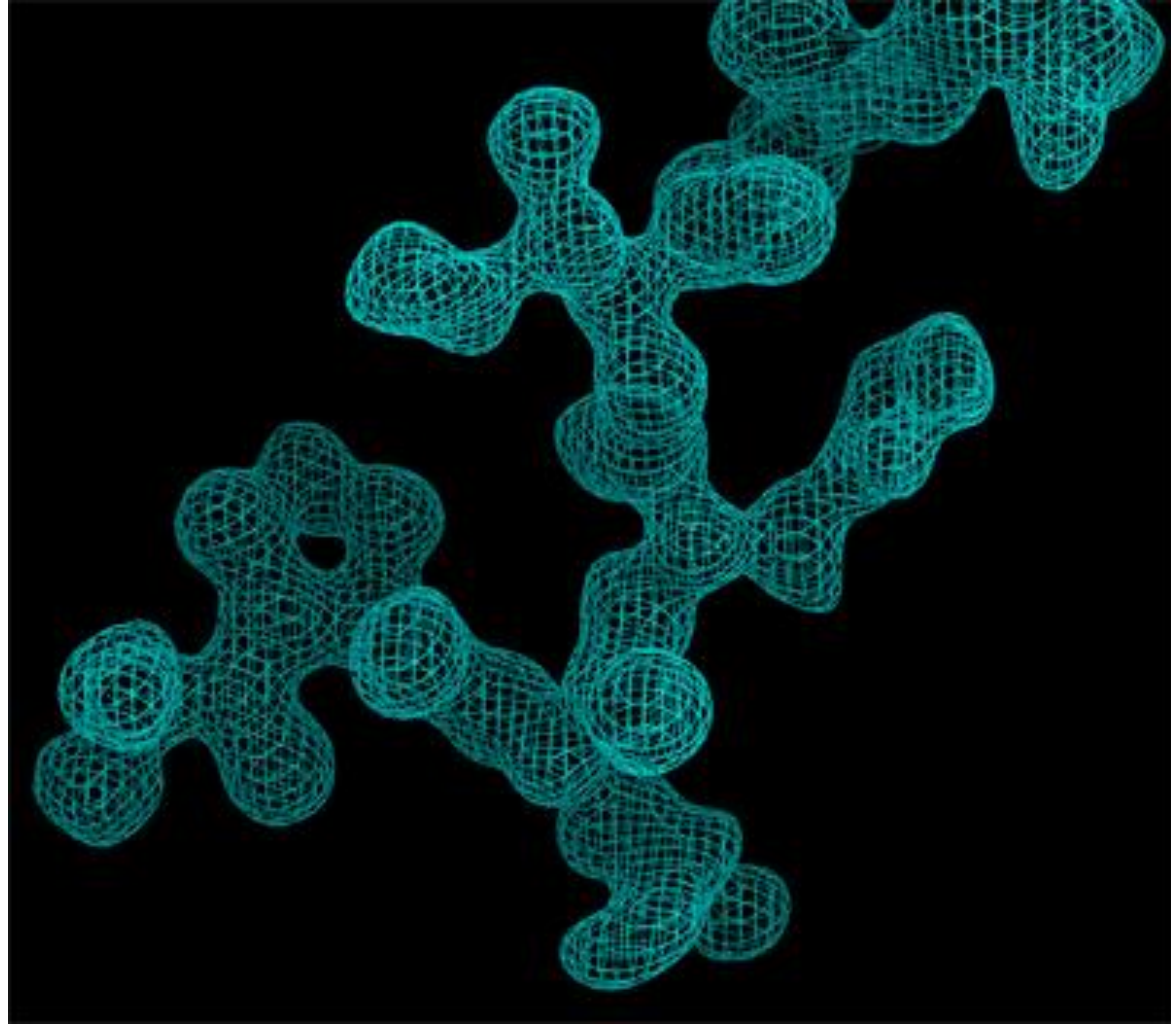
# Reciproký prostor

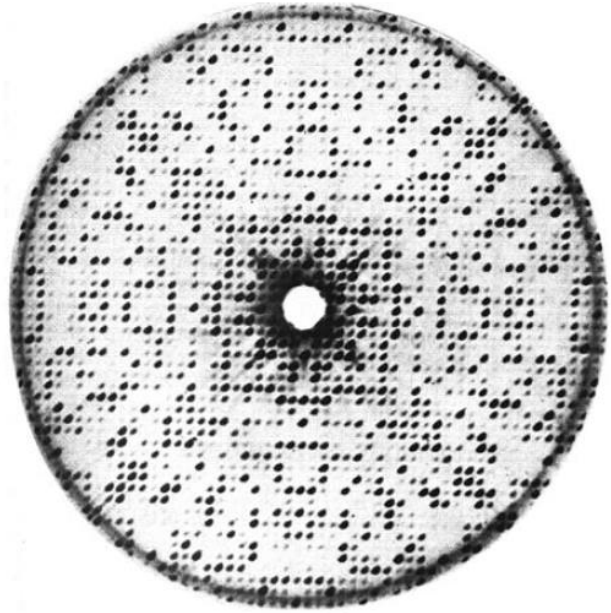


<https://youtu.be/DFFU39A3fPY?si=sW5zmz1TGpILVImL>

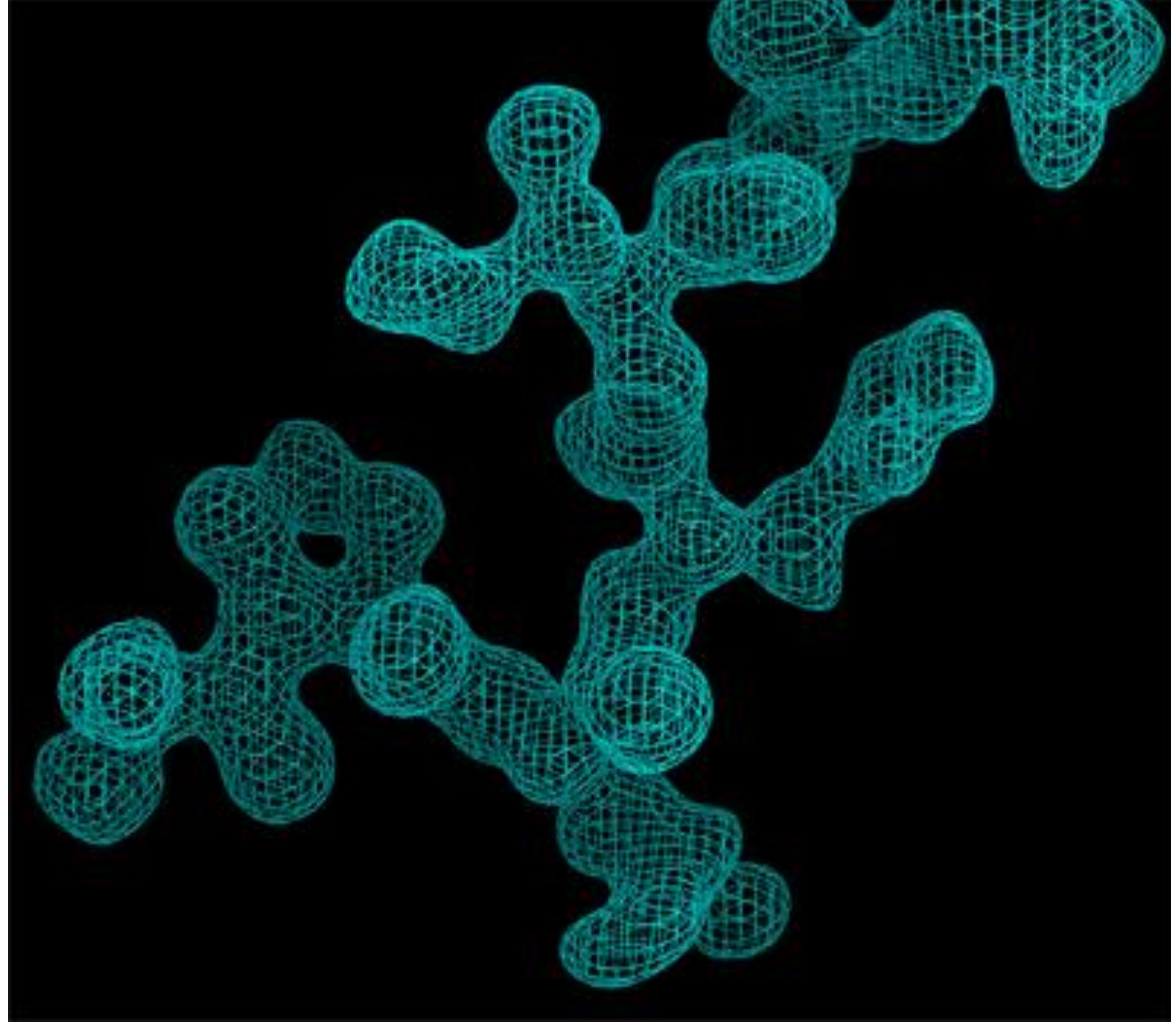


FT  
→

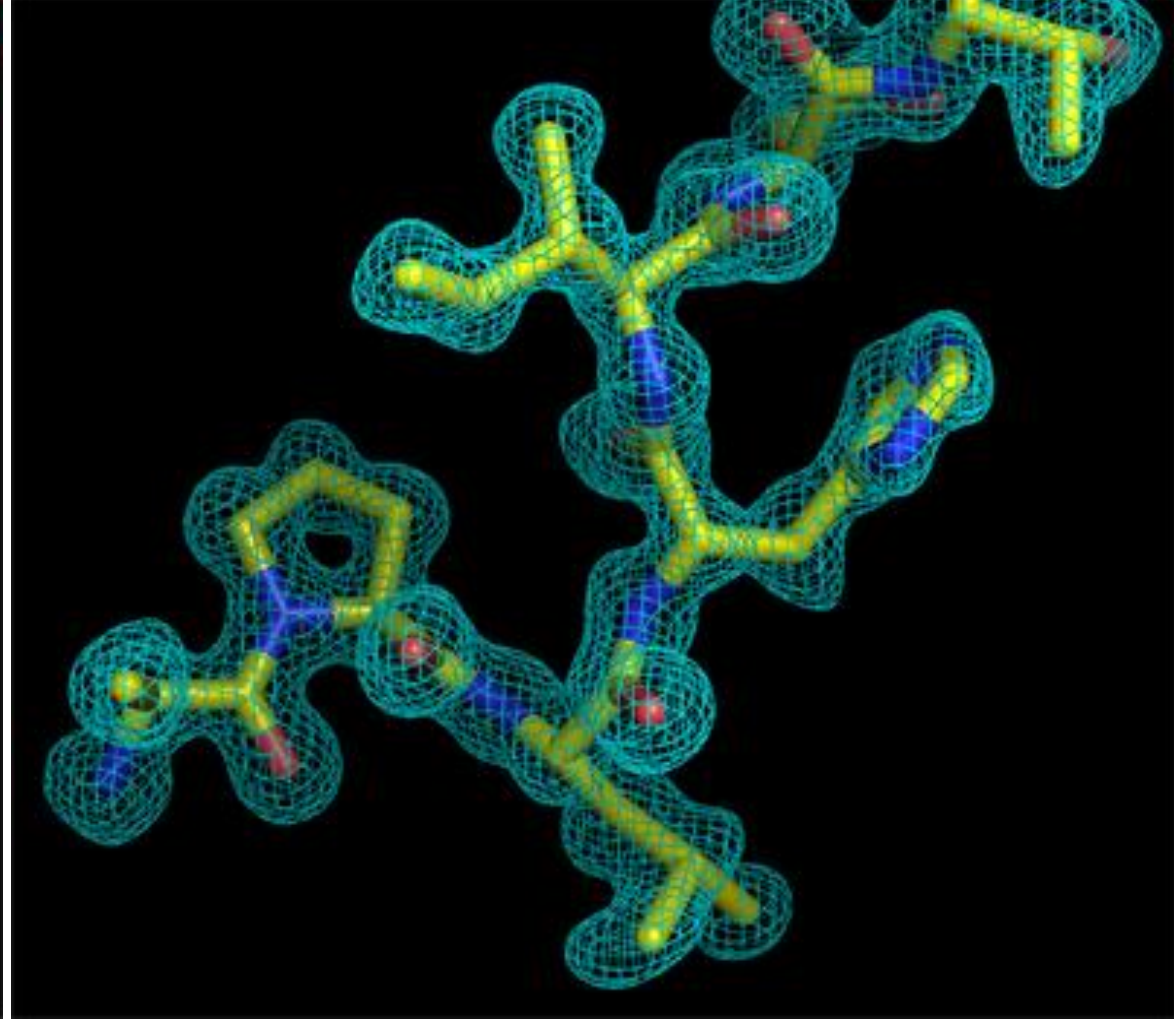
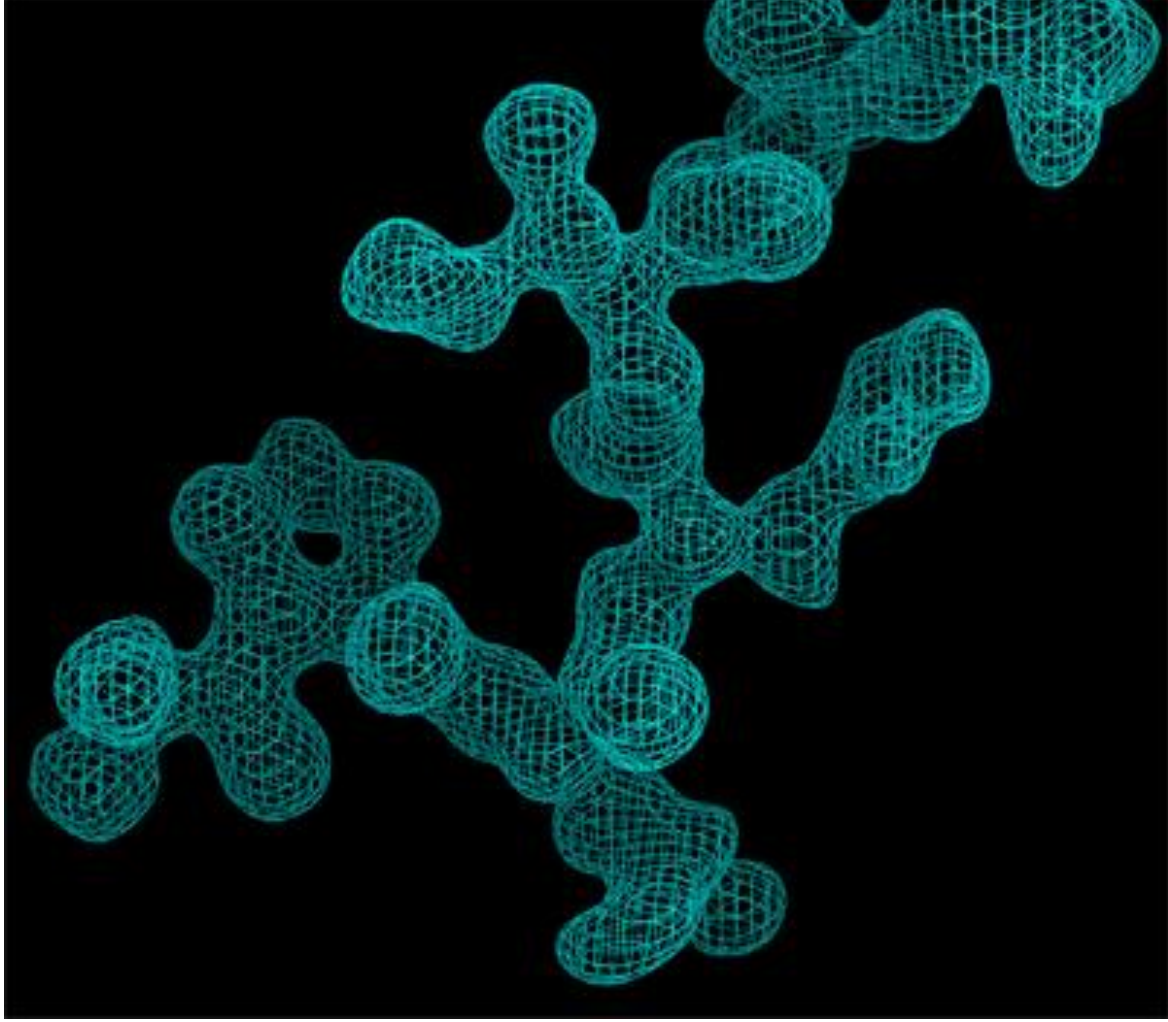




FT  
←





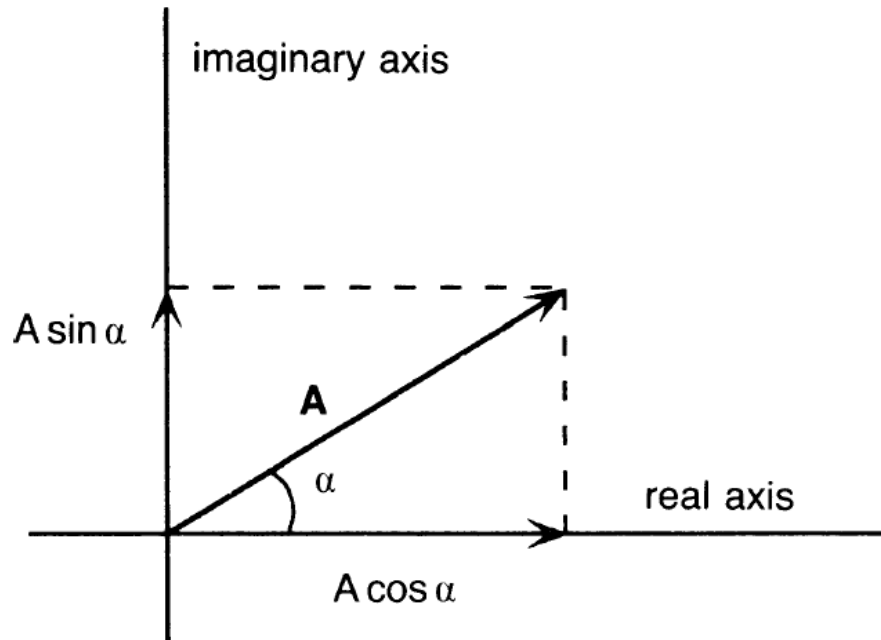




# Argandův diagram

$$A = |A| (\cos \alpha + i \sin \alpha)$$

$$A = |A| \exp i \alpha$$



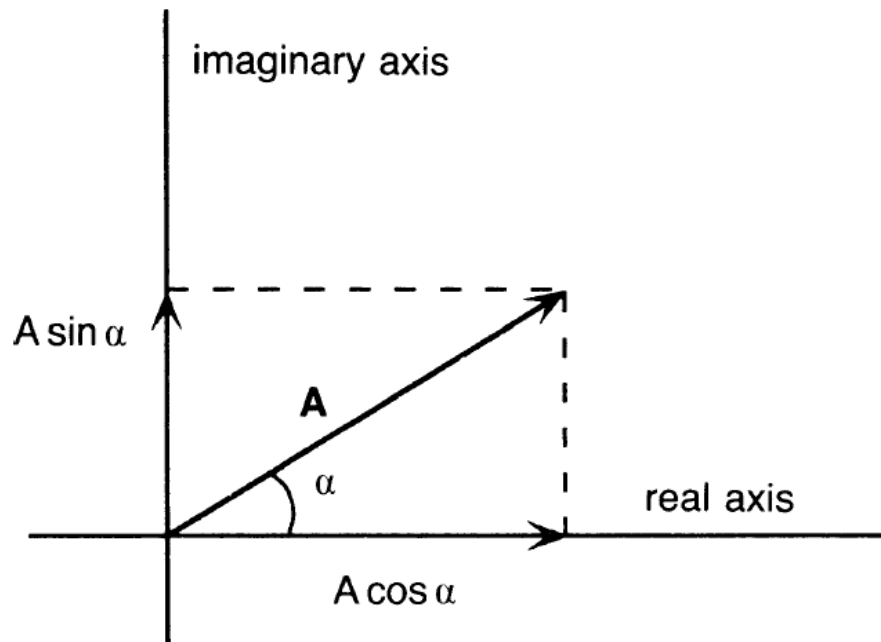
# Argandův diagram

$$A = |A| (\cos \alpha + i \sin \alpha)$$

$$A = |A| \exp i \alpha$$

$$F_{(hkl)} = |F_{(hkl)}| (\cos \alpha_{(hkl)} + i \sin \alpha_{(hkl)})$$

$$F_{(hkl)} = |F_{(hkl)}| \exp [i \alpha_{(hkl)}]$$



# Argandův diagram

$$A = |A| (\cos \alpha + i \sin \alpha)$$

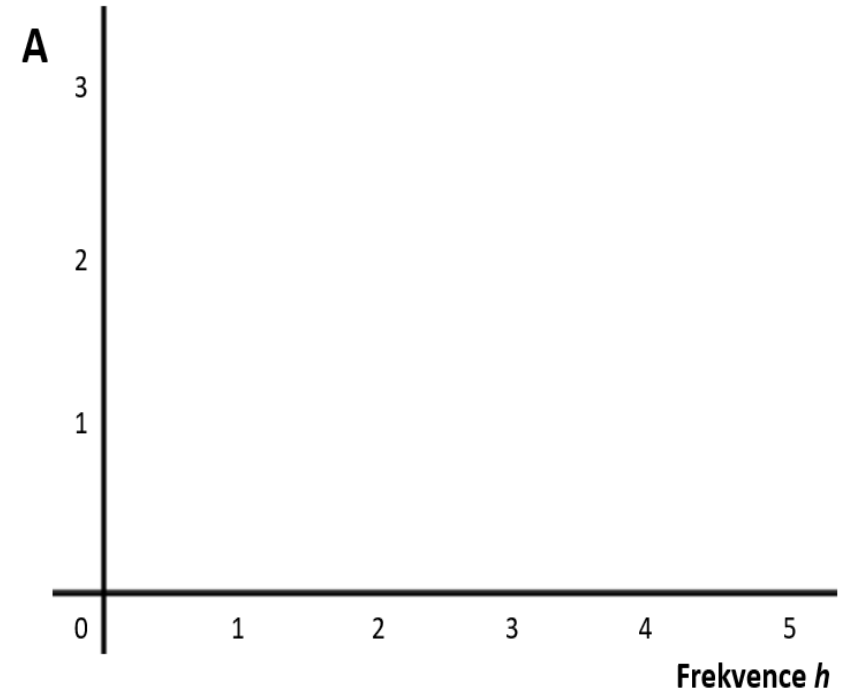
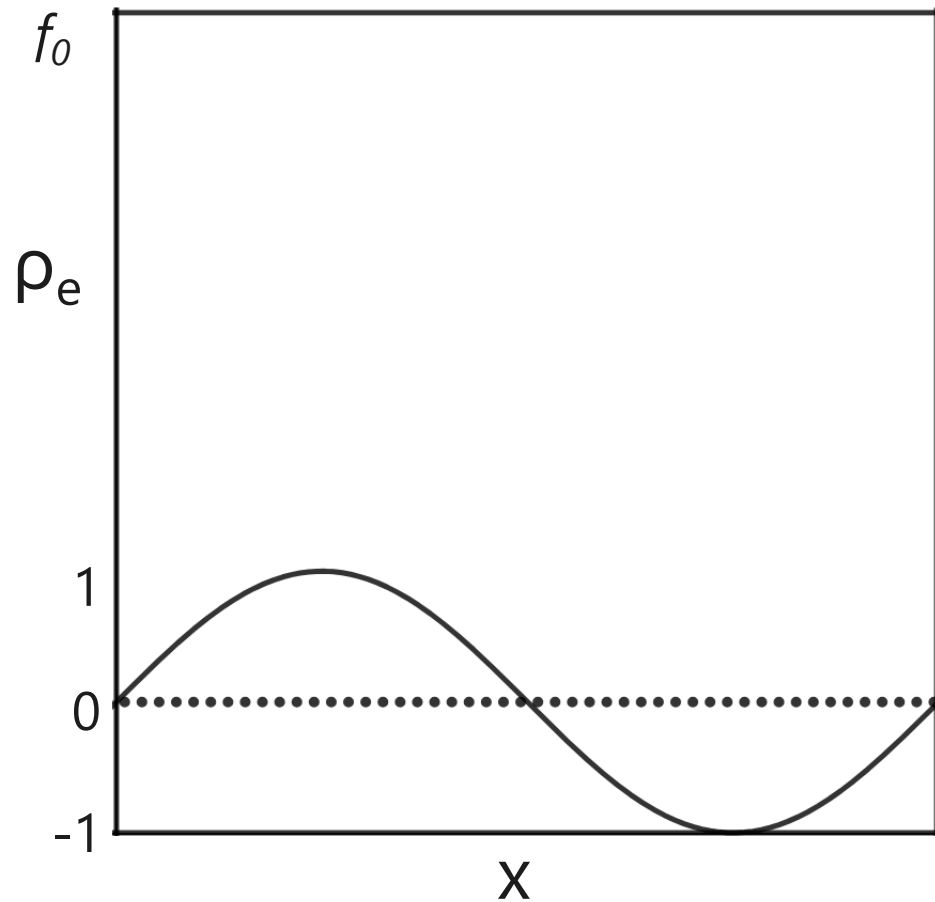
$$A = |A| \exp i \alpha$$

$$F_{(hkl)} = |F_{(hkl)}| (\cos \alpha_{(hkl)} + i \sin \alpha_{(hkl)})$$

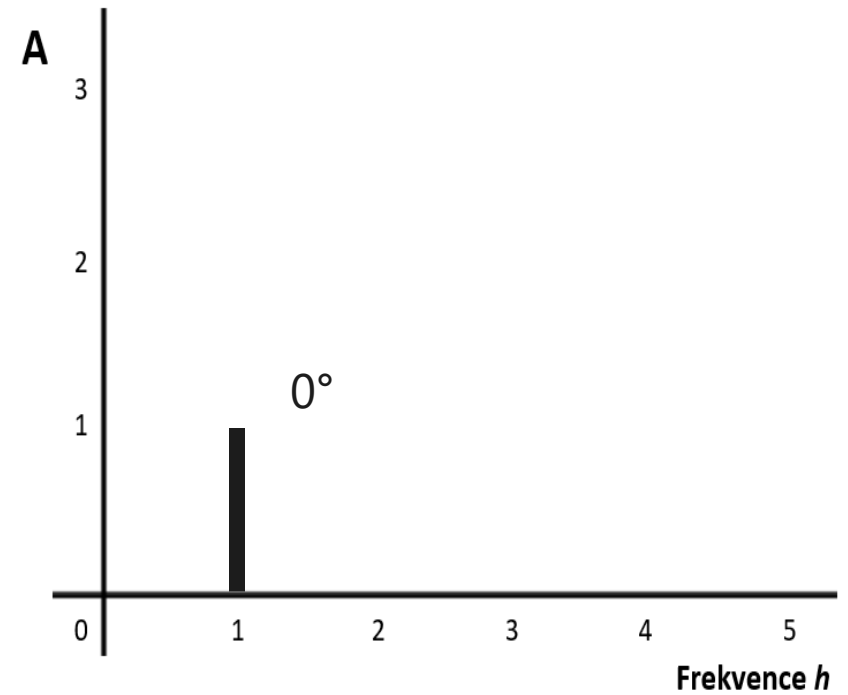
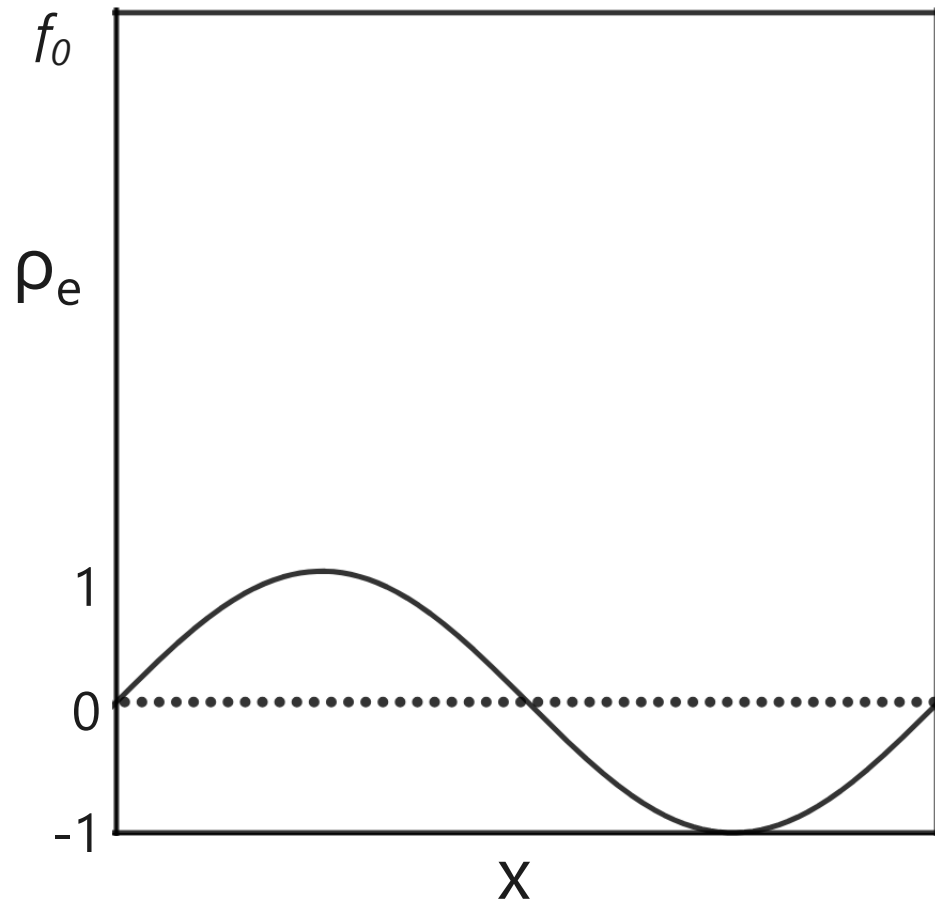
$$F_{(hkl)} = |F_{(hkl)}| \exp [i \alpha_{(hkl)}]$$

$$\rho_{(xyz)} = \frac{1}{V_C} \sum_h \sum_k \sum_l |F_{(hkl)}| \exp [-2\pi i (hx + ky + lz) + i \alpha_{(hkl)}]$$

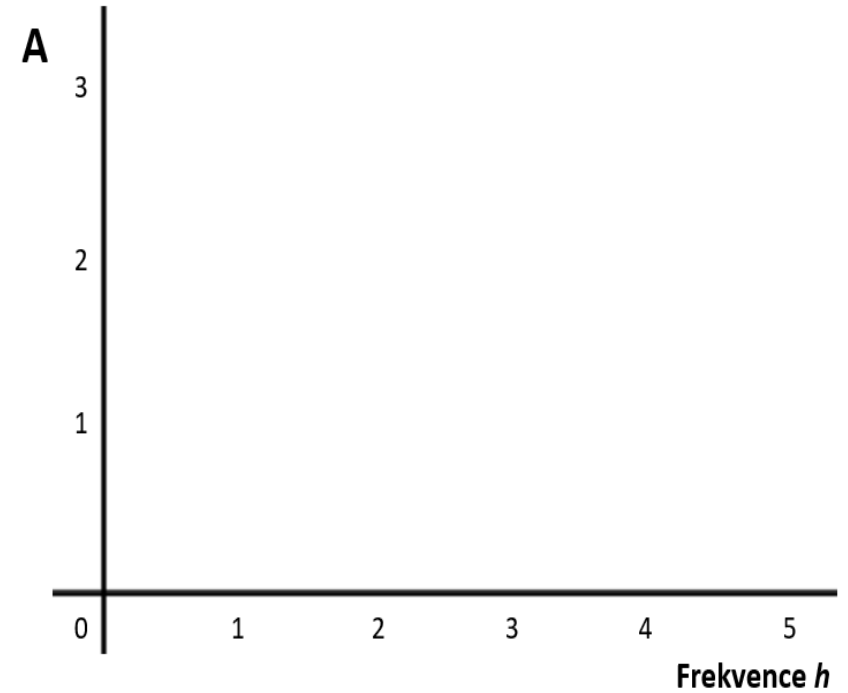
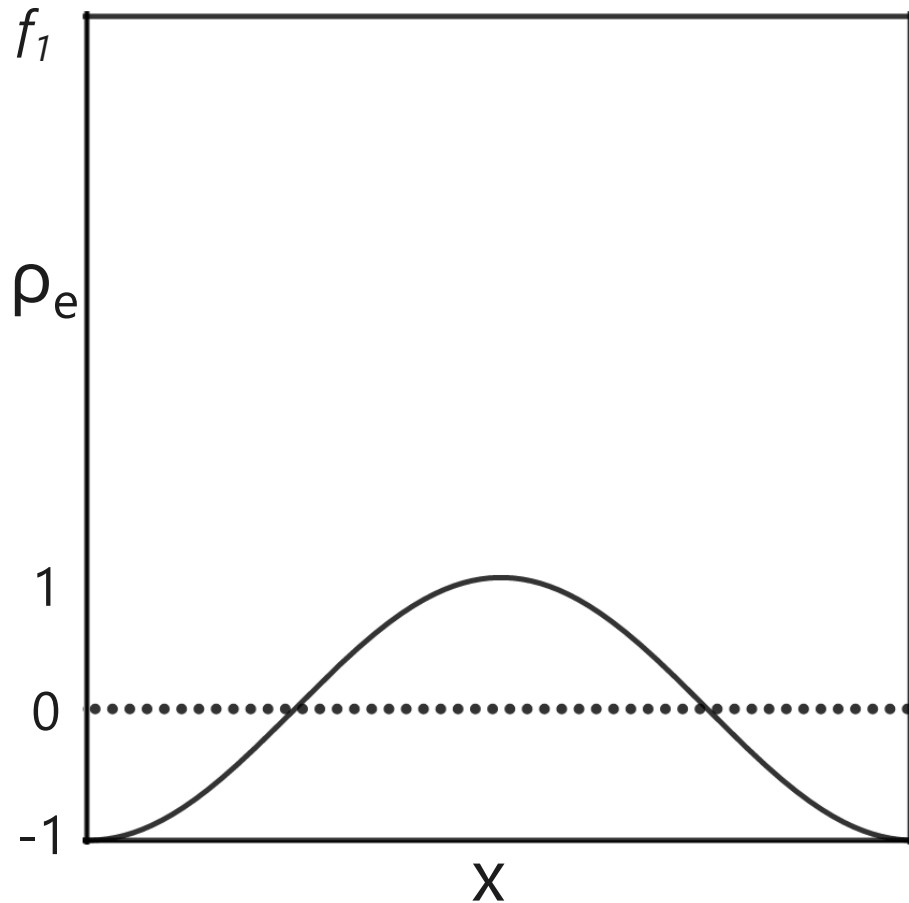
# FT jednoduché funkce



# FT jednoduché funkce

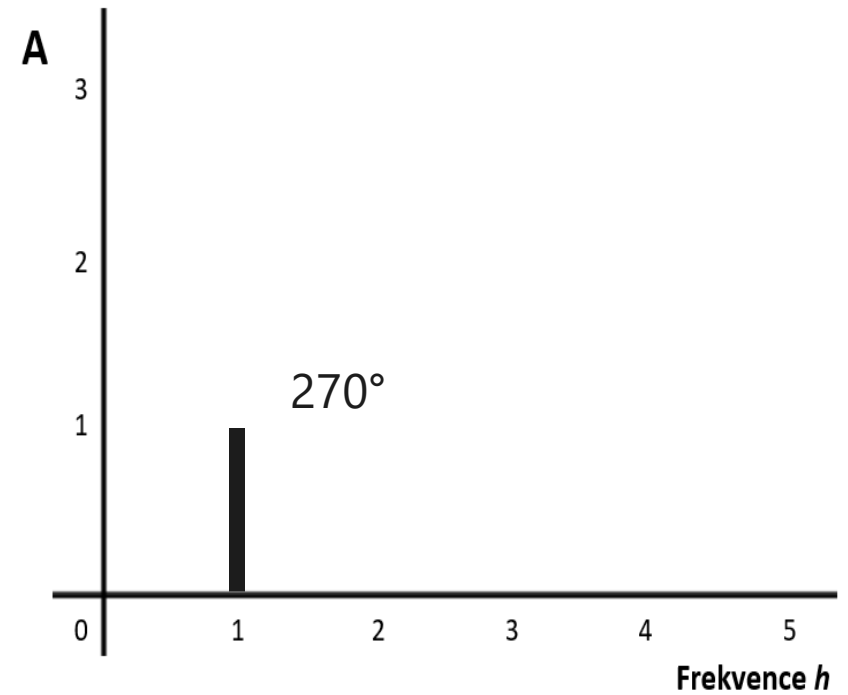
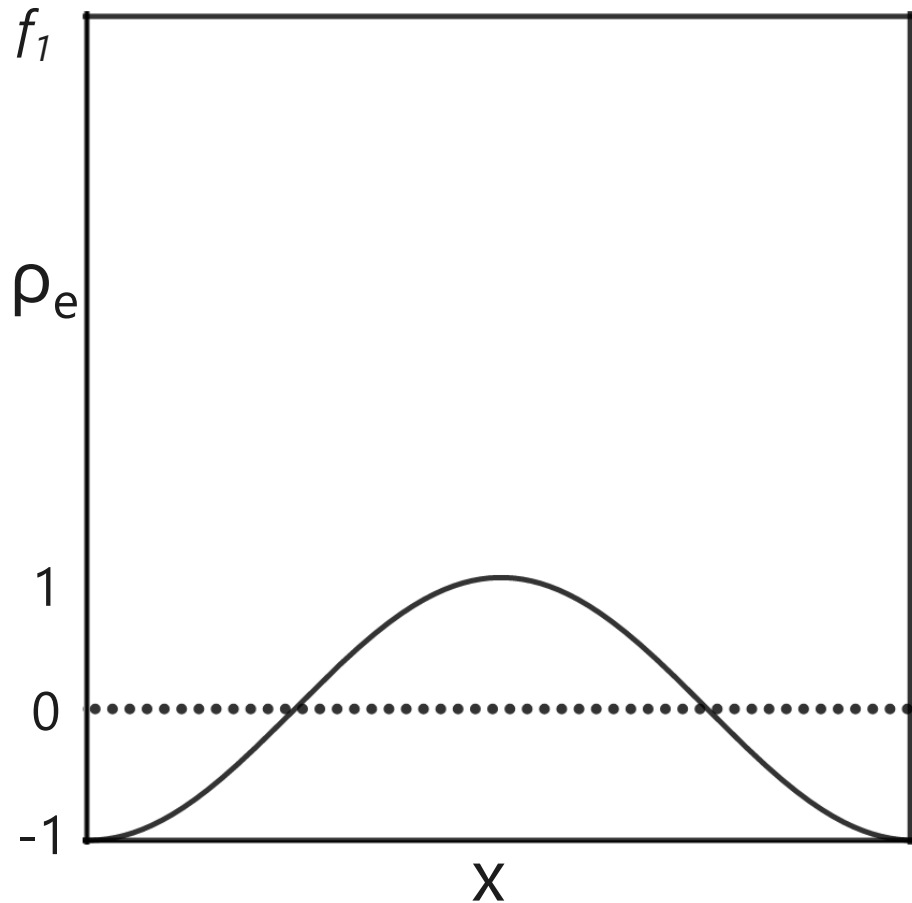


# FT jednoduché funkce $f_1$

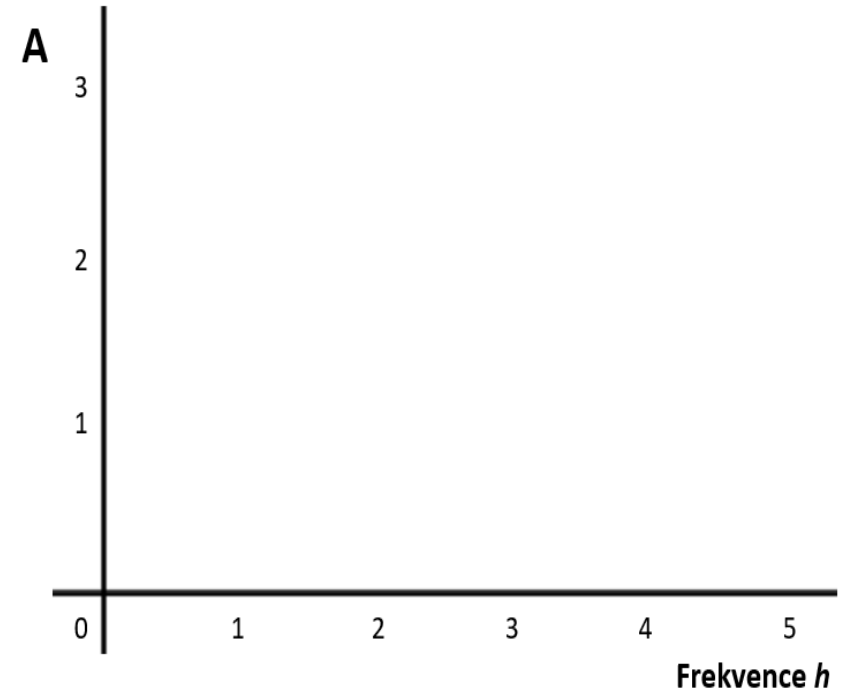
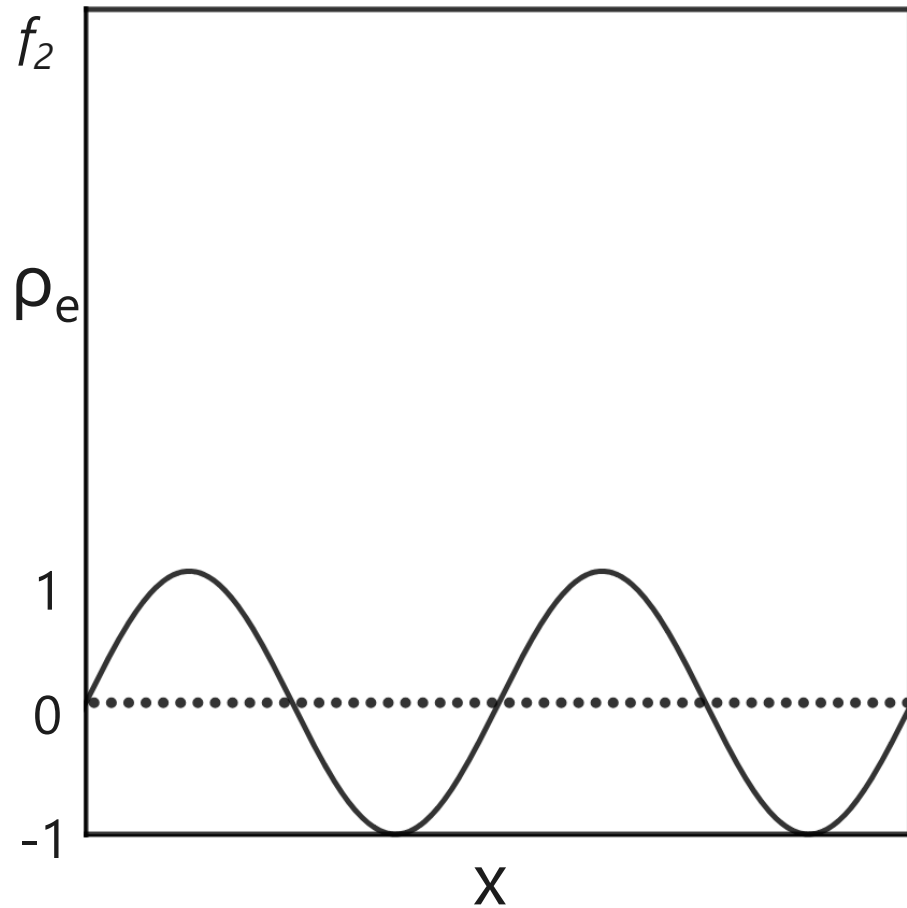




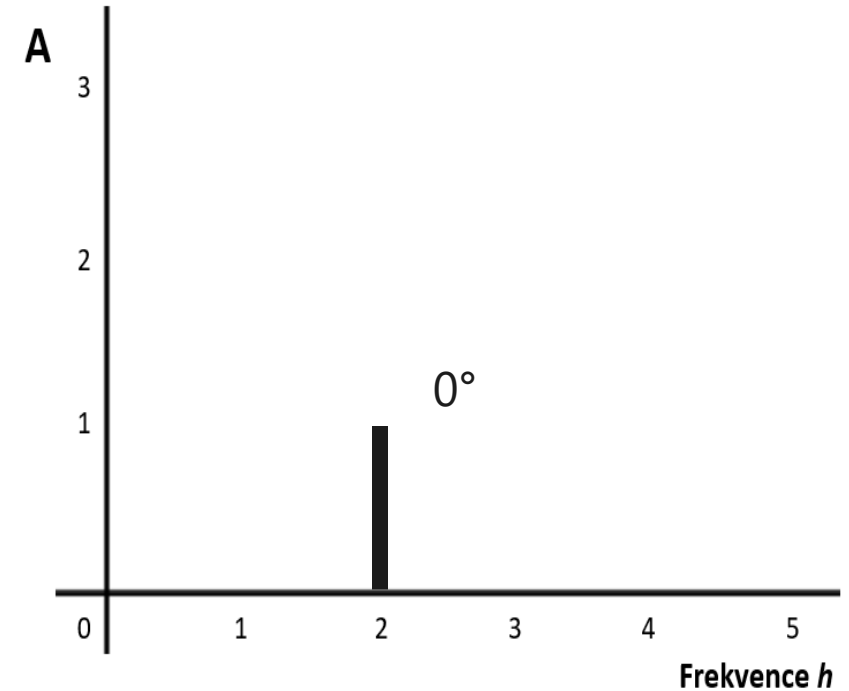
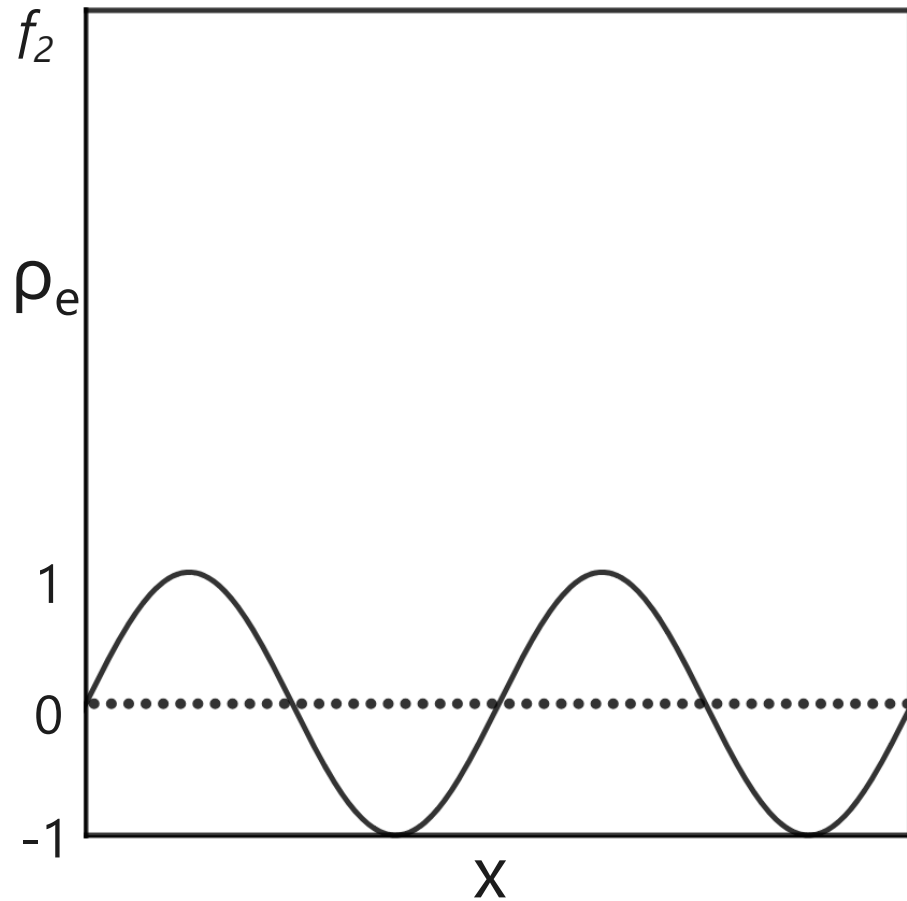
# FT jednoduché funkce $f_1$



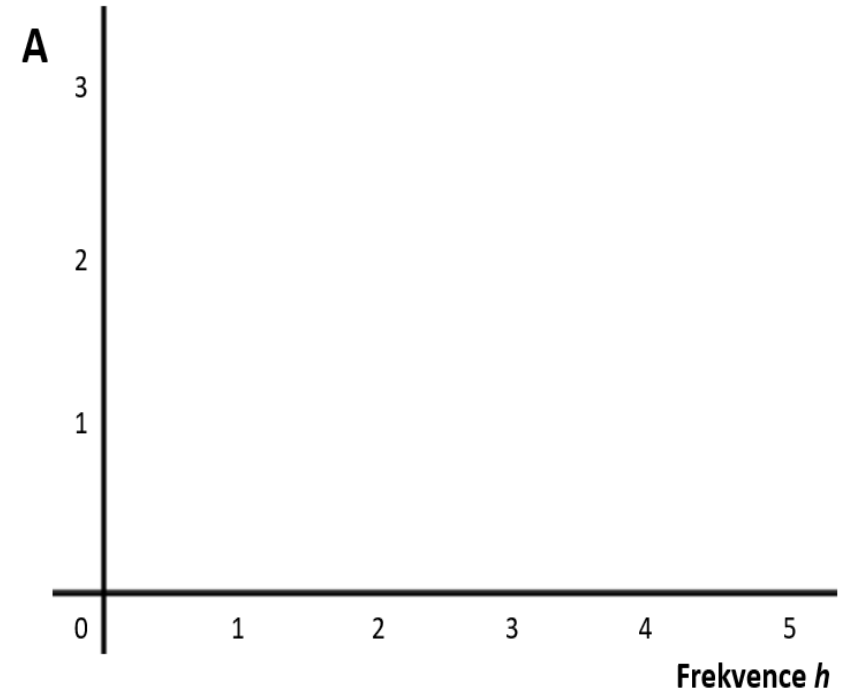
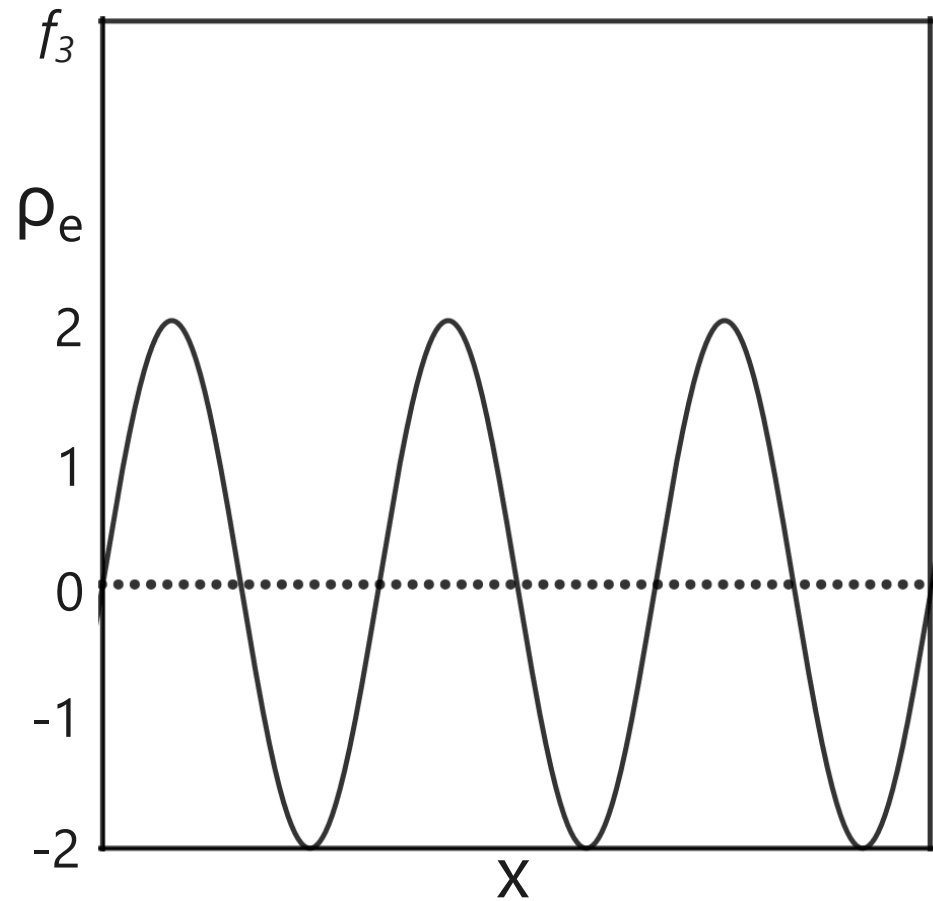
# FT jednoduché funkce $f_2$



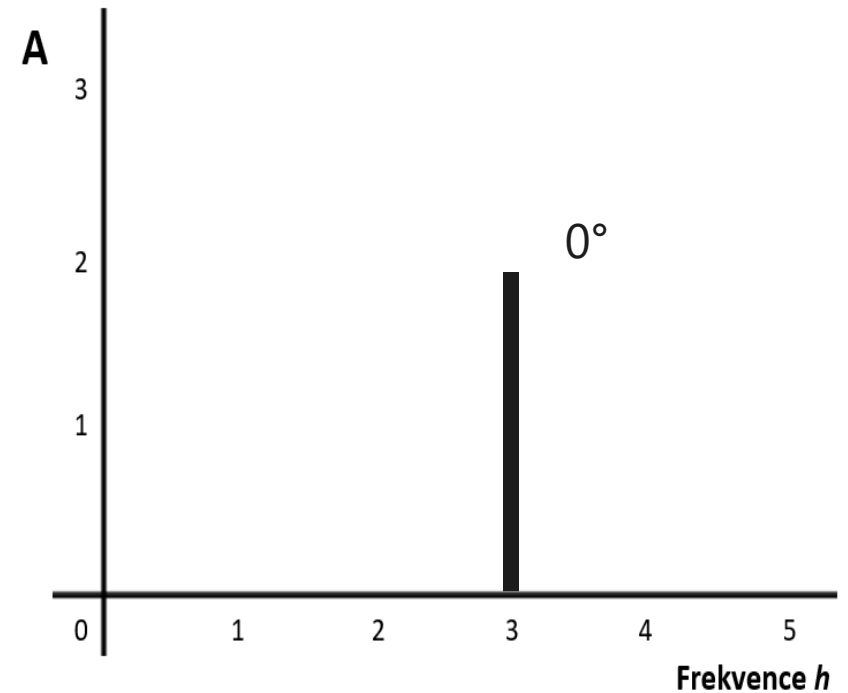
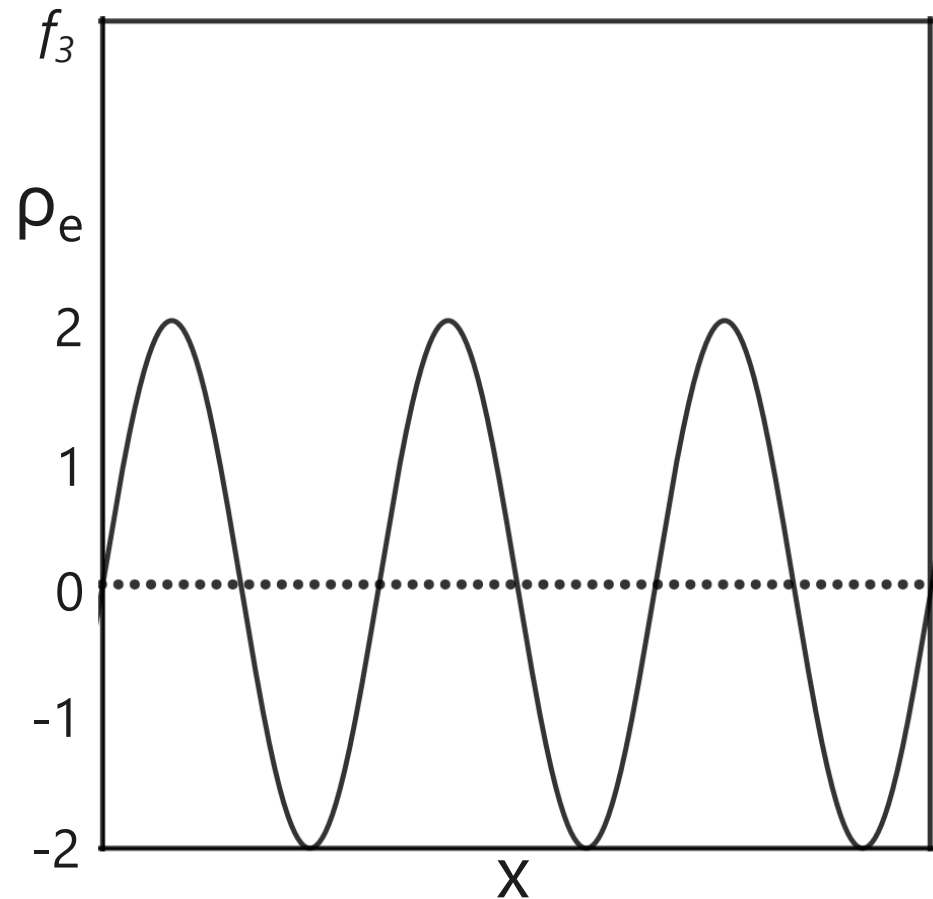
# FT jednoduché funkce $f_2$



# FT jednoduché funkce $f_3$

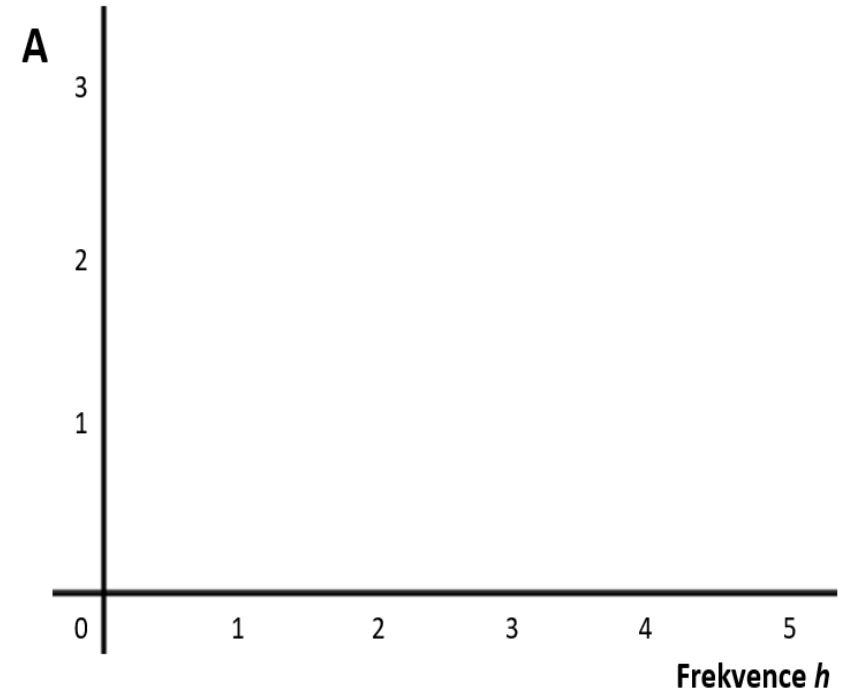
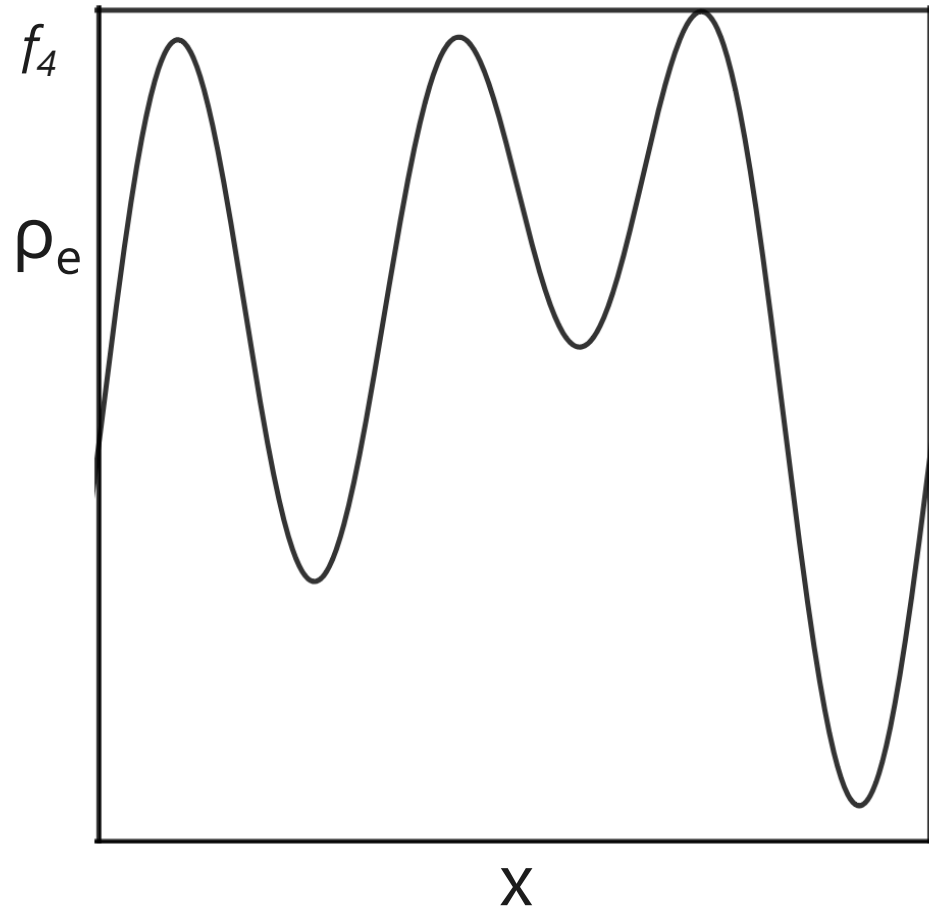


# FT jednoduché funkce $f_3$



# FT složené funkce $f_4$

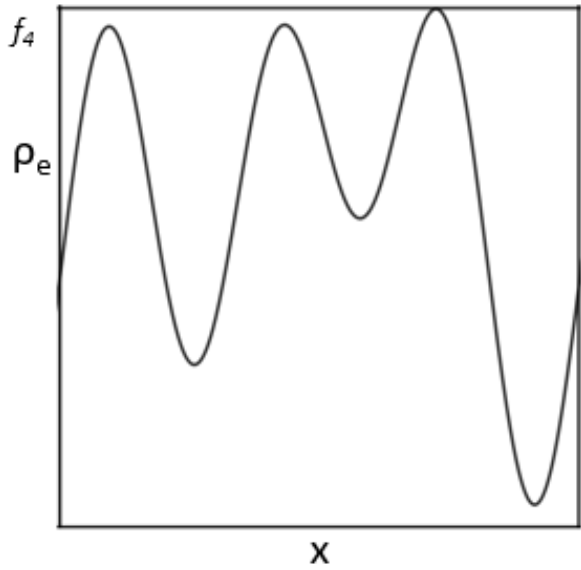
$$f_4 = f_1 + f_2 + f_3$$



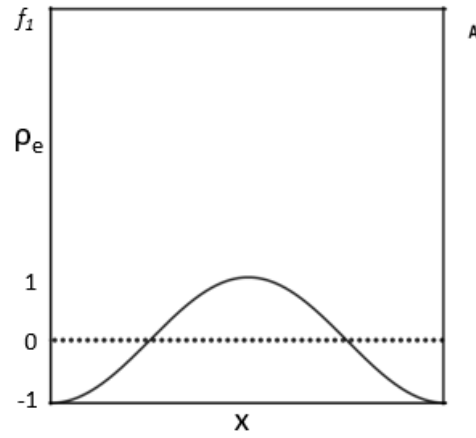


# FT složené funkce $f_4$

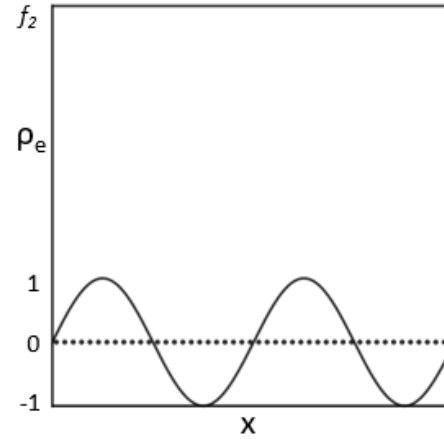
$$f_4 = f_1 + f_2 + f_3$$



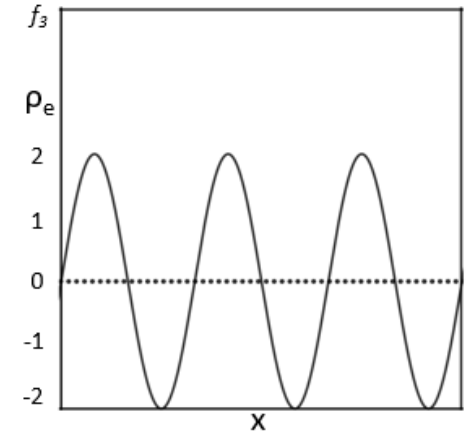
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+

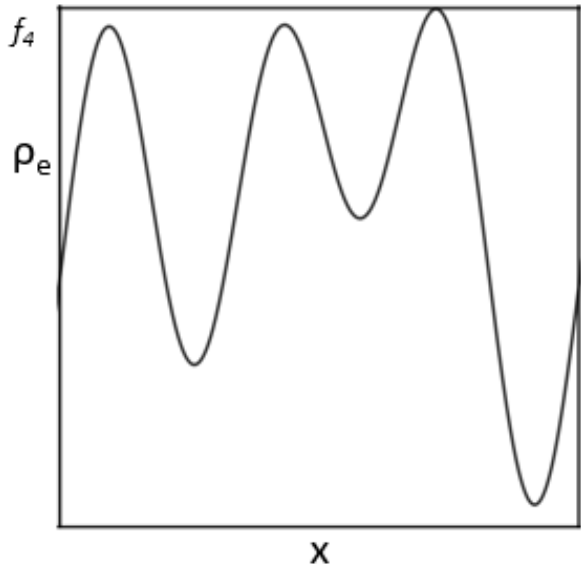


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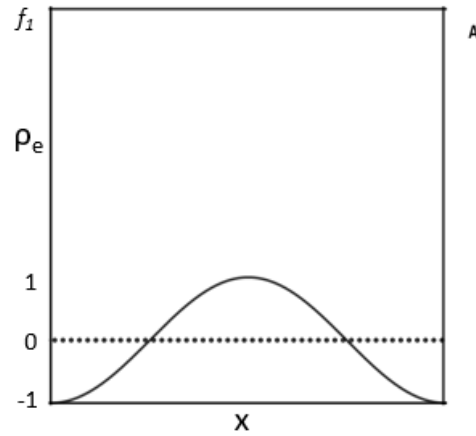


# FT složené funkce $f_4$

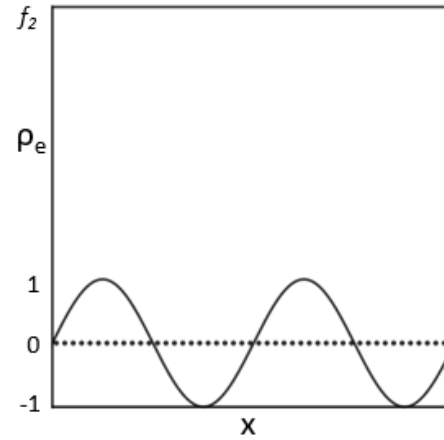
$$f_4 = f_1 + f_2 + f_3$$



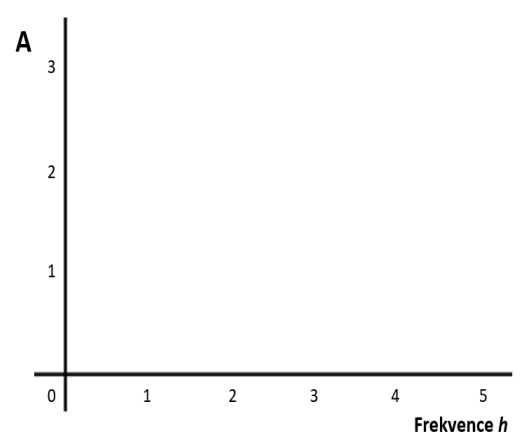
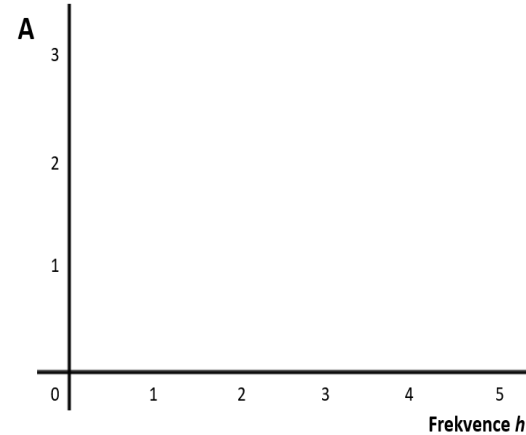
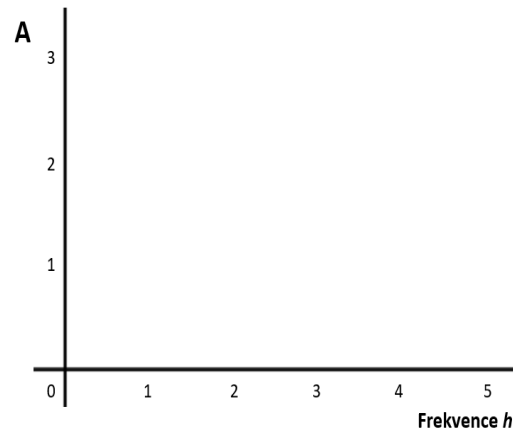
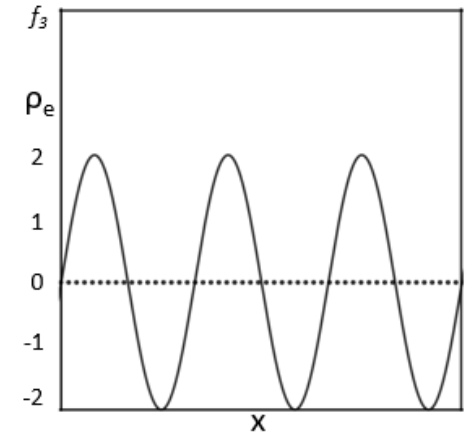
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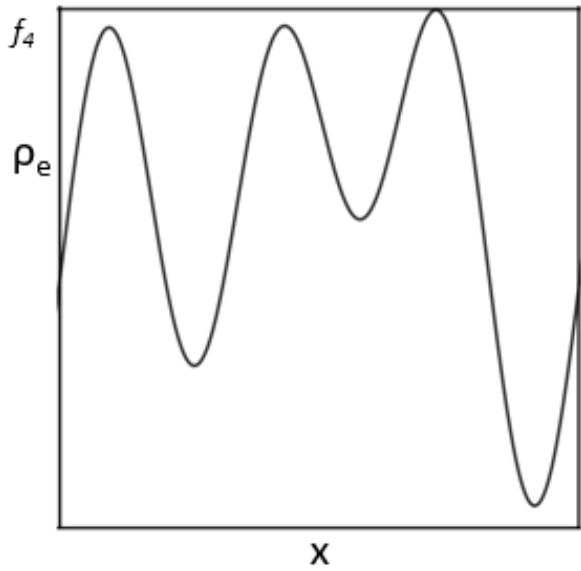


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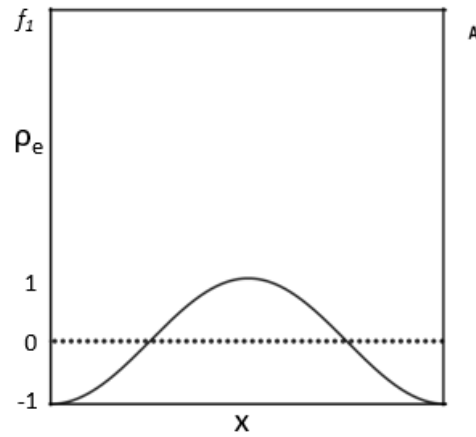


# FT složené funkce $f_4$

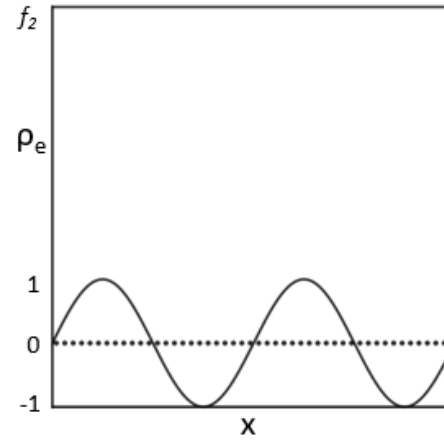
$$f_4 = f_1 + f_2 + f_3$$



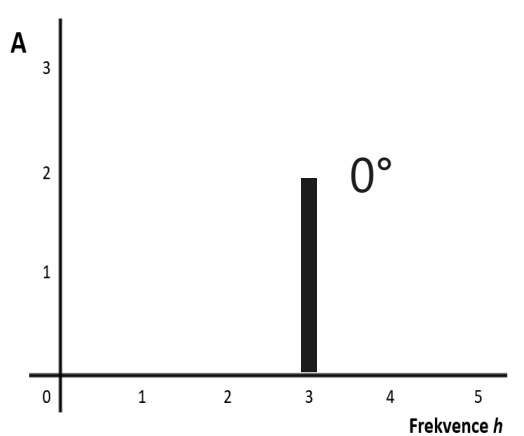
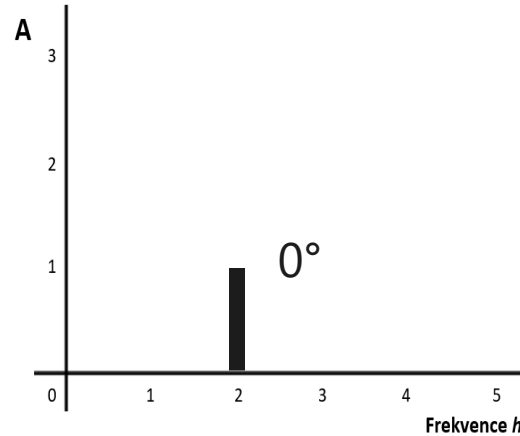
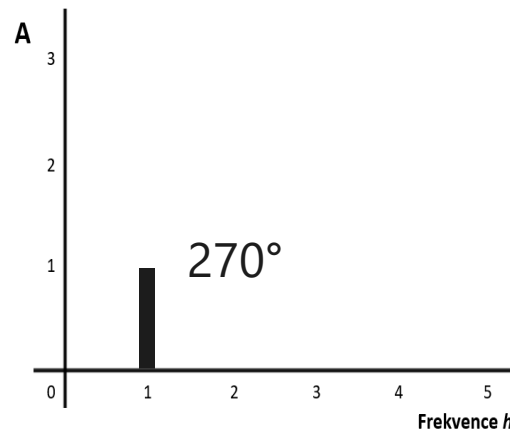
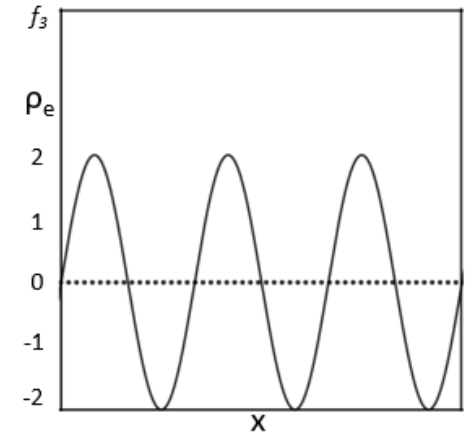
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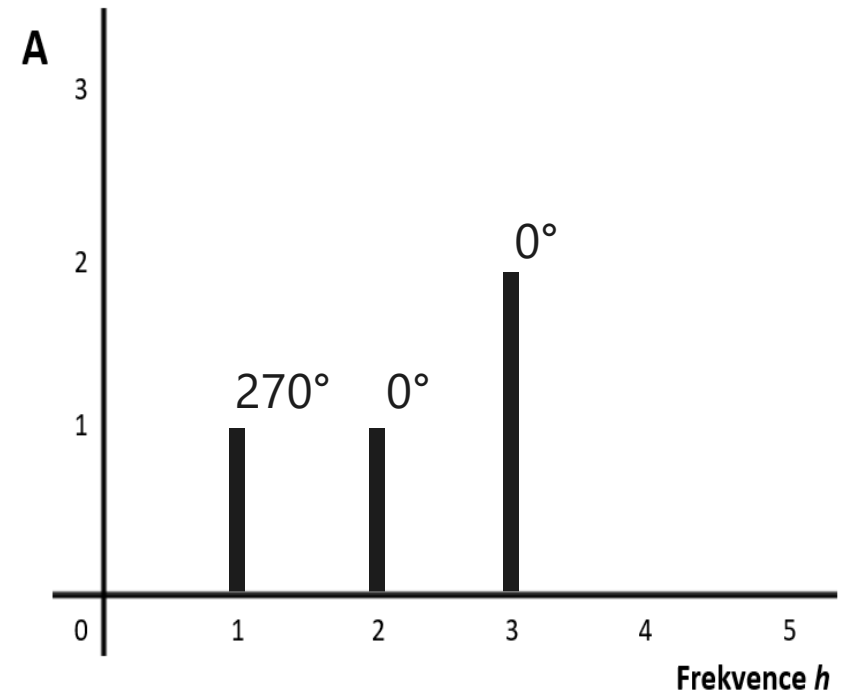
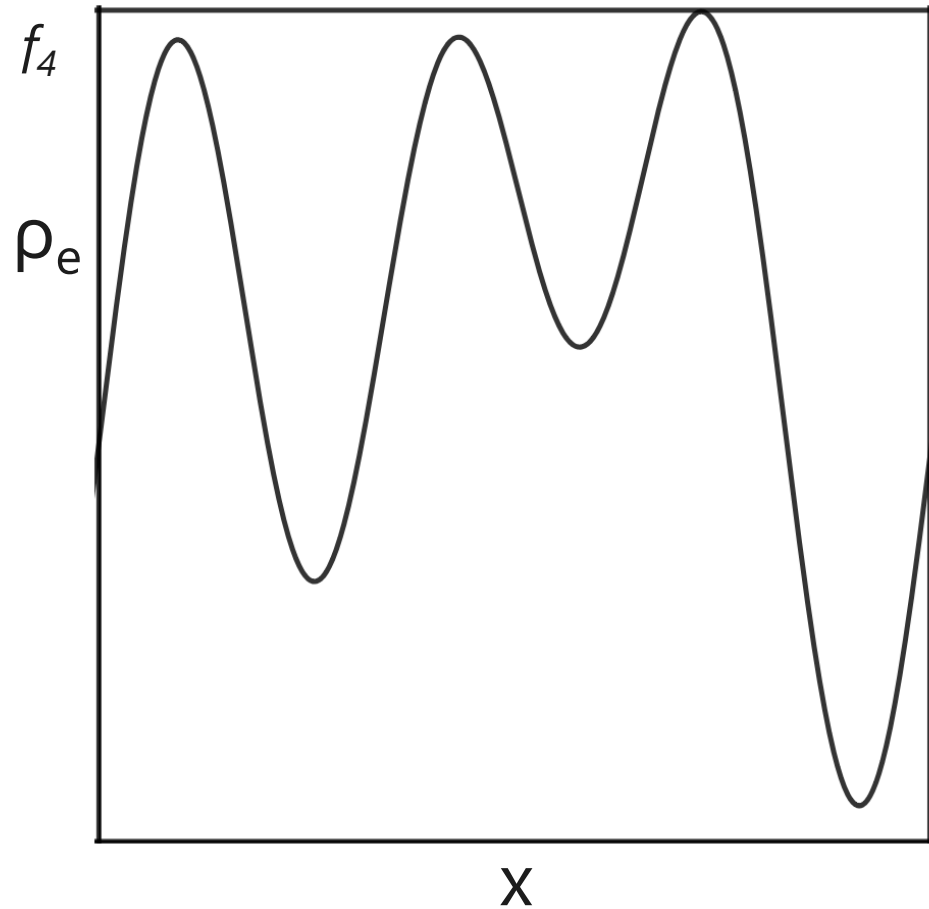


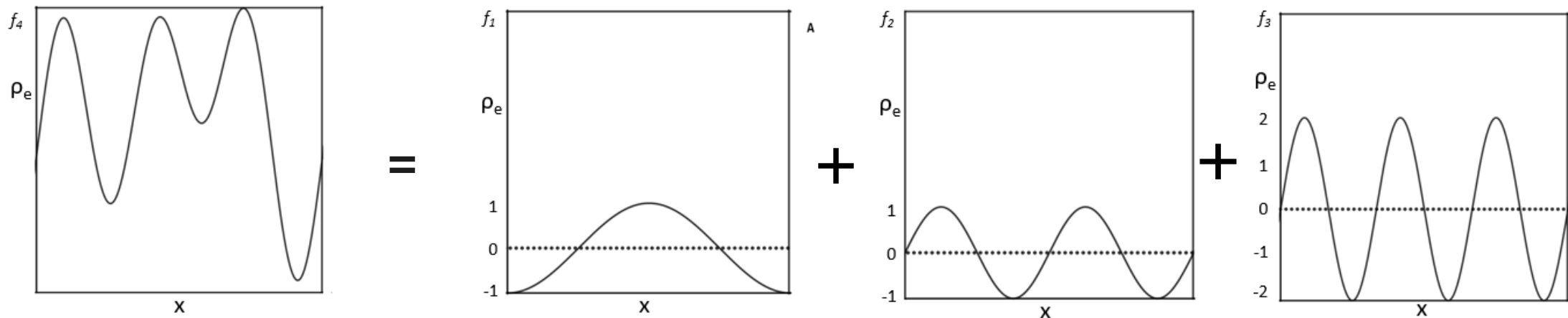
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# FT složené funkce $f_4$

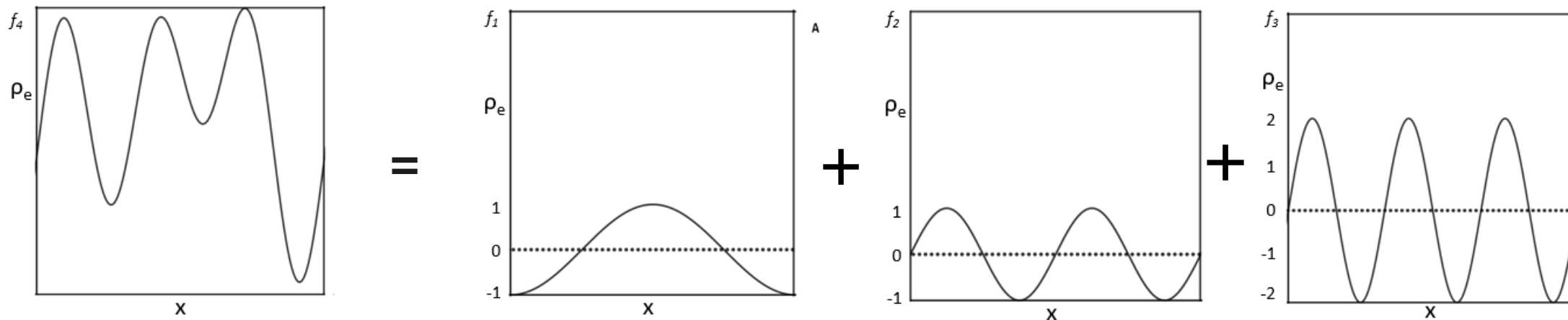
$$f_4 = f_1 + f_2 + f_3$$





$$\rho_{(xyz)} = \frac{1}{V_C} \sum_h \sum_k \sum_l |F_{(hkl)}| \exp [-2\pi i(hx + ky + lz) + i\alpha_{(hkl)}]$$

**Elektronová hustota** ←  $\rho(x) = \frac{1}{l} \sum_{n=1}^N |F_n| \exp [-2\pi i hx + i\alpha_{(n)}]$

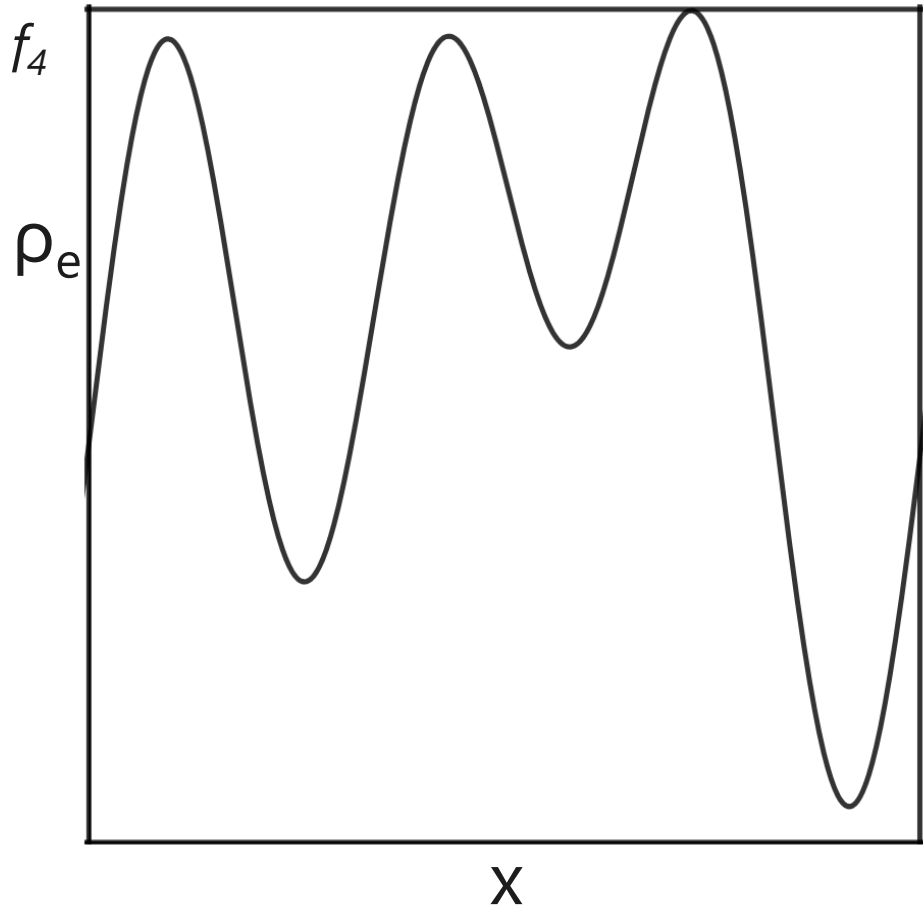


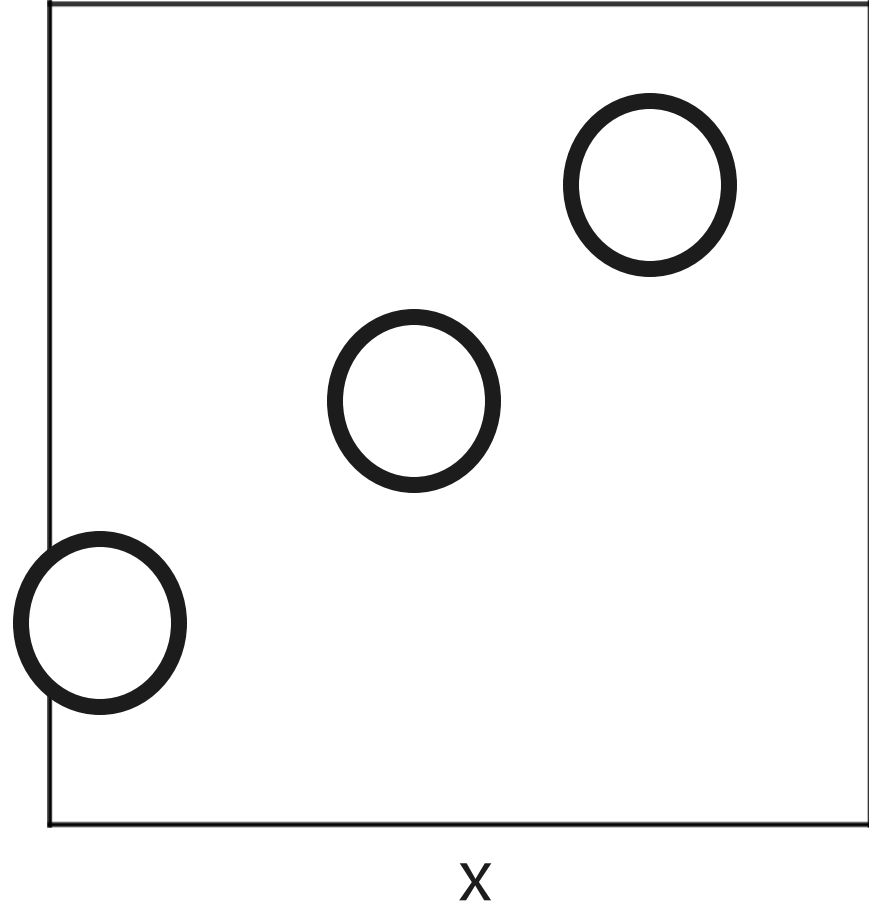
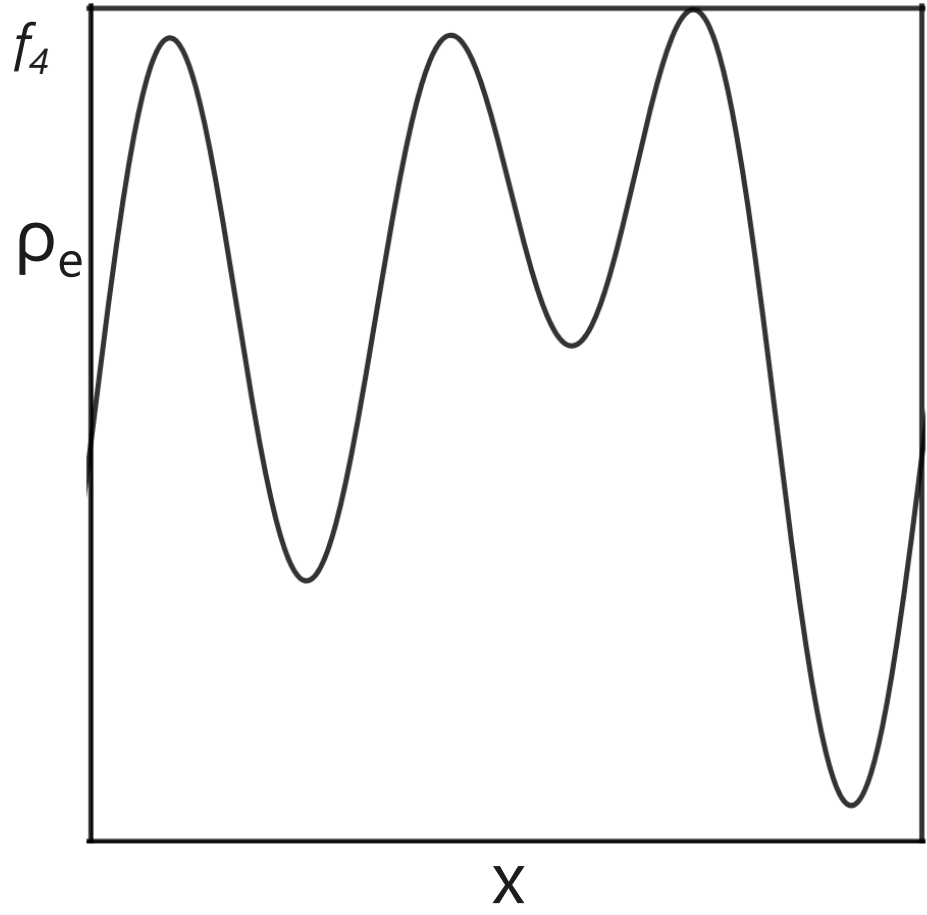
**Elektronová hustota** ←  $\rho(x) = \frac{1}{l} \sum_{n=1}^N |F_h| \exp \left[ -2\pi i h x + i \alpha_{(h)} \right]$

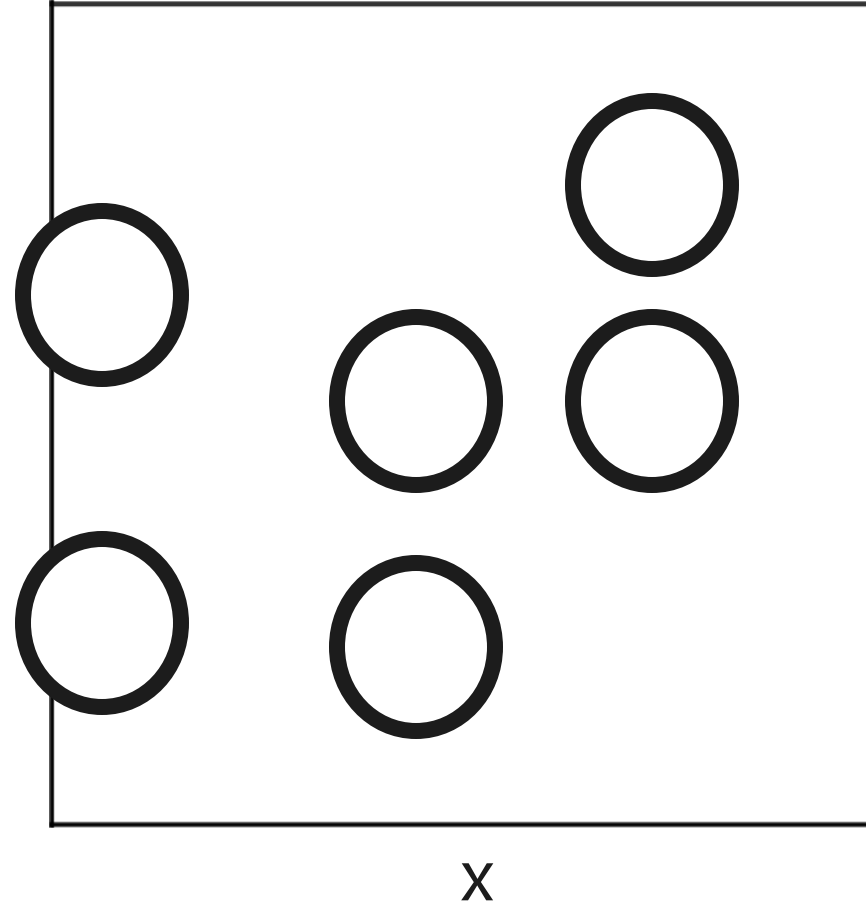
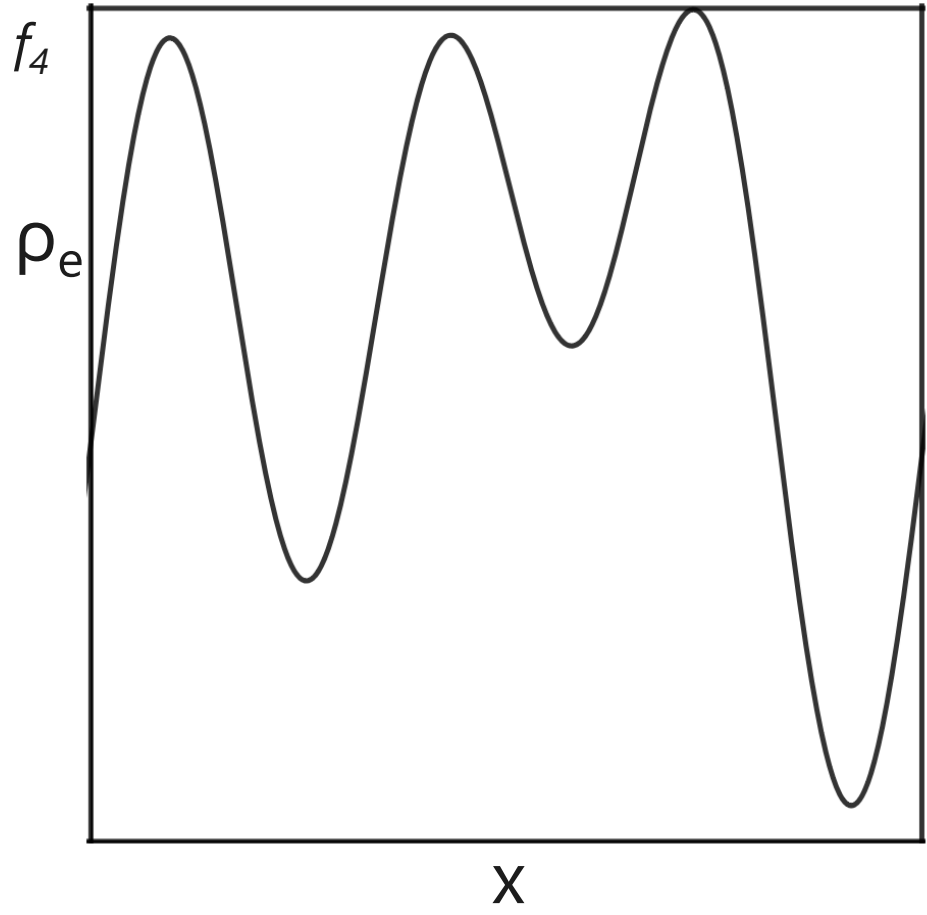
↓ Amplituda
↑ Frekvence
↓ Fáze



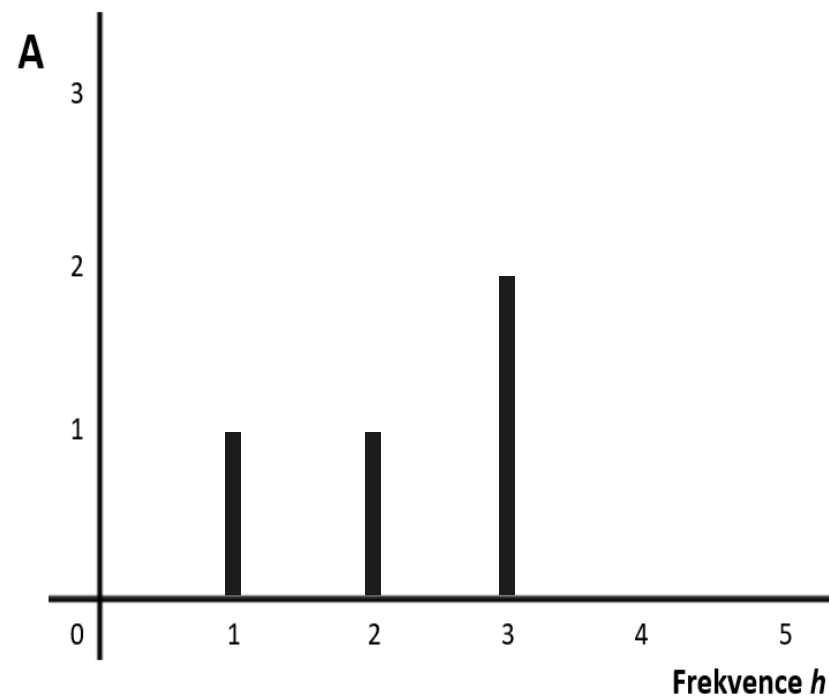
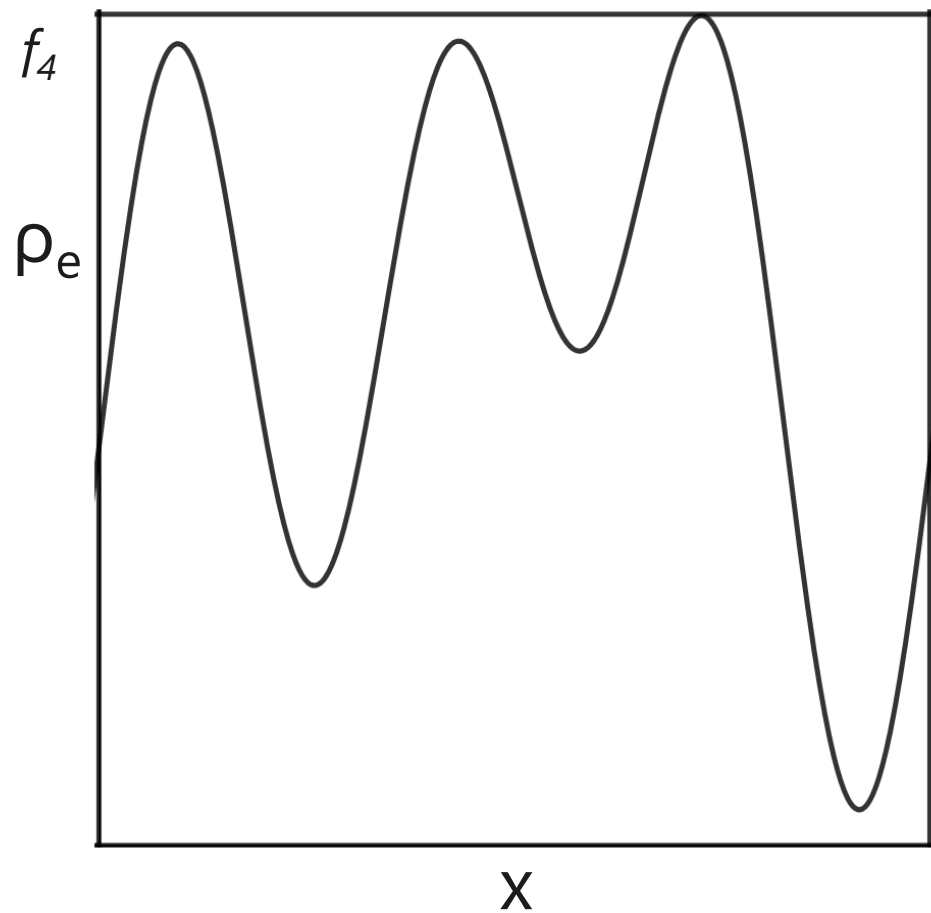
# Kolik atomů je ukryto ve funkci $f_4$



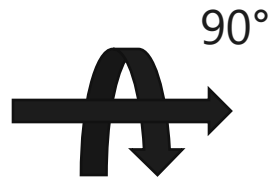
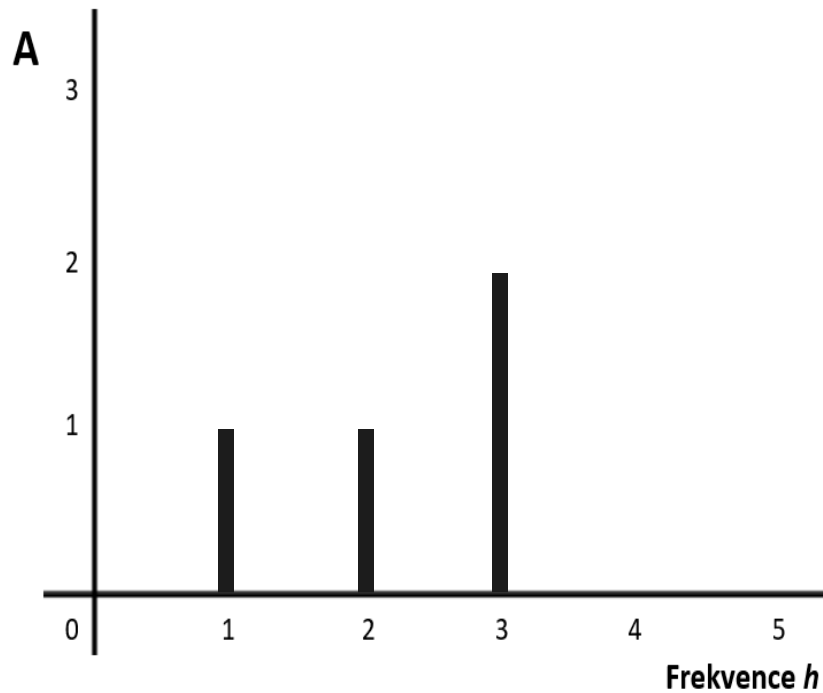




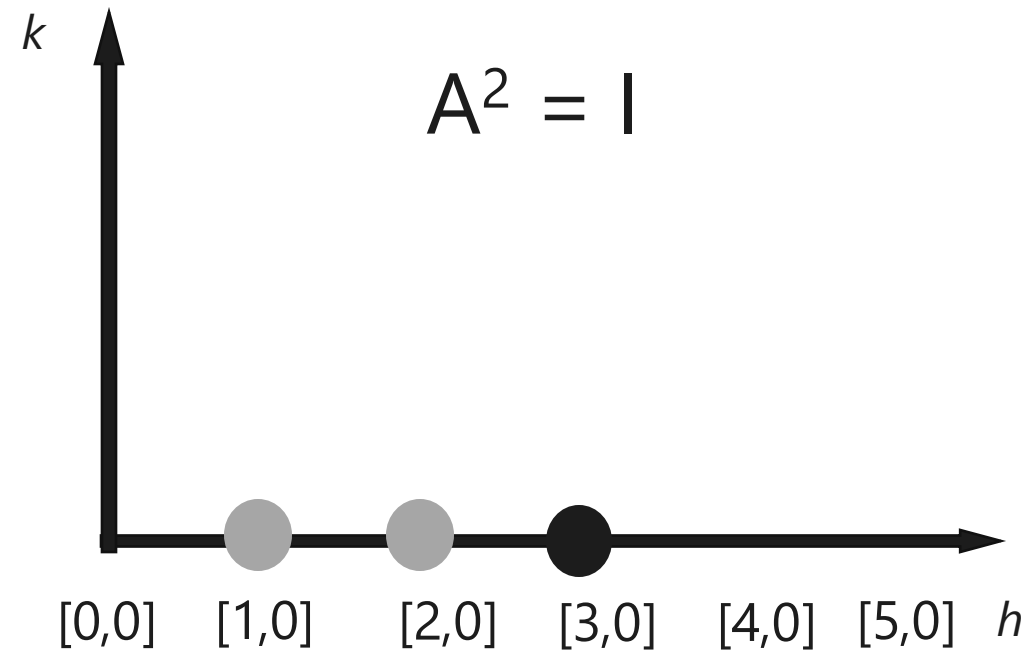
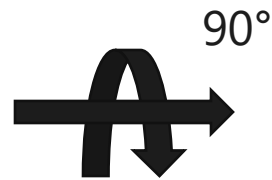
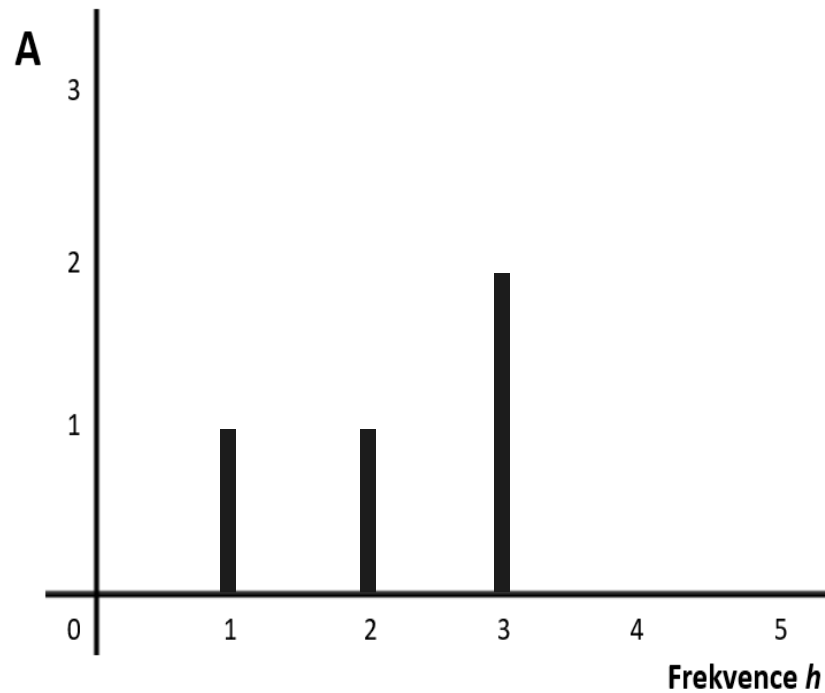
# 1D experiment



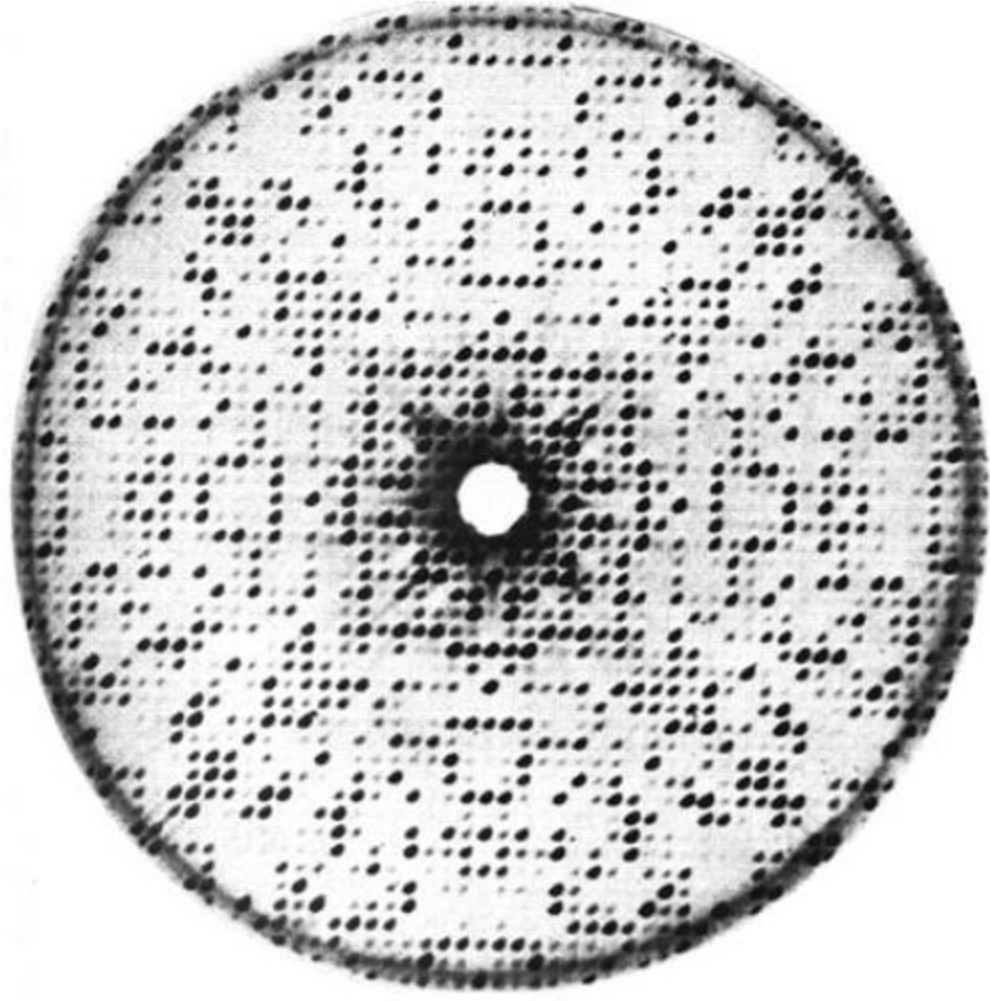
# Vícedimenzionální experiment



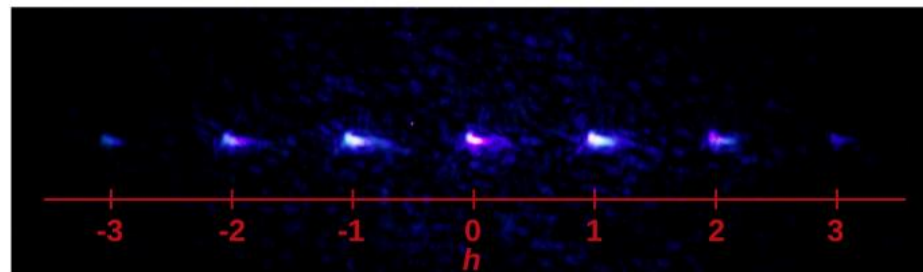
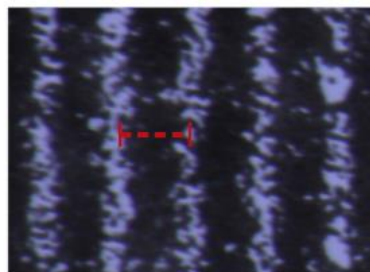
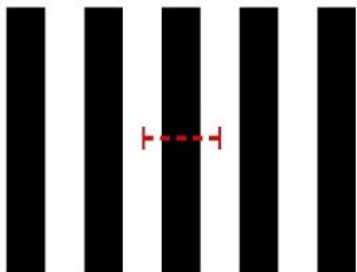
# Vícedimenzionální experiment



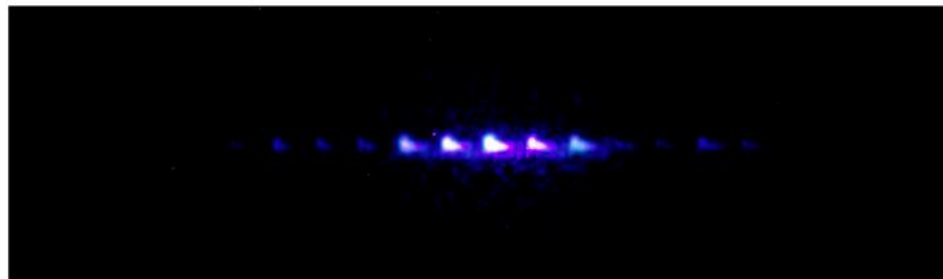
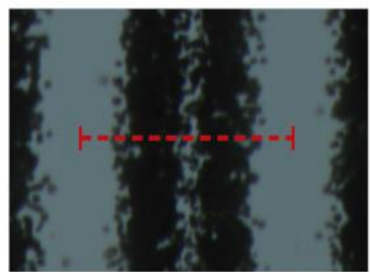
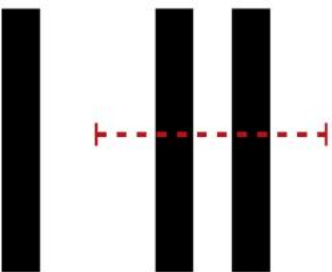




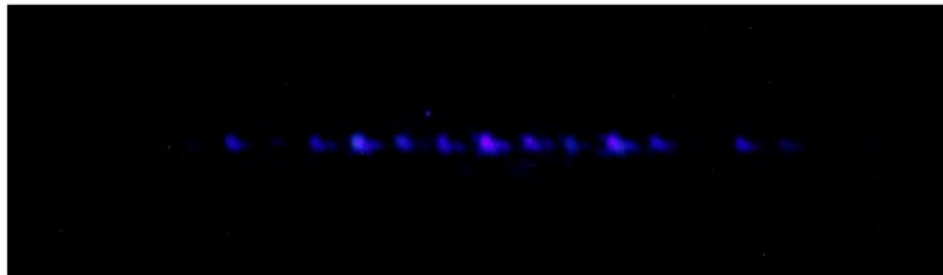
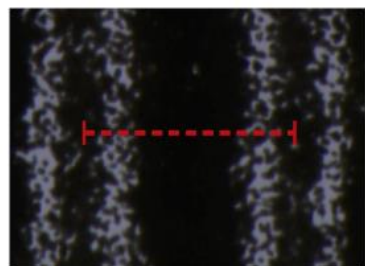
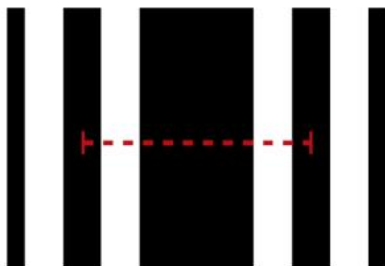
A)



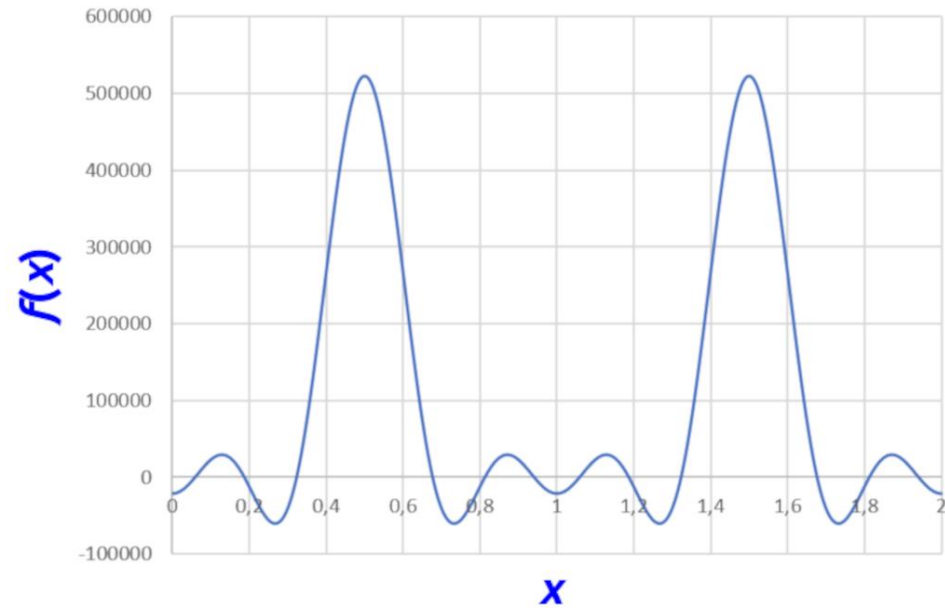
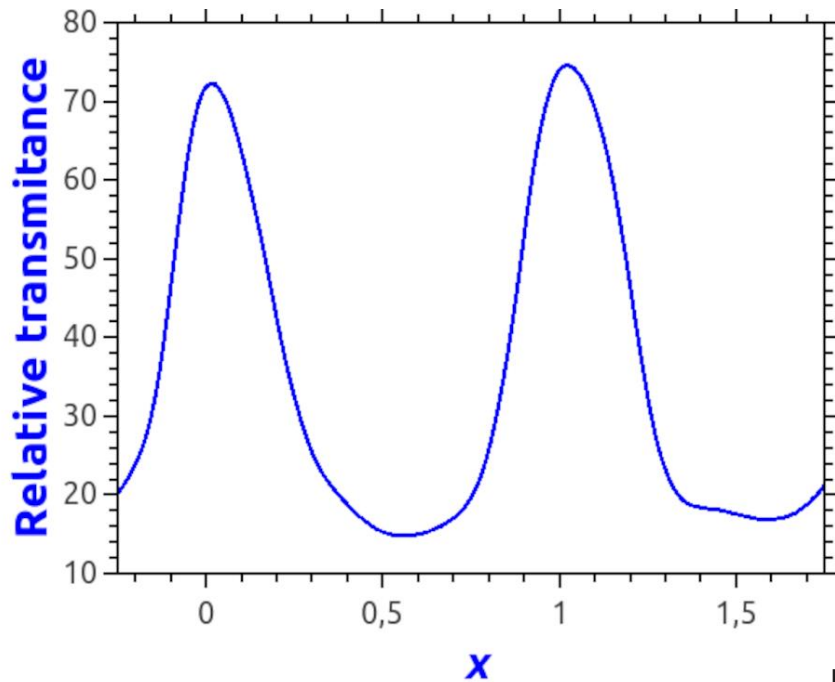
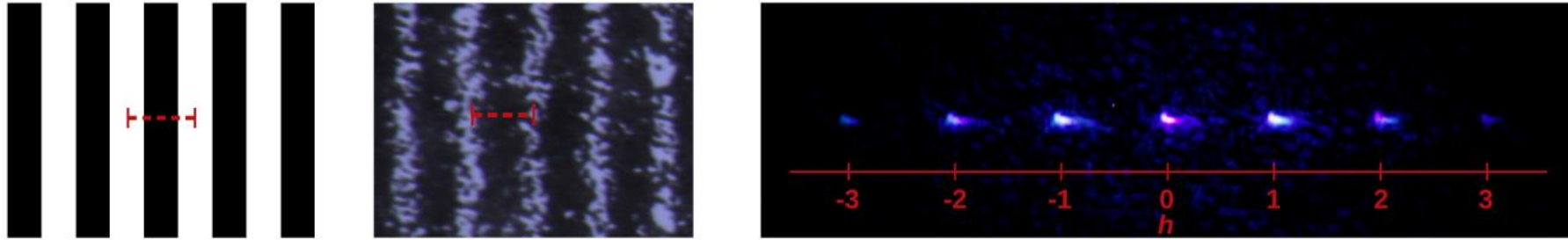
B)



C)

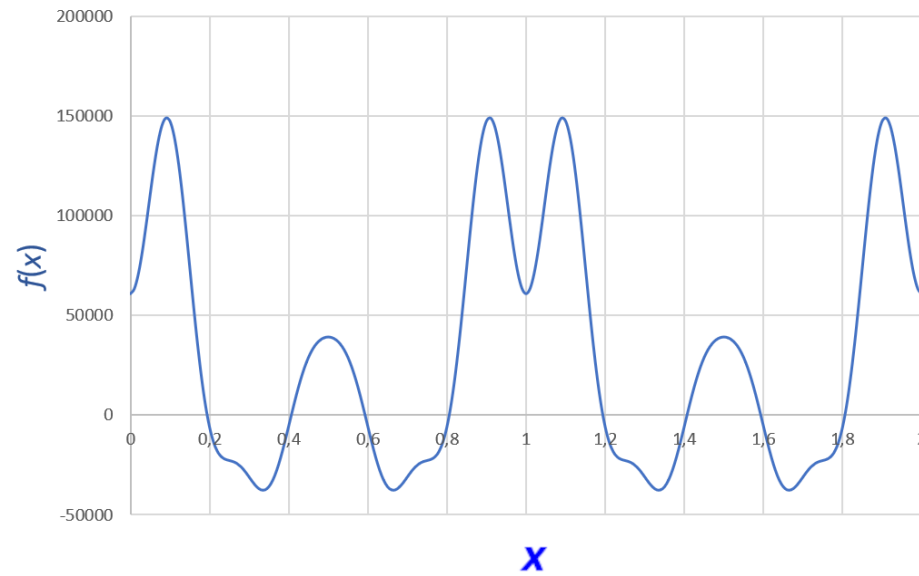
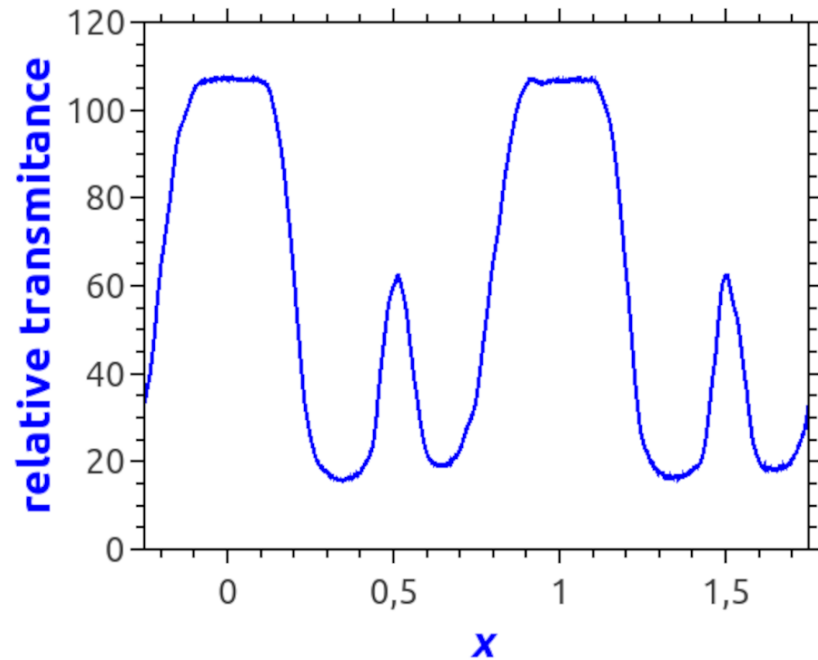
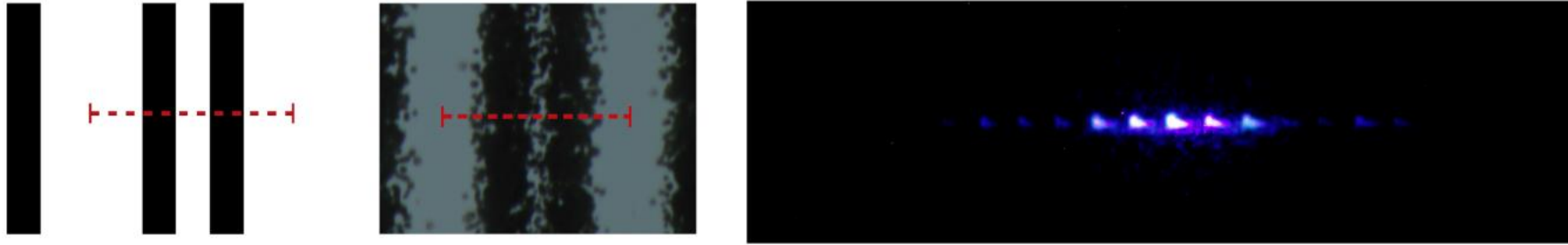


# Fourierova transformace mřížky „A“



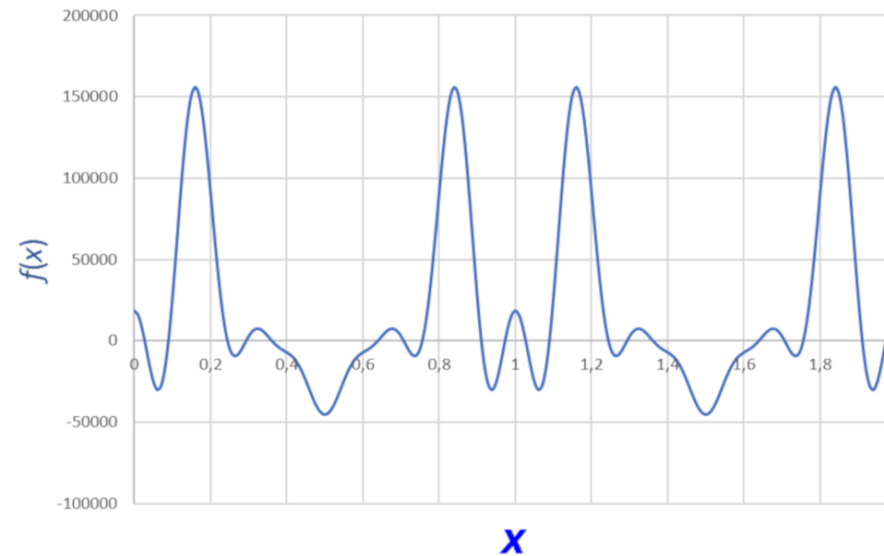
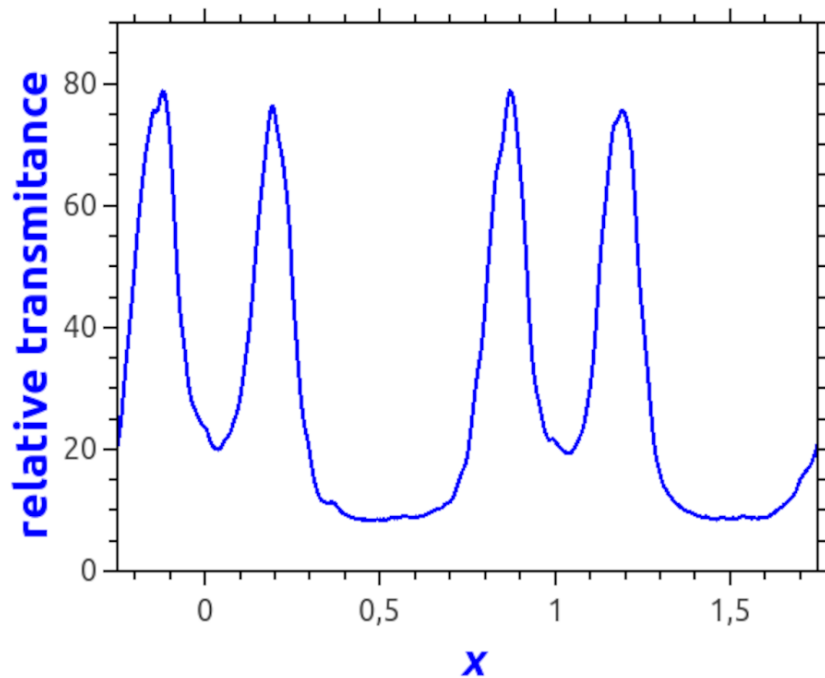
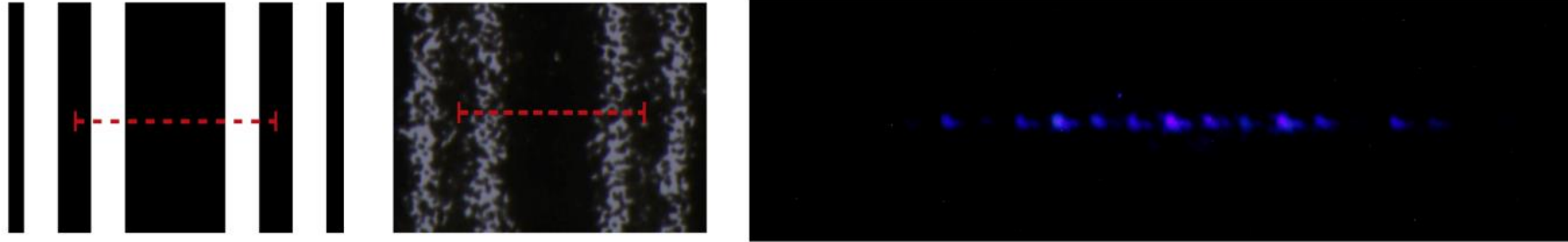
Excel soubor pro vyzkoušení v materiálech je nazvaný "Mrizka\_A"

# Fourierova transformace mřížky „B“



Excel soubor pro vyzkoušení v materiálech je nazvaný "Mrizka\_B"

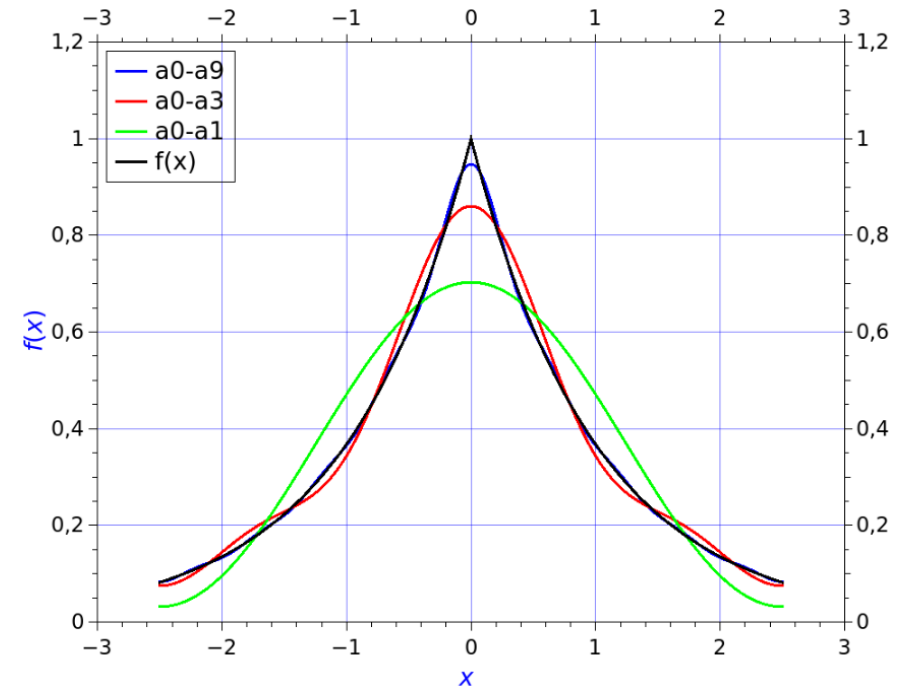
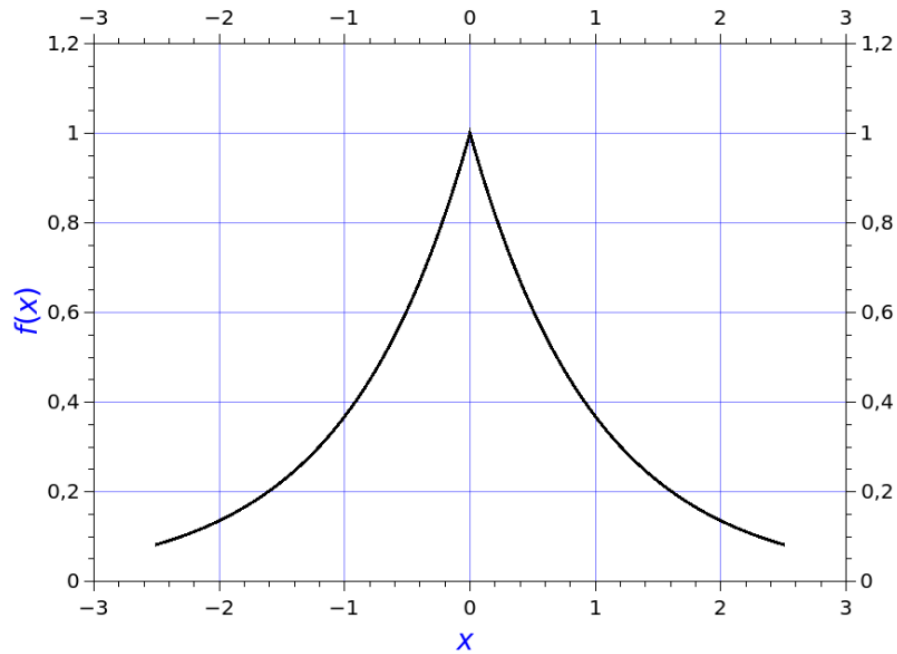
# Fourierova transformace mřížky „C“



Excel soubor pro vyzkoušení v materiálech je nazvaný "Mrizka\_C"

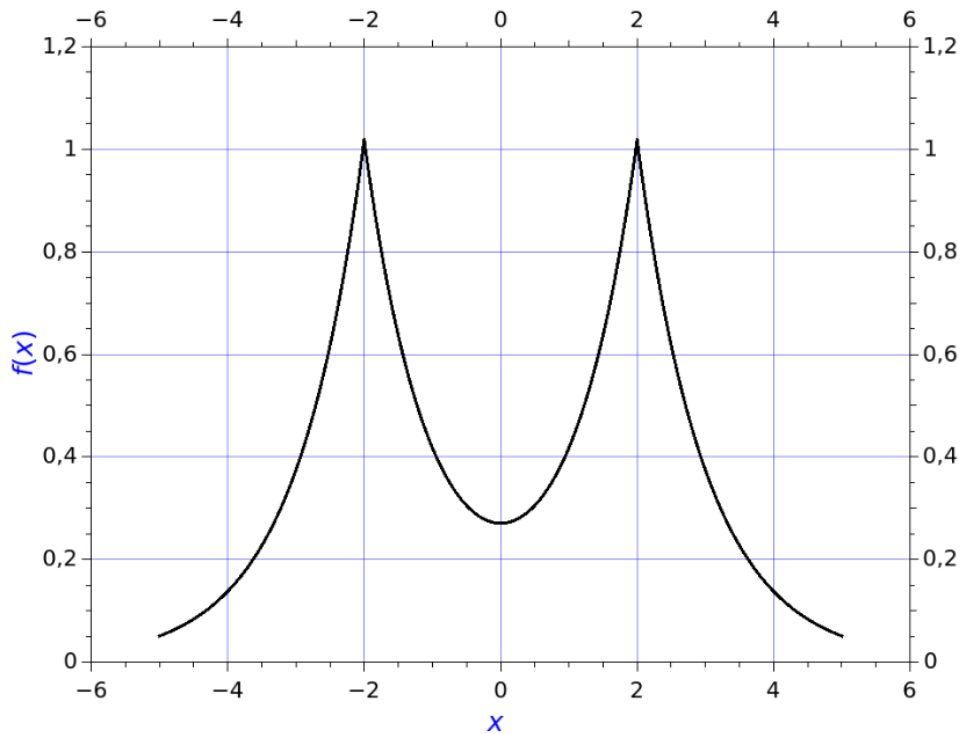
# Fourierova série jednoduché funkce

- Jedna perioda funkce  $f(x) = \exp(-|x|)$



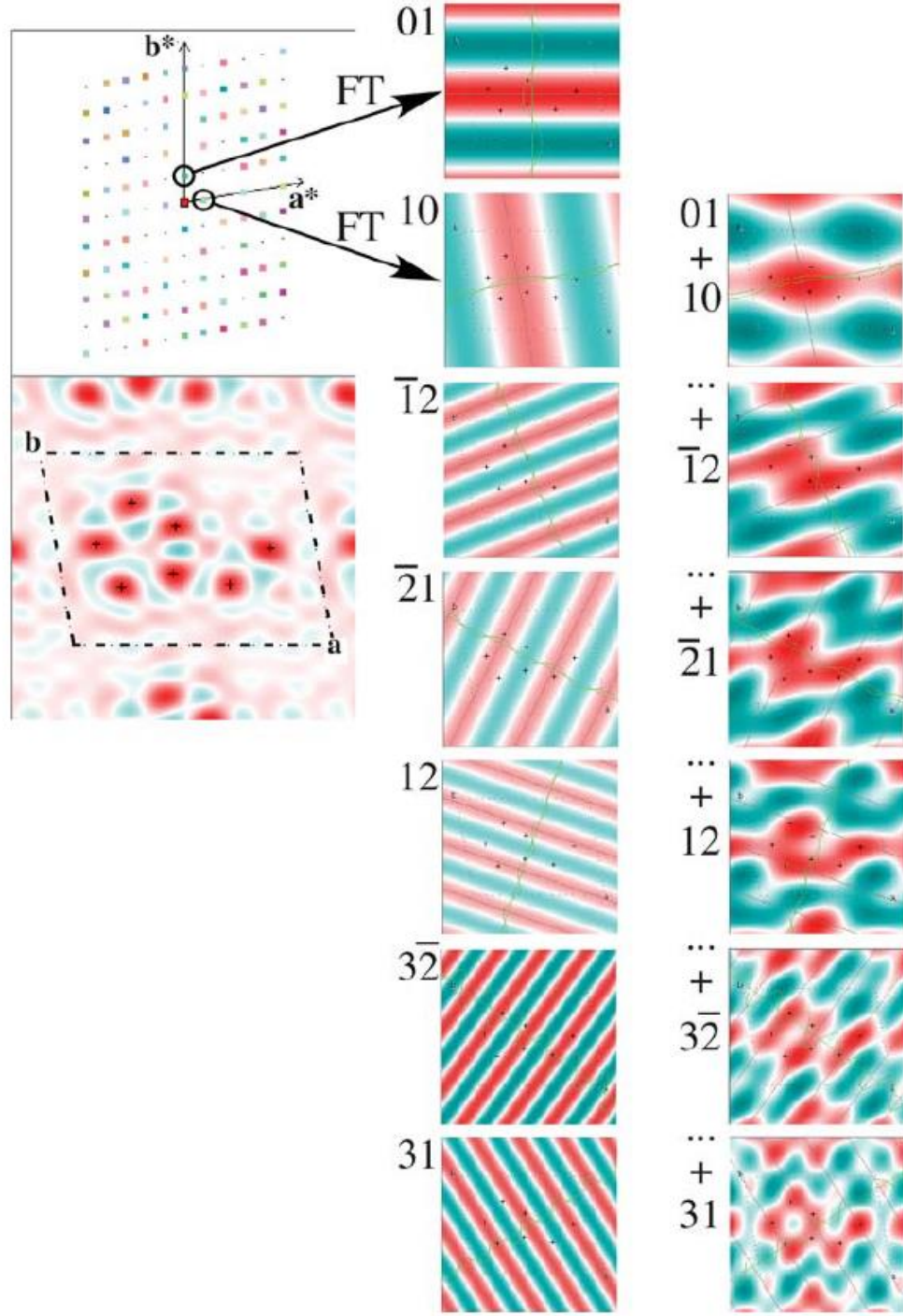
# Fourierova série funkce

- Jedna perioda funkce  $f(x) = \exp(-|x + 2|) + \exp(-|x - 2|)$

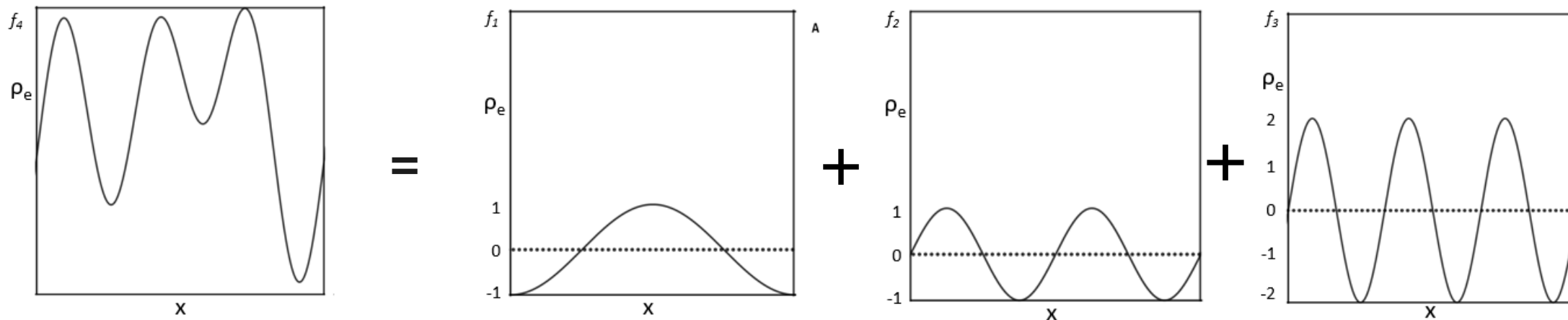


Excel soubor pro vyzkoušení v materiálech je nazvaný "Cviceni\_Fourierova\_serie"







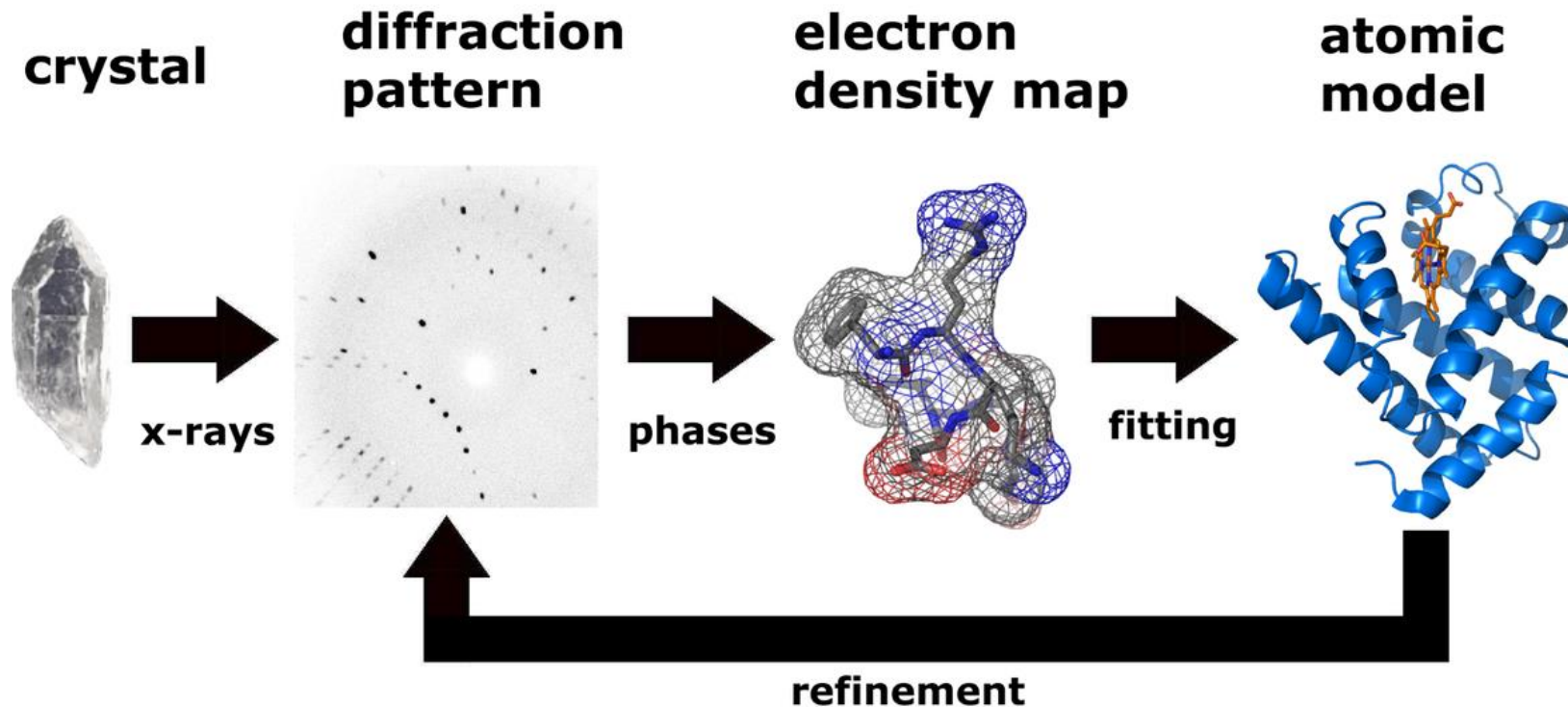


**Elektronová hustota** ←  $\rho(x) = \frac{1}{l} \sum_{n=1}^N |F_h| \exp \left[ -2\pi i h x + \underbrace{\varphi}_\times \right]$

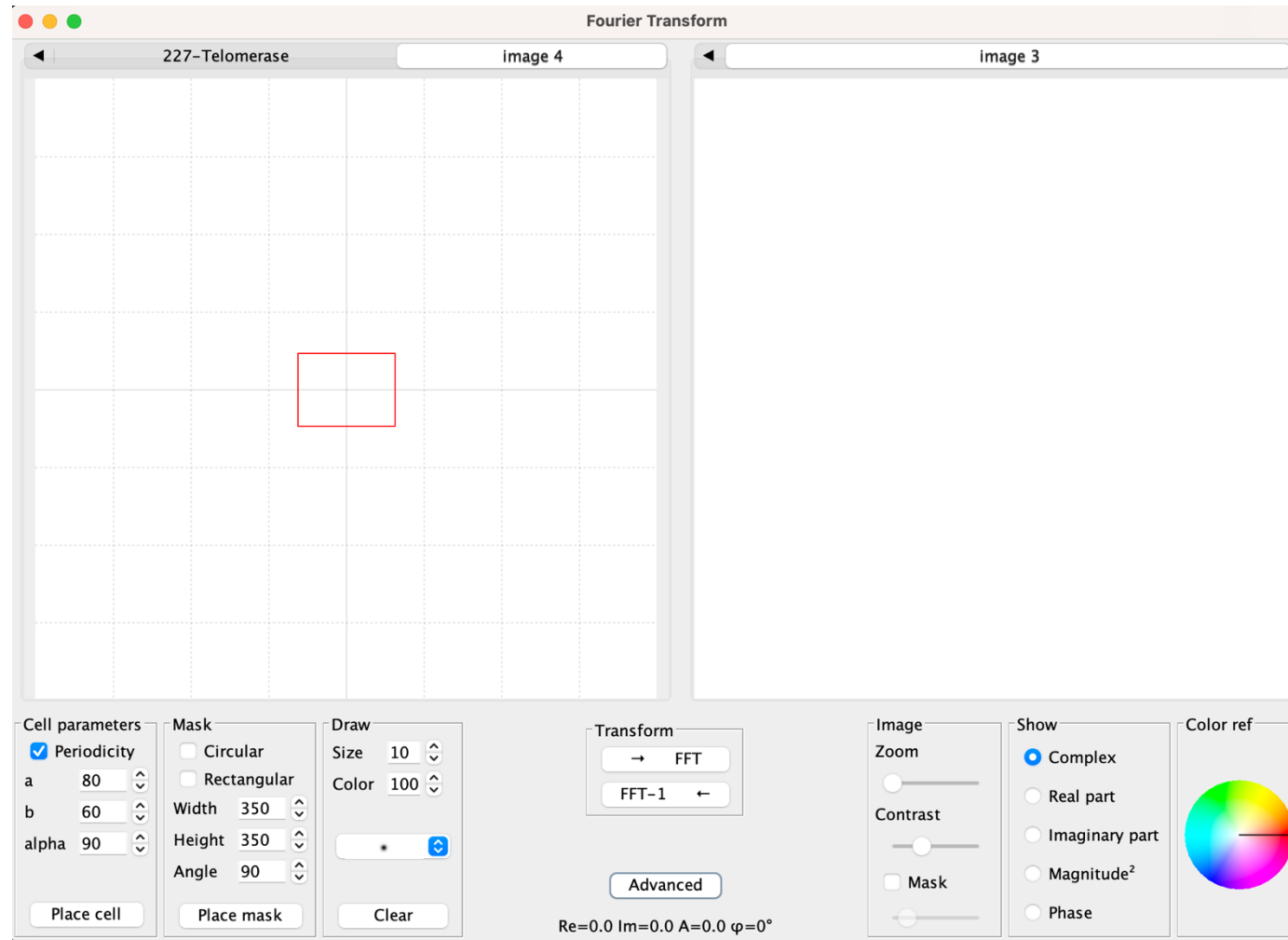
↓ Amplituda
↑ Frekvence
↓ Fáze

# Metody řešení fázového problému

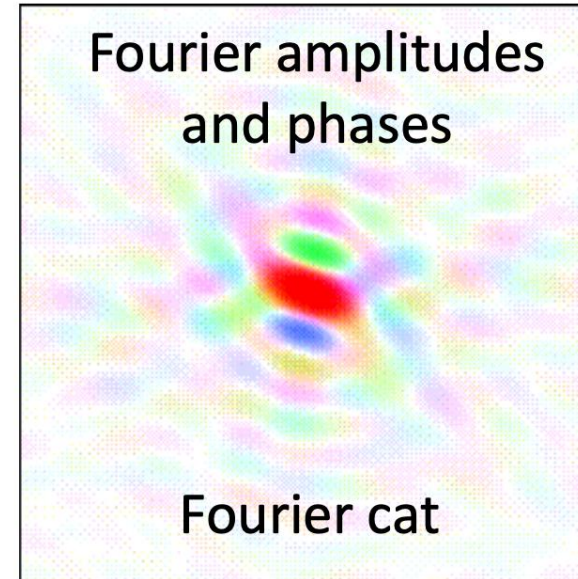
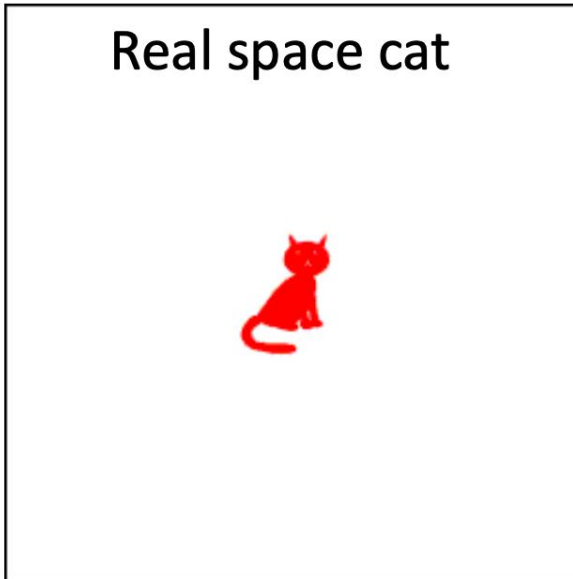
- Metoda molekulárního nahrazení
- Metoda izomorfního nahrazení
- Metoda anomálního rozptylu



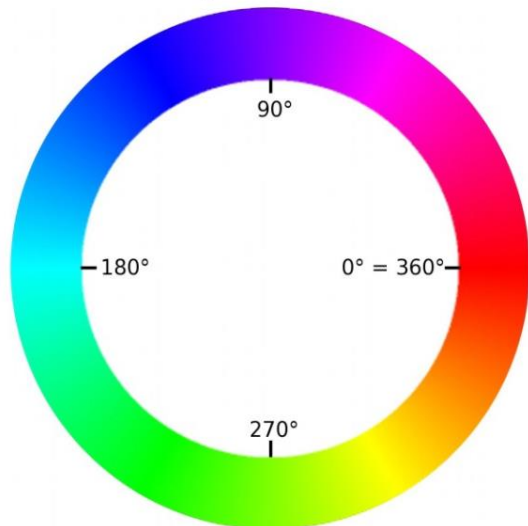
# Fourierova transformace obrázku



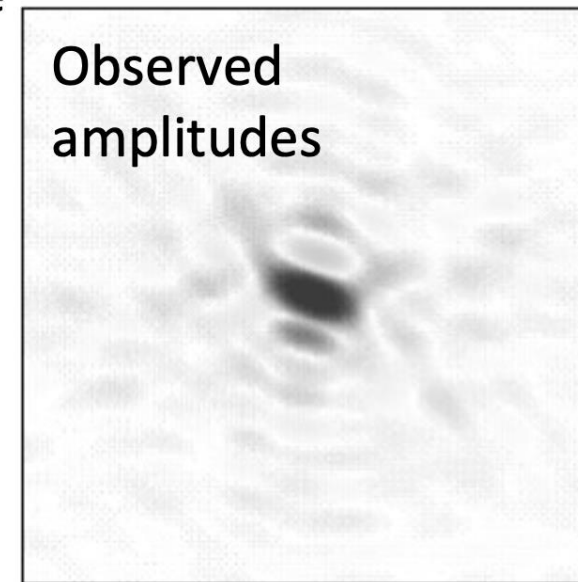
[Odkaz program ZDE](#) je potřeba mít java na PC




Circular rainbow scale of phases



Linear intensity scale of amplitude size

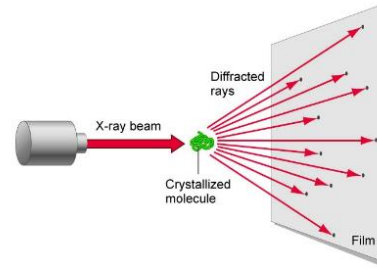


**Unknown structure,  
unknown orientation**

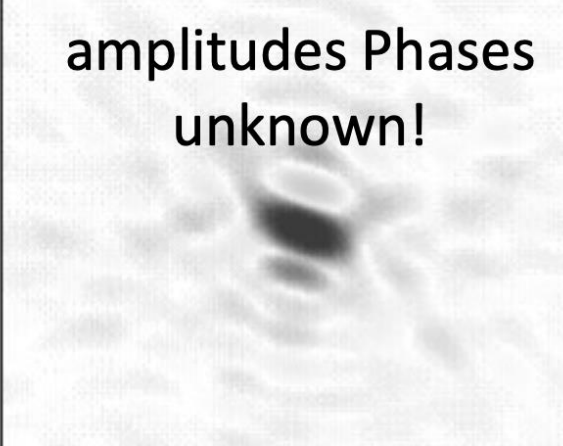


Cat

Diffraction  
experiment




Observed  
amplitudes Phases  
unknown!

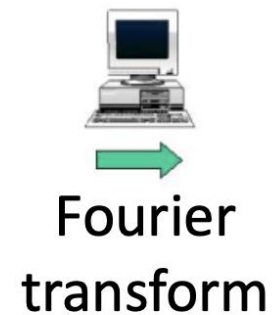


Fourier cat

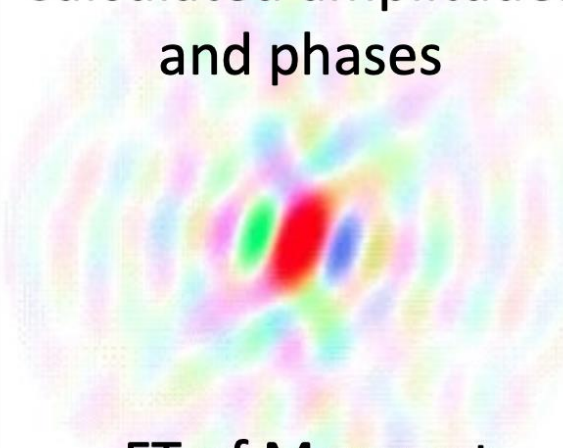
Known structure



Manx cat



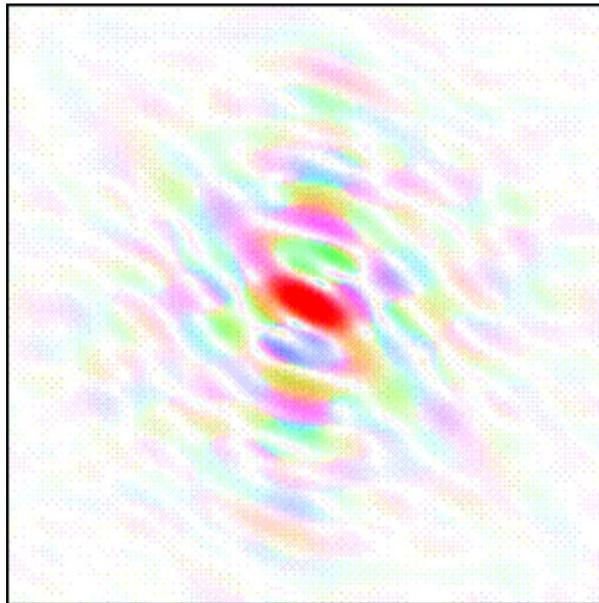
Calculated amplitudes  
and phases




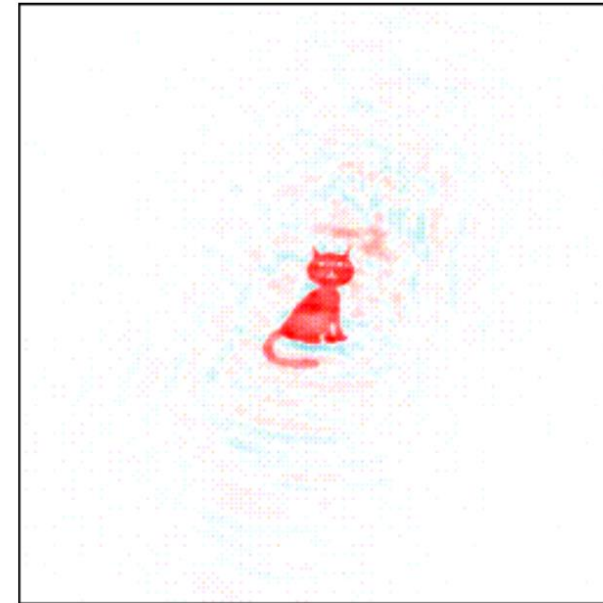
FT of Manx cat

**Wrong orientation!**

# Observed **amplitudes** (tailed cat), calculated **phases** (Manx cat)



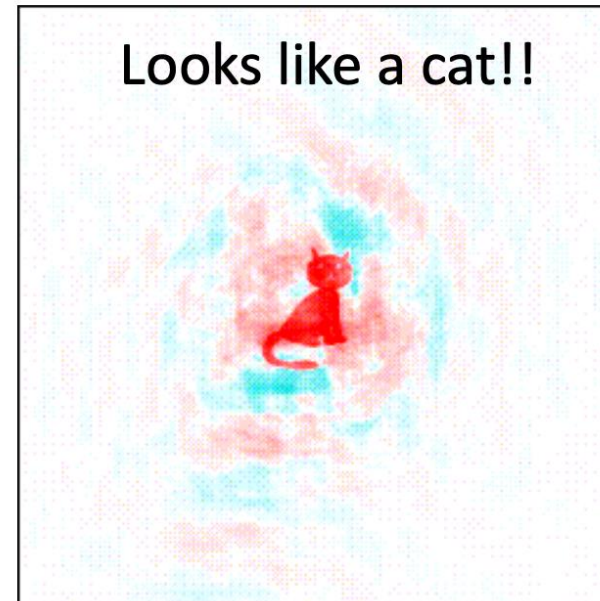
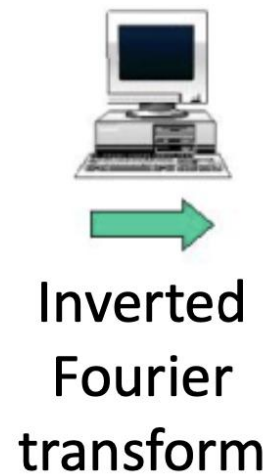
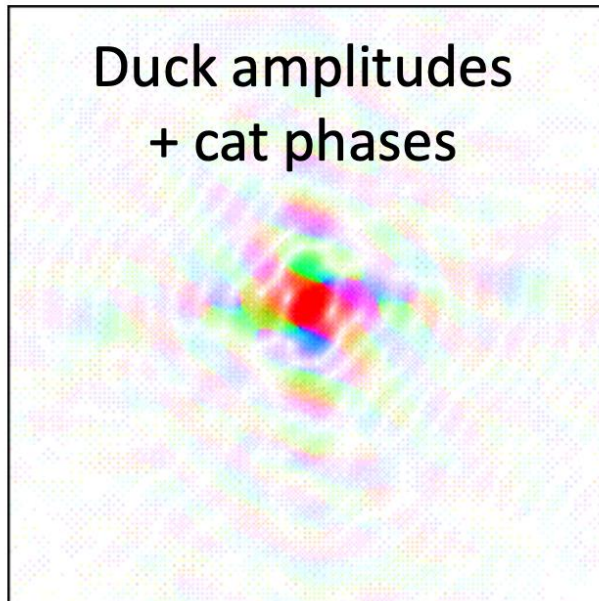
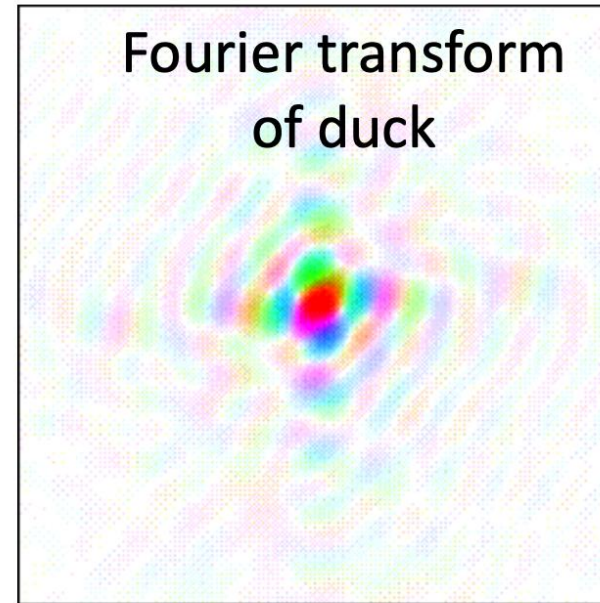
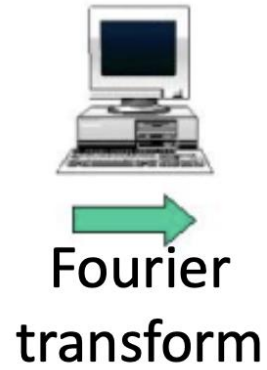
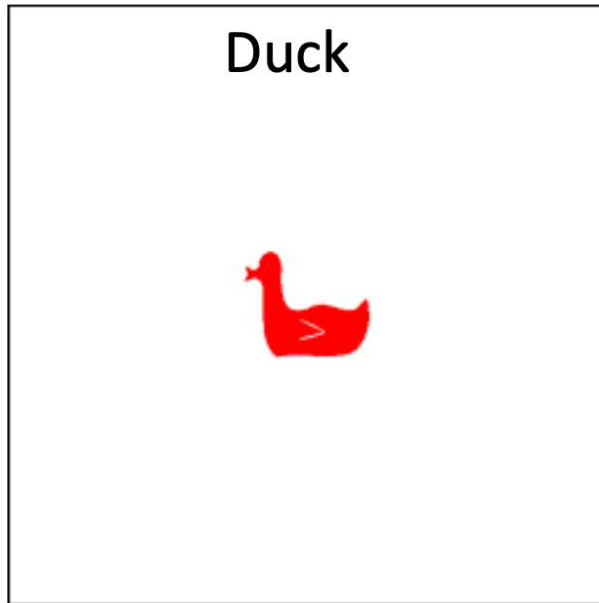
  
→  
Inverted  
Fourier  
transform



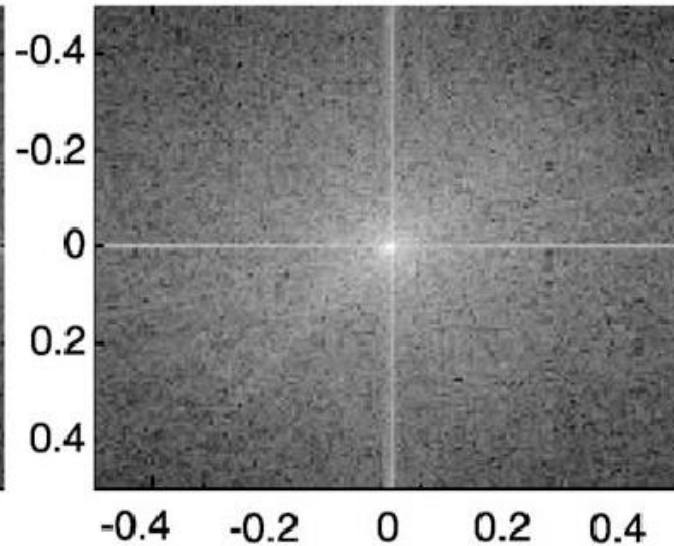
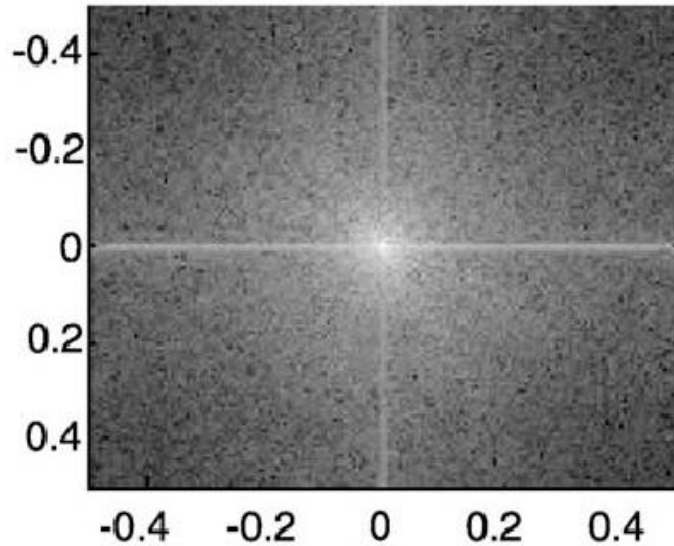
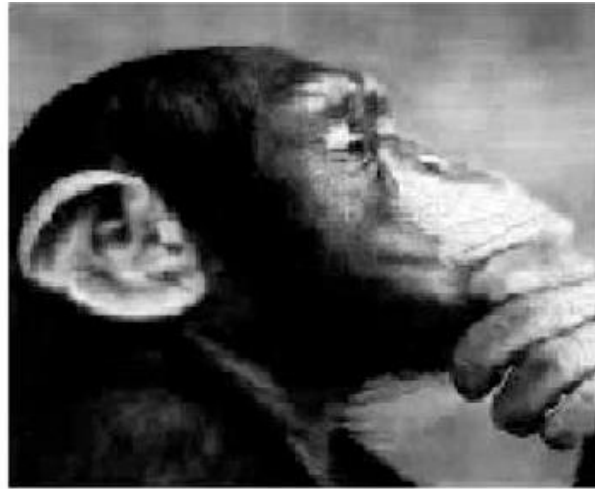
Even the tail becomes visible!



# Model Bias

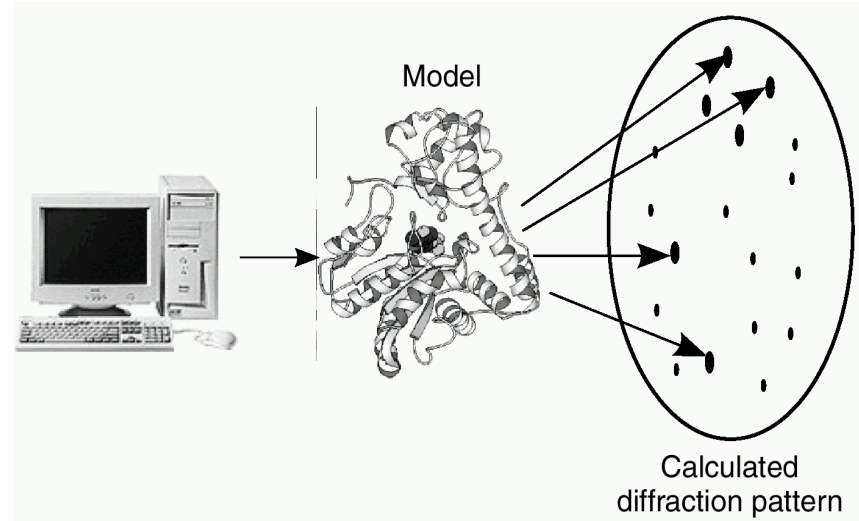
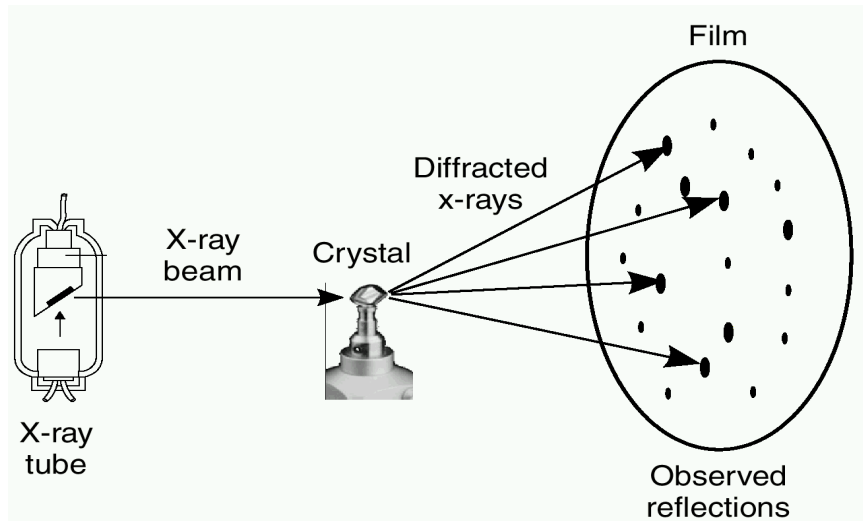


# Fourierova transformace obrázku





# Opakování R-factor, $R_{\text{free}}$ factor



R-factor

$$R = \frac{\sum_{hkl} ||F_{\text{obs}}| - k|F_{\text{calc}}||}{\sum_{hkl} |F_{\text{obs}}|}$$

$R_{\text{free}}$  factor

$$R_{\text{free}} = \frac{\sum_{hkl \subset T} ||F_{\text{obs}}| - k|F_{\text{calc}}||}{\sum_{hkl \subset T} |F_{\text{obs}}|}$$

# Výpočet struktury z náhodných fází

The interface is divided into several sections:

- Original structure:** A grid for drawing the initial structure.
- Reconstructed structure:** A grid for displaying the reconstructed structure.
- Flowchart:** A central diagram showing the iterative process: **Draw a Structure** (orange box) leads to **FFT**, which produces **F**. **F** is processed by **Random Phases** to produce **ρ**. **ρ** is processed by **Flip charges ( $\rho < \delta$ )** to produce **g**. **g** is processed by **FFT** to produce **G**. **G** is processed by **Restore amplitudes** to produce **F**. **F** is processed by **FFT-1** to produce **ρ**.
- Graph:** A plot showing the progress of the reconstruction. The y-axis ranges from 0% to 100%. The legend indicates: **Total Charge G(0)** (red line) and **R factor** (blue line).
- Control Panels:**
  - Drawing:** Pen size (10), Darkness (100), Position (-109 95), Clear button.
  - Run:** FFT, Do one cycle, Loop, Reset buttons.
  - Parameters:** Mask Radius (checked), Delta (0.4279), Dynamic (checked, 10%), Weak reflections (0%), Re=0.0 Im=0.0 A=0.0  $\varphi=0^\circ$ , Default button.
  - Image:** Zoom, Contrast, Rotate 180° buttons.
  - Show:** Complex (checked), Real part, Imaginary part, Magnitude<sup>2</sup>, Phase radio buttons.
  - Color ref:** A color wheel for reference.

[Odkaz program ZDE](#) je potřeba mít java na PC