

Exercise 2 — adding waves -- due Mon. Oct 26

Draw/write on these slides.

Save as PDF.

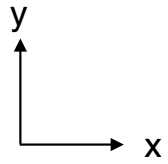
Upload to <http://www.bioinfo.rpi.edu/bystrc/courses/bcbp4870/homework.html>

part 1

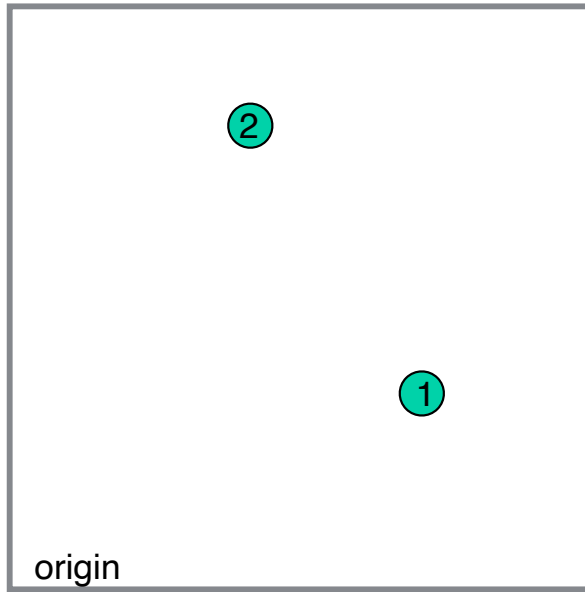
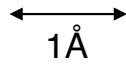
- (1) Look at the setup on the next page, a square unit cell of width 5.00\AA , with 2 hydrogen atoms in it. Xrays come in from the left, scatter at $2\theta=90^\circ$.
- (2) Measure the distance traveled from Wall A to Atom 1 (r_1) to Wall B, traveling along beam direction $\mathbf{s}_0 = (1, 0, 0)$ and scattered wave $\mathbf{s} = (0, 1, 0)$, respectively. Divide by the wavelength. Multiply by 2π (or 360) to get the phase in radians (or degrees).
- (3) Do the same for Atom 2 (r_2). Fill in Table 1.
- (4) Add the two waves in Argand space (slide 20 of this lecture). Measure the resulting length (amplitude A) and phase (α).

Exercise 2 — copy this page and draw on it — due Mon. Oct 26

Wall B the wave detector

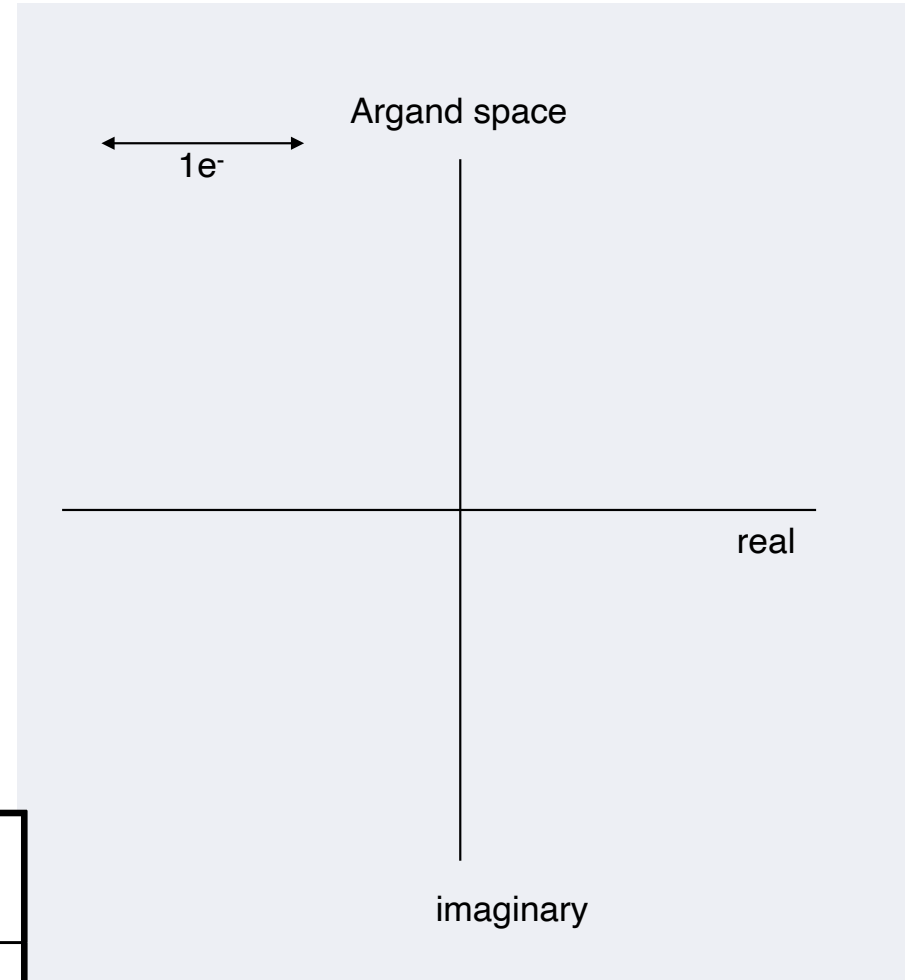
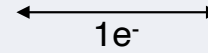


Real space



add the two scattered waves in

Argand space



Wall A

the wave generator

Table 1	Distance traveled	subtract origin distance traveled	phase (°) if wavelength = 1.54Å
origin			
r ₁			
r ₂			

Amplitude (A)	
phase (α)	

Exercise 2 — part 2

Calculate the wave sum using the Fourier transform

$$F(S) = \sum_k \rho(r_k) e^{i2\pi S \cdot r_k}$$

$$\lambda = 1.54 \text{ \AA}$$

$$s_0 = (1, 0, 0)$$

$$s = (0, 1, 0)$$

$$S = (s - s_0)/\lambda = (\quad \quad \quad)$$

Table 2	Measure Å coordinates of r_k relative to origin from previous page.	$A_k = \rho(r_k)$	$\alpha_k = 2\pi S \cdot r_k$	$A_k \cos(\alpha_k)$	$i A_k \sin(\alpha_k)$
k=1					
k=2					
sum					
Amplitude (A) = (imag, real)					
phase (α) = $\tan^{-1}(\text{imag}/\text{real})$ (in degrees)					