Problem

'One dimensional crystallography'.

Consider a one dimensional crystal consisting of two carbon atoms ($n_c = 7$ electrons.) located at positions $x = +0.2$, and $x = -0.2$

The unit cell dimension is $a = 10\text{Å}$

Calculate the values of $F_h = \sum_j n_j e^{2\pi i h x_j}$

for $h = -10$ to 10

What are the phases of each reflection α_h

Any comment on why the phases have rather special values? & Why $F_h = F_{-h}$

Imagine now that you actually measured these as I_h for $h = -10$ to $+10$, took the square root to give $|F_h|$, and determined α_h for $h = -10$ to $+10$. Don't forget F_0!

Reconstruct the electron density to different 'resolutions' as follows. 5Å, 2Å, 1Å.

Note: • Resolution $= |S_{max}| = \frac{a}{h}$

• Hint: Use $\rho(x) = \sum_{h=0}^{+h} F_h e^{2\pi i h x} + F_{-h} e^{-2\pi h x} = F_0 + \sum_{h=1}^{+h_{max}} 2F_h \cos(2\pi h x)$

Hint: If $\alpha_h = 180°$, use $F_h = -|F_h|$

Plot $\rho(x)$ in 0.5Å intervals, or sketch the terms and sketch the answers.