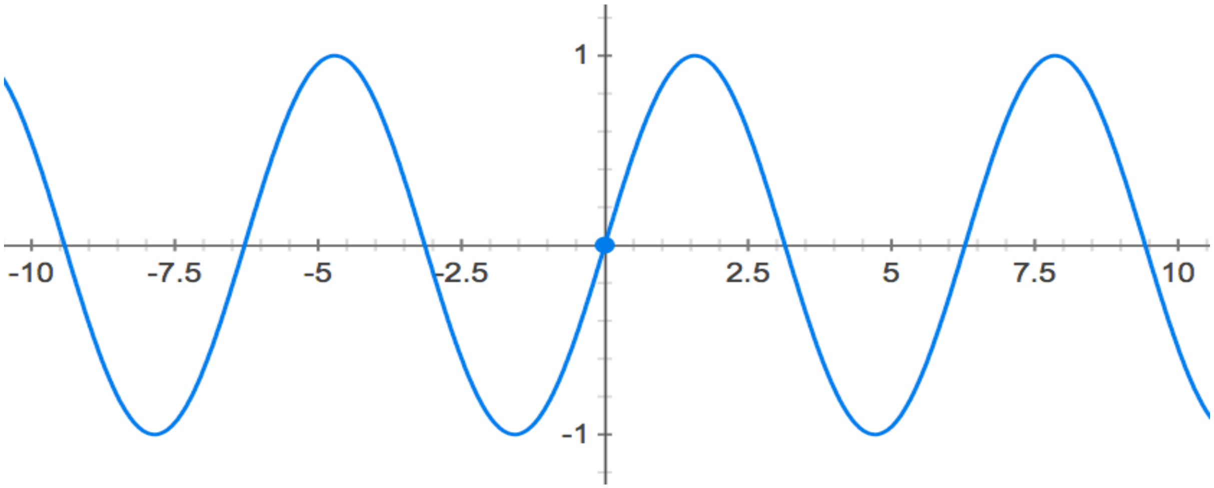
Part 2: Fourier transforms

Key to understanding NMR,
X-ray crystallography,
and all forms of microscopy

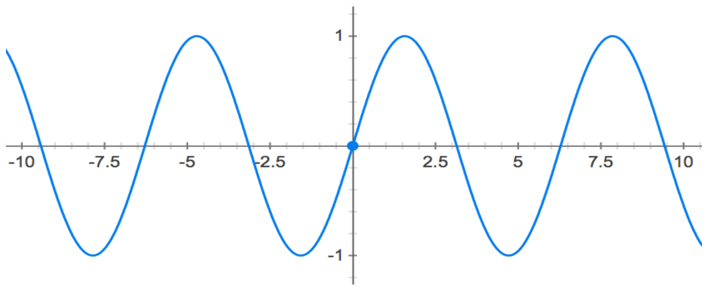
Sine waves



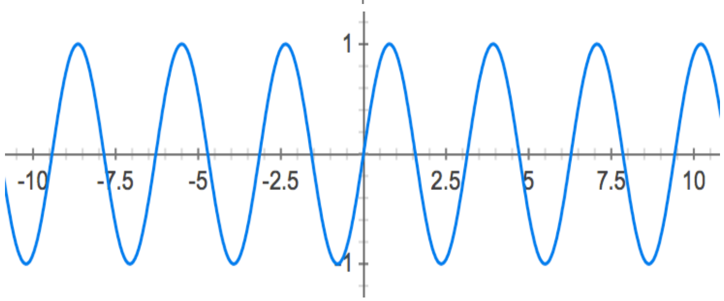
$y(t) = A \sin(wt + p)$
$y(x) = A \sin(kx + p)$

To completely specify a sine wave, you need its
(1) direction,
(2) wavelength or frequency,
(3) amplitude, and
(4) phase shift

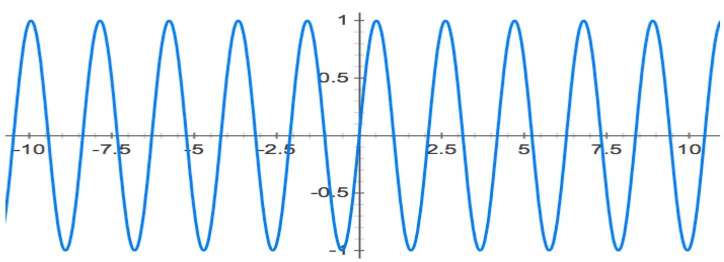
Adding sine waves



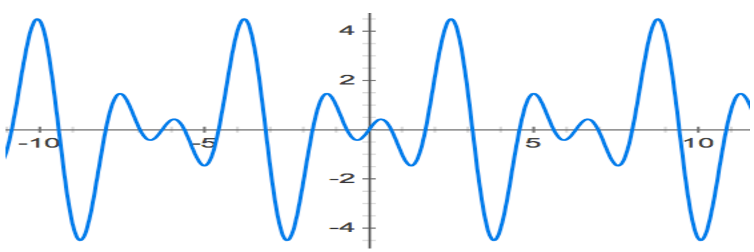
$y = \sin(x)$



$y = \sin(2x)$



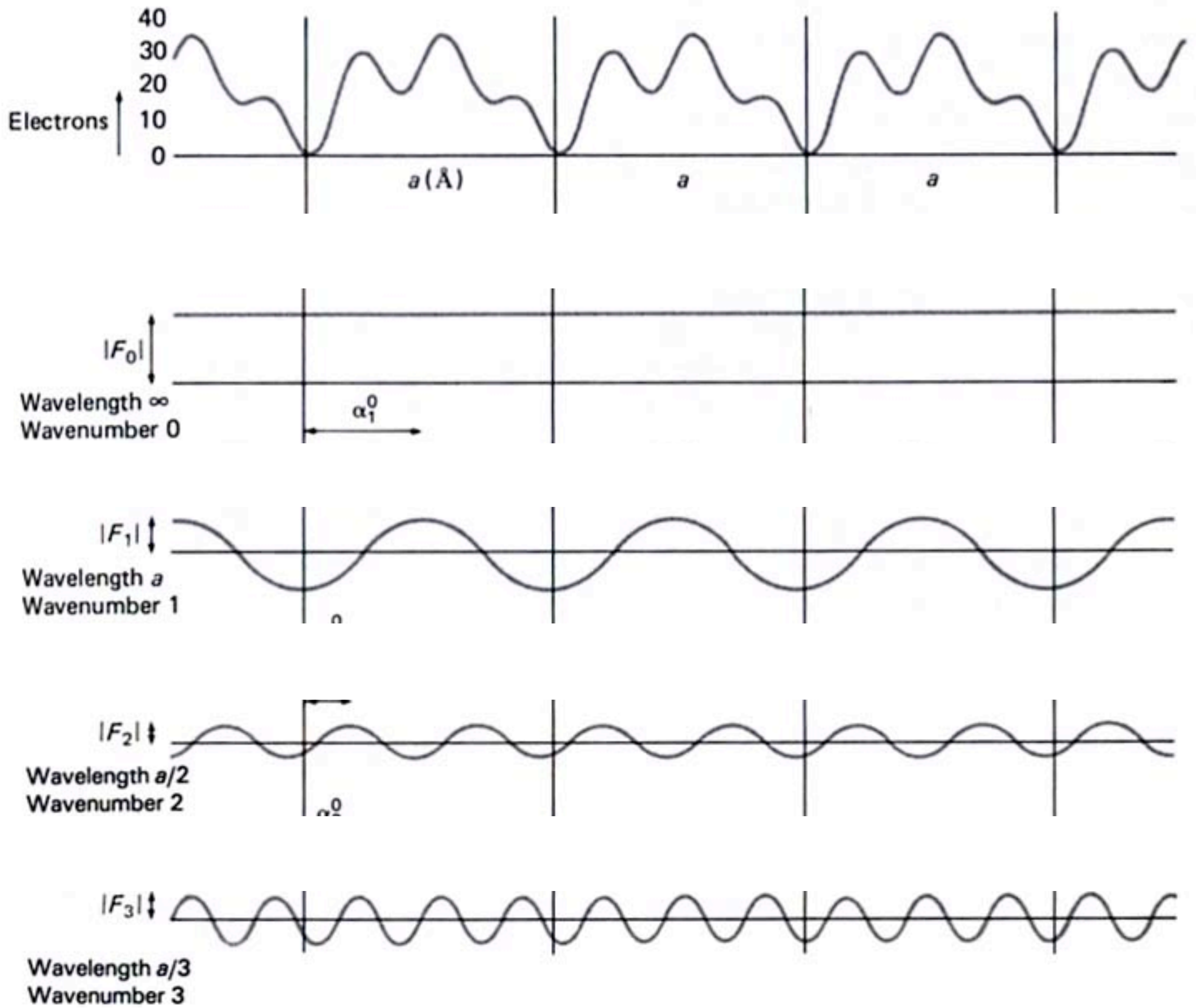
$y = \sin(3x)$



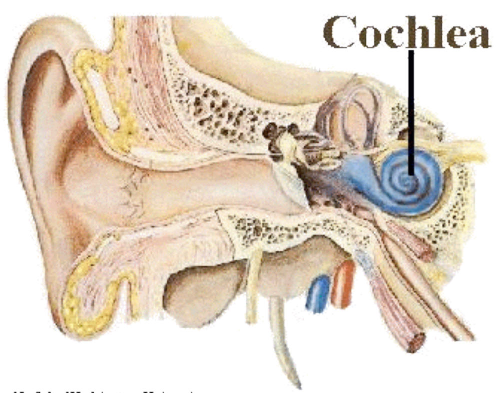
$y = \sin(x) - 2.3\sin(2x) + 1.8\sin(3x)$

Taking sine wave sums apart

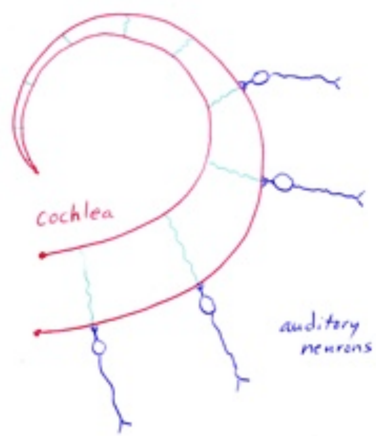
(a Fourier “decomposition”, or “transform”)

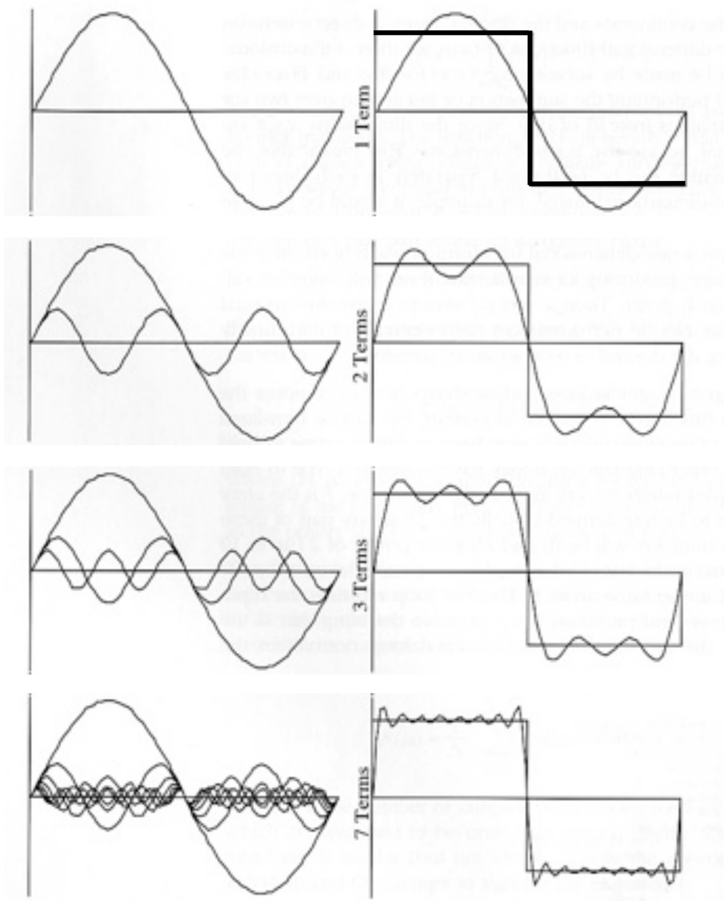


Fourier transforms in music and hearing



Alec N. Salt, Washington University





Fourier decompositions may not be exact - depends on how many terms you use ("resolution")

The mathematical details

$$f(x) = \frac{A_0}{2} + \sum_{m=1}^{\infty} A_m \cos\left(\frac{2\pi m x}{\lambda}\right) + \sum_{m=1}^{\infty} B_m \sin\left(\frac{2\pi m x}{\lambda}\right)$$

$$A_m = \frac{2}{\lambda} \int_0^{\lambda} f(x) \cos\left(\frac{2\pi m x}{\lambda}\right) dx$$

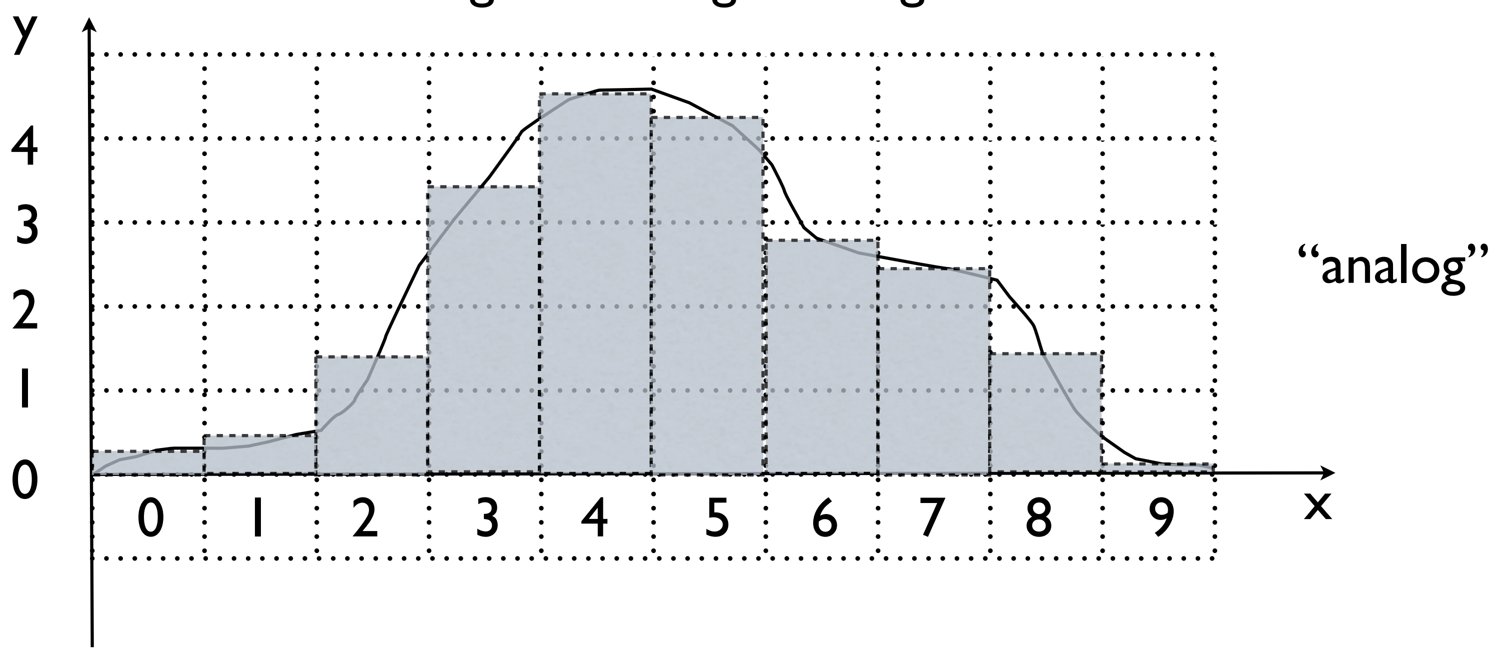
$$B_m = \frac{2}{\lambda} \int_0^{\lambda} f(x) \sin\left(\frac{2\pi m x}{\lambda}\right) dx$$

The balance between sine and cosine terms can be equivalently introduced by giving each sine term a "phase"

One-dimensional sine waves and their sums
Concept check questions:

- What four parameters define a sine wave?
- What is the difference between a temporal and a spatial frequency?
- What in essence is a "Fourier transform"?
- How can the amplitude of each Fourier component of a waveform be found?

Analog versus digital images



0.3	0.4	1.3	3.4	4.5	4.2	2.8	2.4	1.4	0.1	“digital”

Consider a one-dimensional array:

0.3	0.4	1.3	3.4	4.5	4.2	2.8	2.4	1.4	0.1

10 numbers

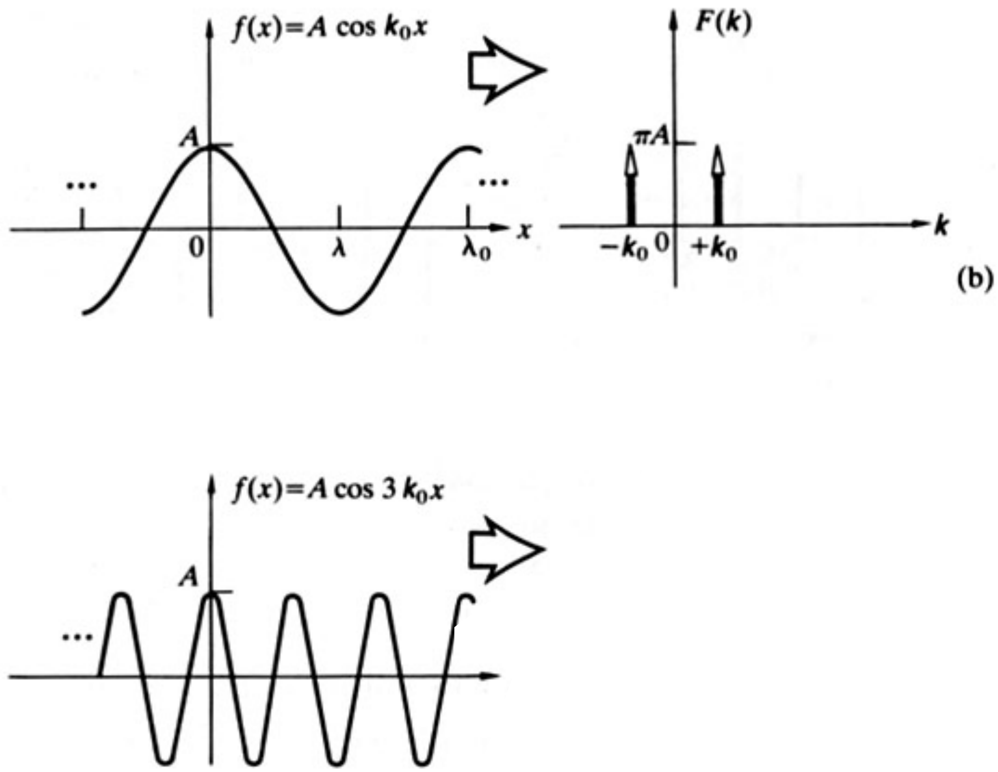
↓ Fourier transform

A_0	P_0	A_1	P_1	A_2	P_2	A_3	P_3	A_4	P_4	A_5	P_5

10 numbers + 2
(5 amps & phases + "DC" component)

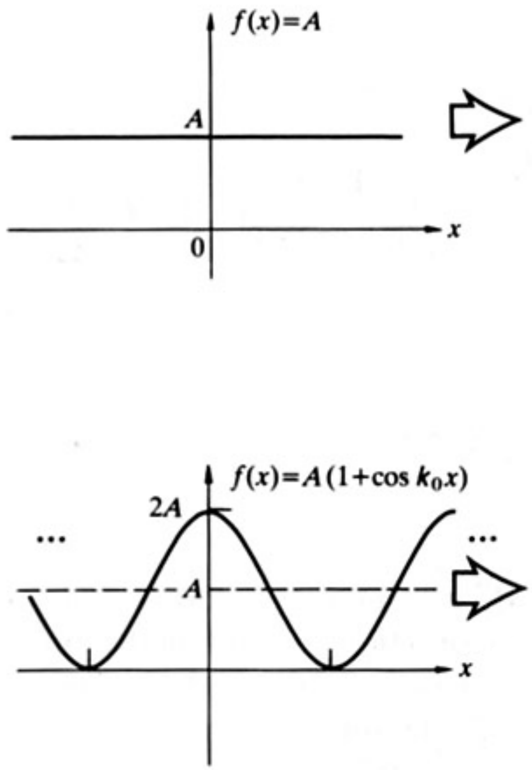
A_0 = amplitude of "DC" component
A_1 = amplitude of "fundamental" frequency (one wavelength across box)
P_1 = phase of "fundamental" frequency component
A_2 = amplitude of first "harmonic" (two wavelengths across box)
P_2 = phase of first harmonic
A_3 = amplitude of second harmonic
P_3 = phase of second harmonic
etc.
A_5 = amplitude of "Nyquist" frequency component

One dimensional functions and transforms (spectra)



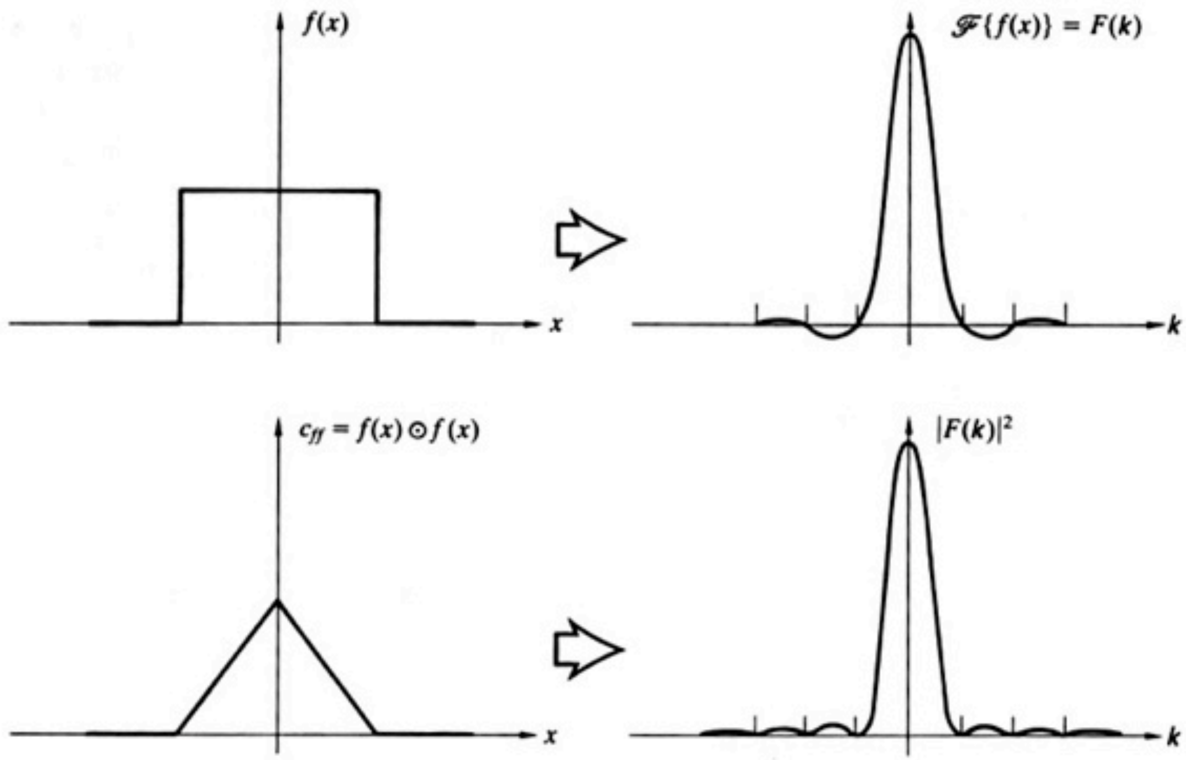
Hecht, Fig. 11.13

One dimensional functions and transforms (spectra)



Hecht, Fig. 11.13

More complicated functions and their spectra

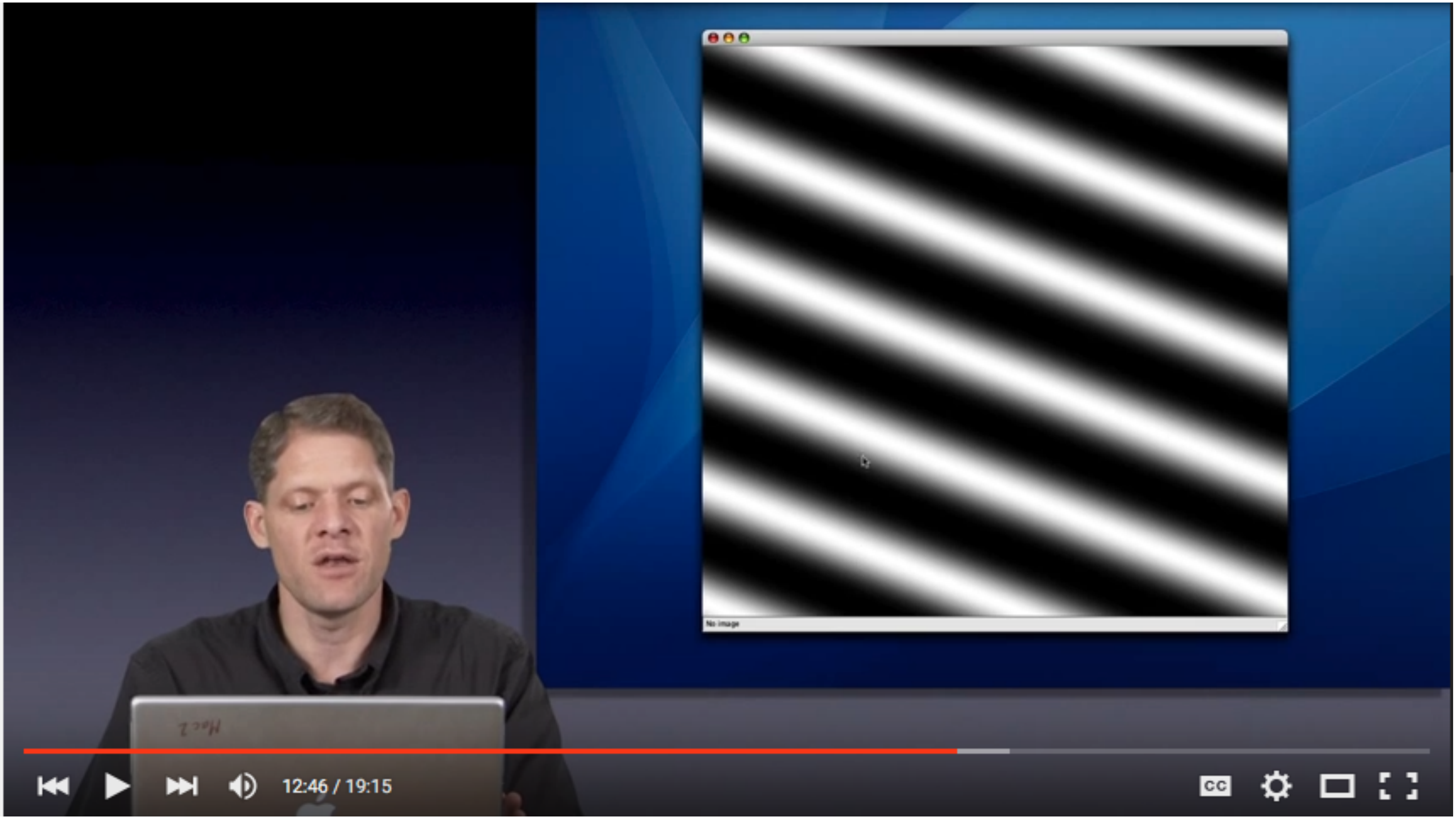


Hecht, Fig. 11.38

One-dimensional reciprocal space
Concept check questions:

- What is the difference between an “analog” and a “digital” image?
- What is the “fundamental” frequency? A “harmonic”? “Nyquist” frequency?
- What is “reciprocal” space? What are the axes?
- What does a plot of the Fourier transform of a function in reciprocal space tell you?

In microscopy we deal with 2-D images and transforms



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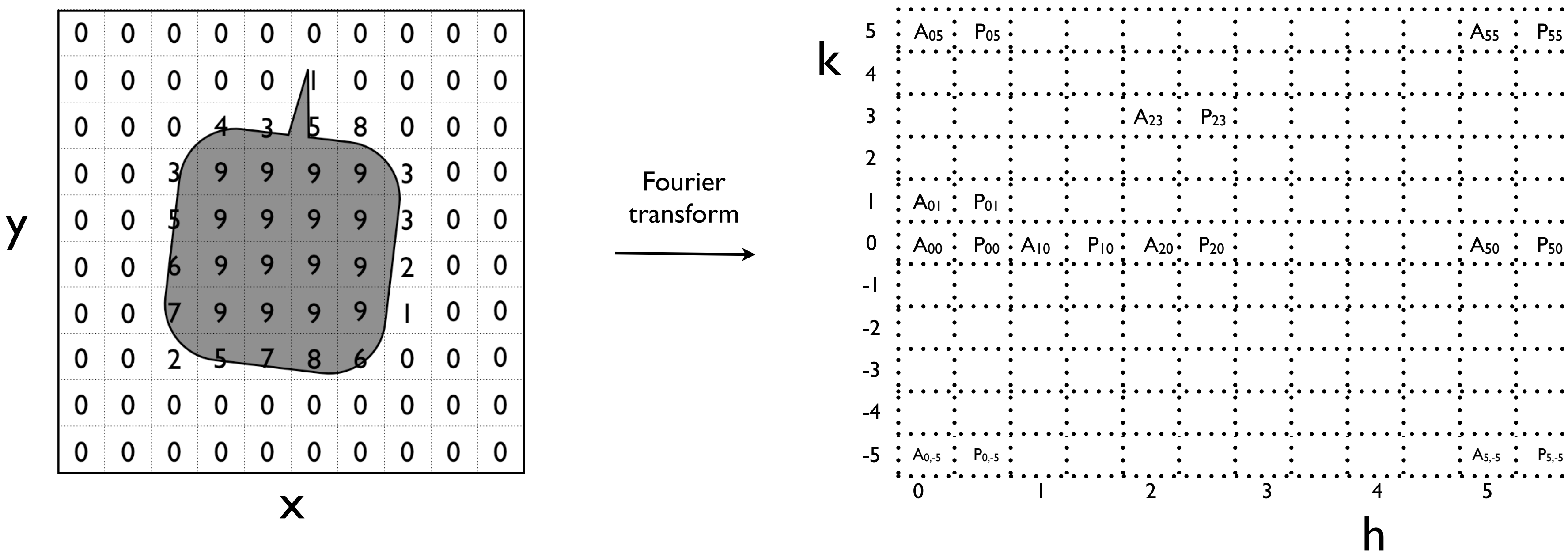
Two-dimensional waves and images
Concept check questions:

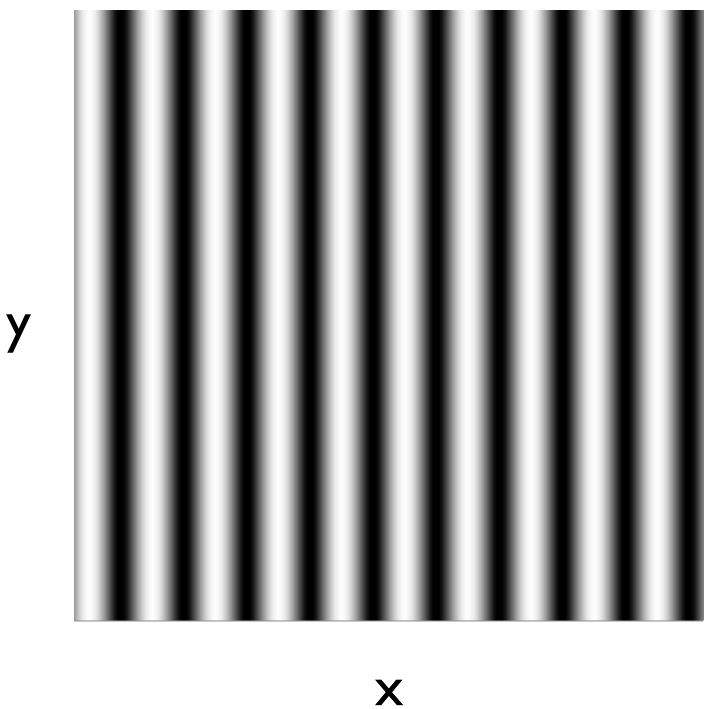
- What does a two-dimensional sine wave look like?
- What do the "Miller" indices "h" and "k" indicate?

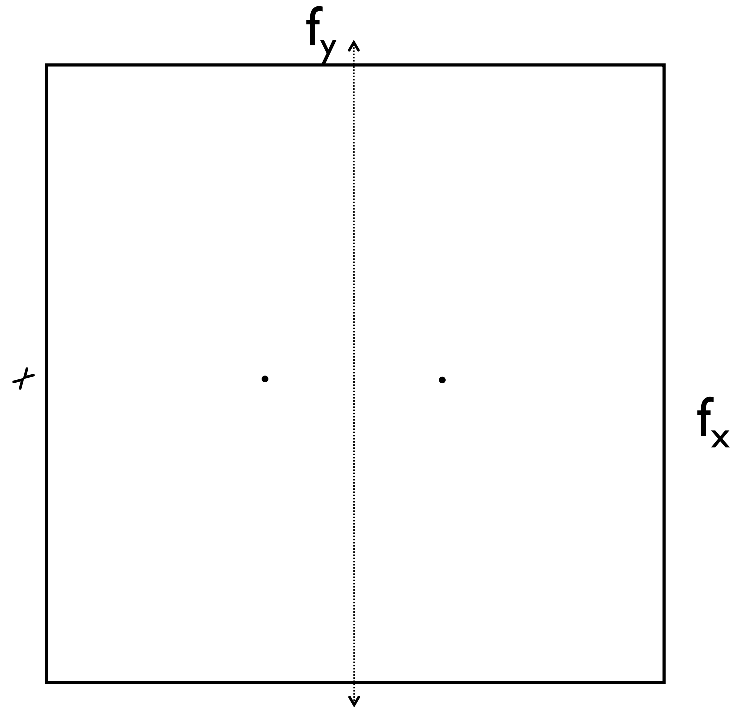


N^2
numbers

$\sim N^2$
numbers

A simple 2-D image and transform (diffraction pattern)

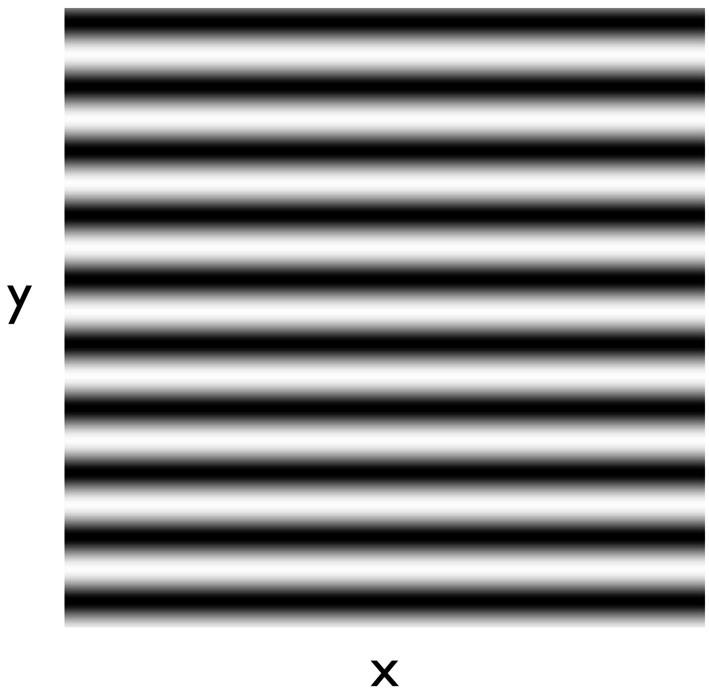


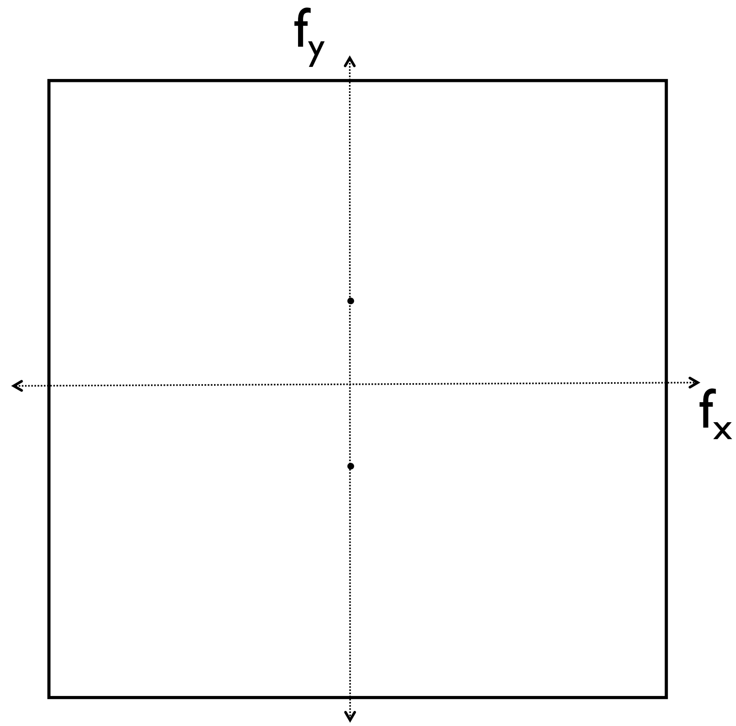


"Real" space : coordinates

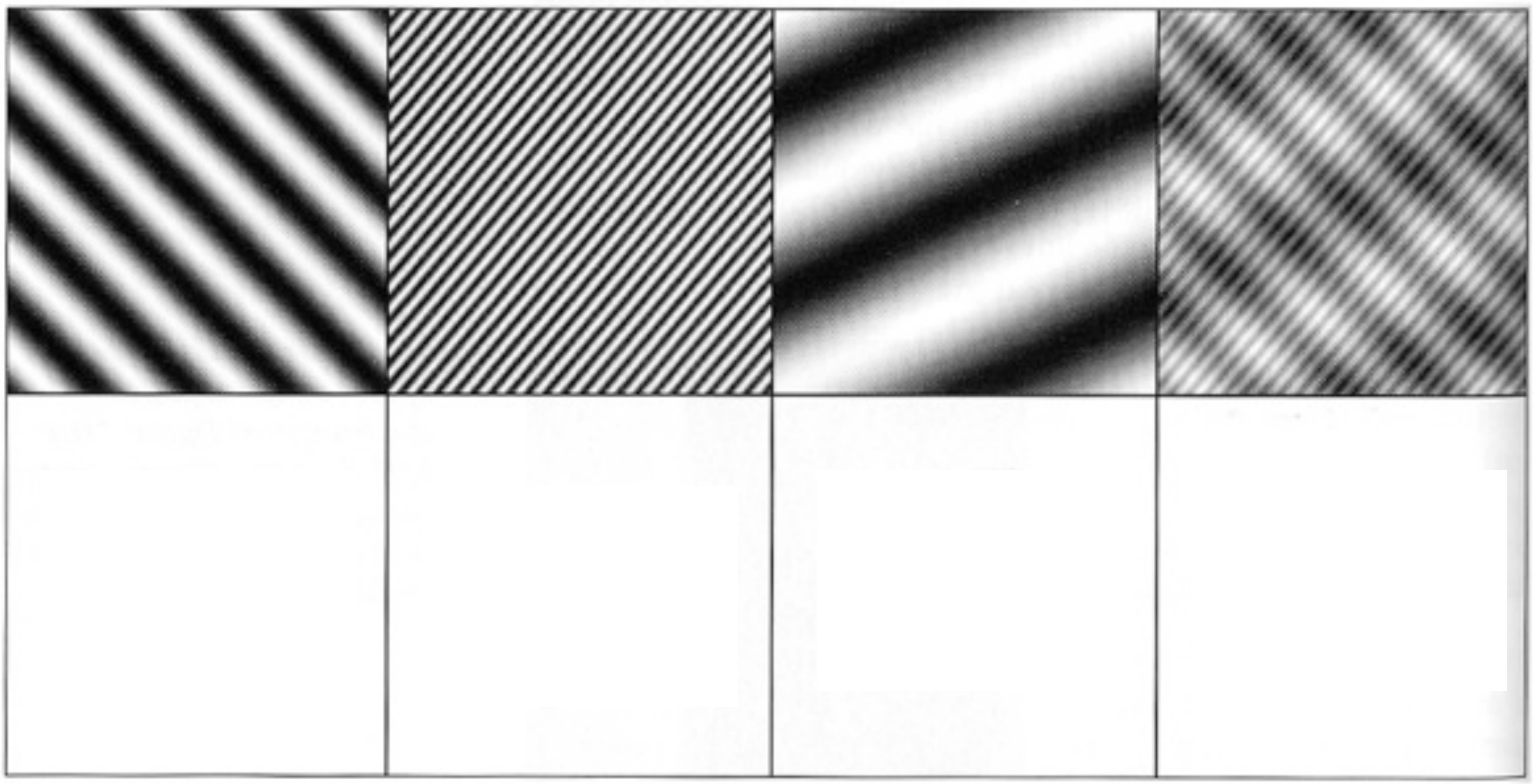
"Reciprocal" space : spatial "frequencies"

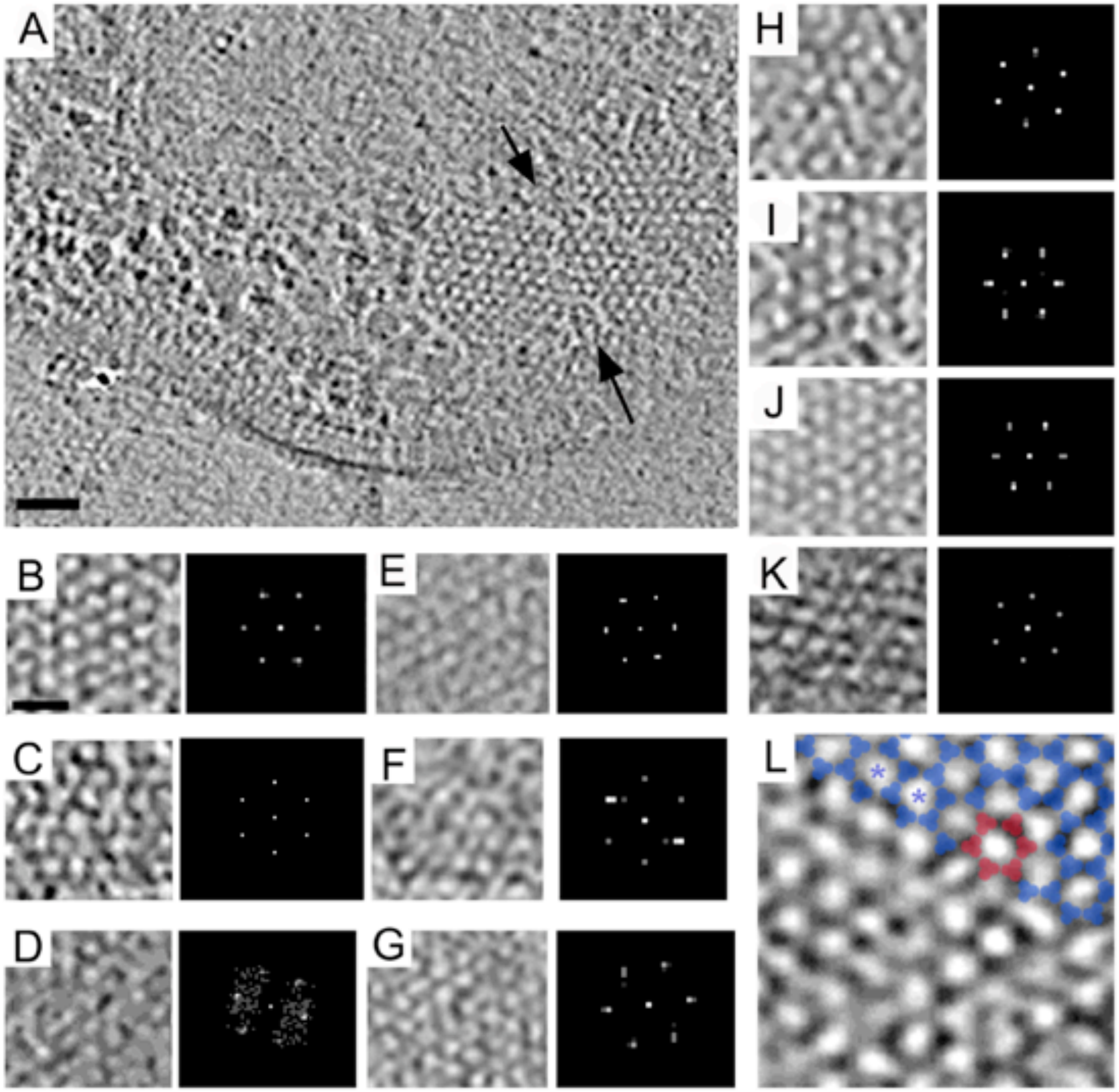
Another simple 2-D image and transform





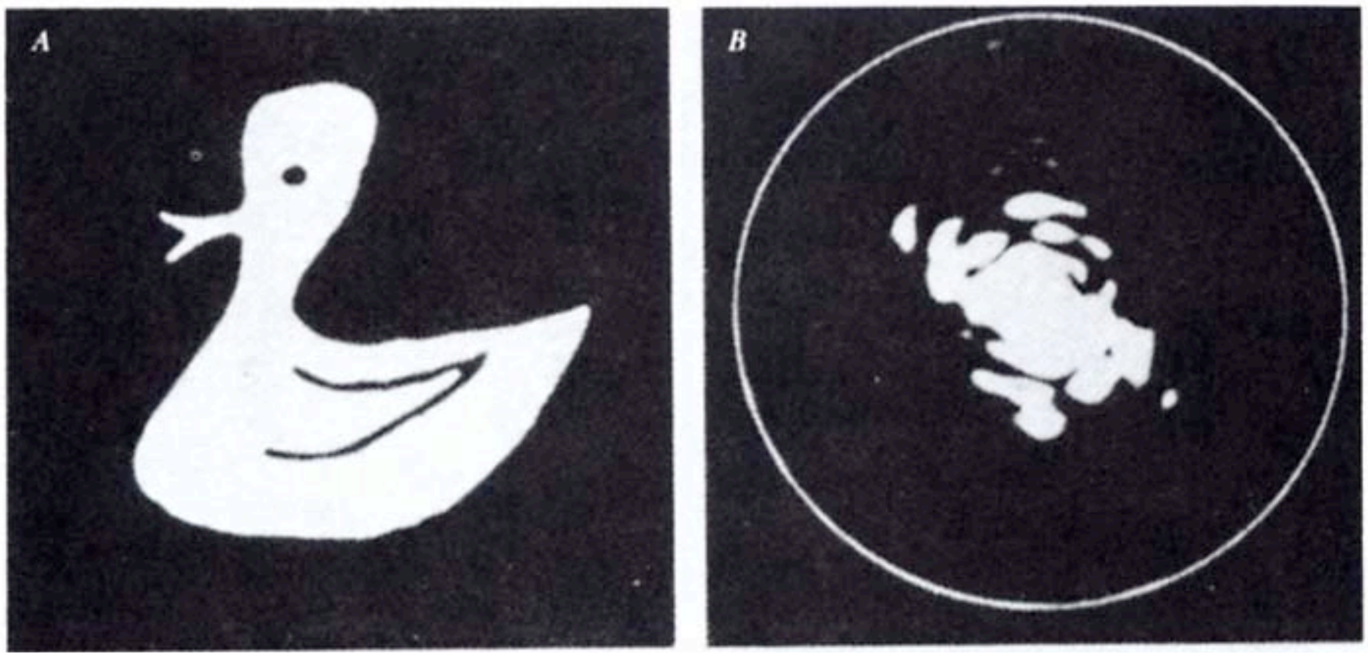
More complex 2-D images and transforms



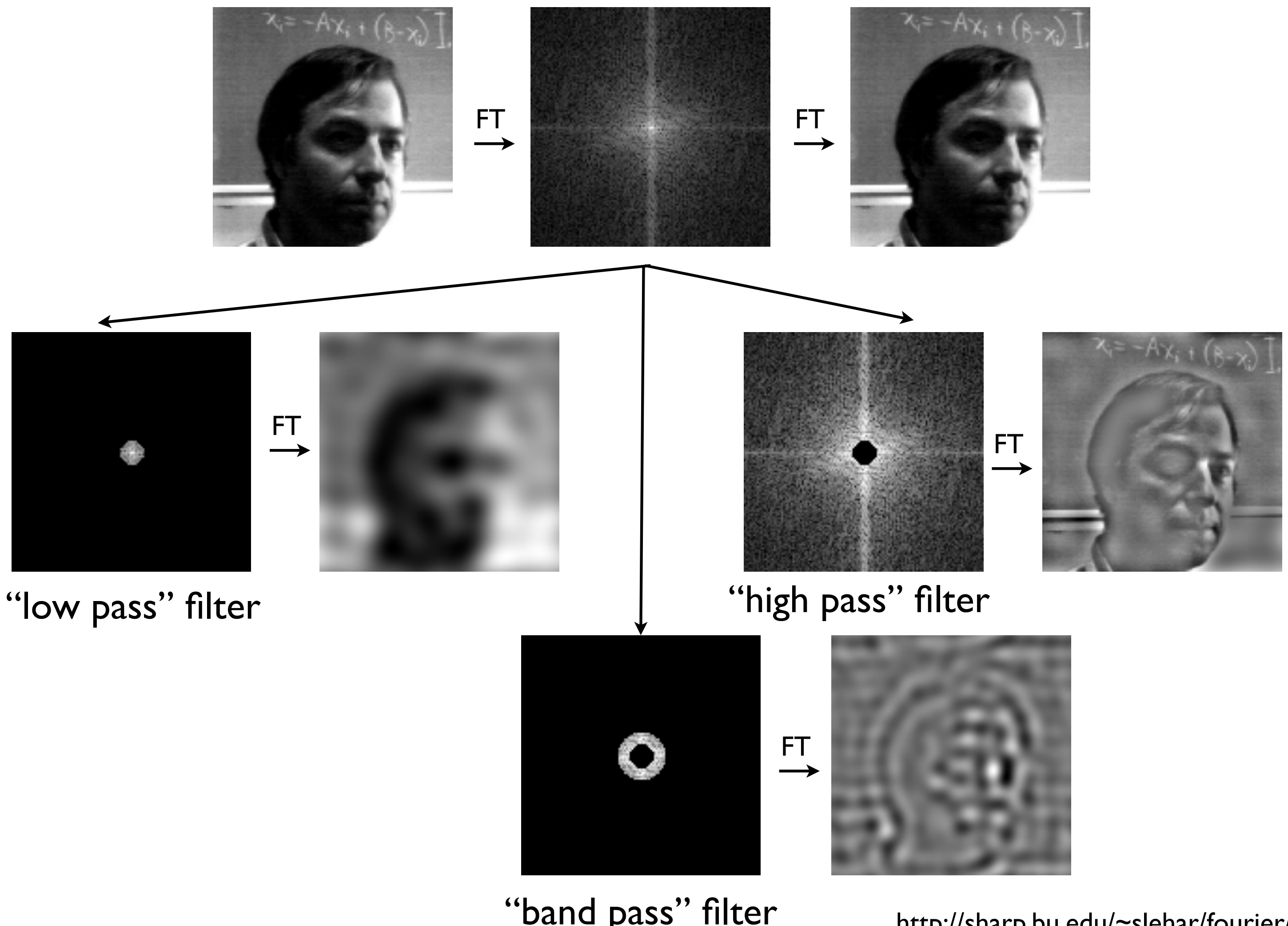


Briegel et al.,
PNAS 2009

“Resolution”



Note here the “power” or intensity of each Fourier component is being plotted, not the phase, and for any real image, the pattern is symmetric



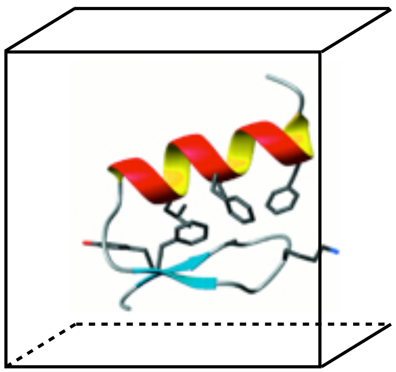
http://sharp.bu.edu/~slehar/fourier/fourier.html

Two-dimensional transforms and filters
Concept check questions:

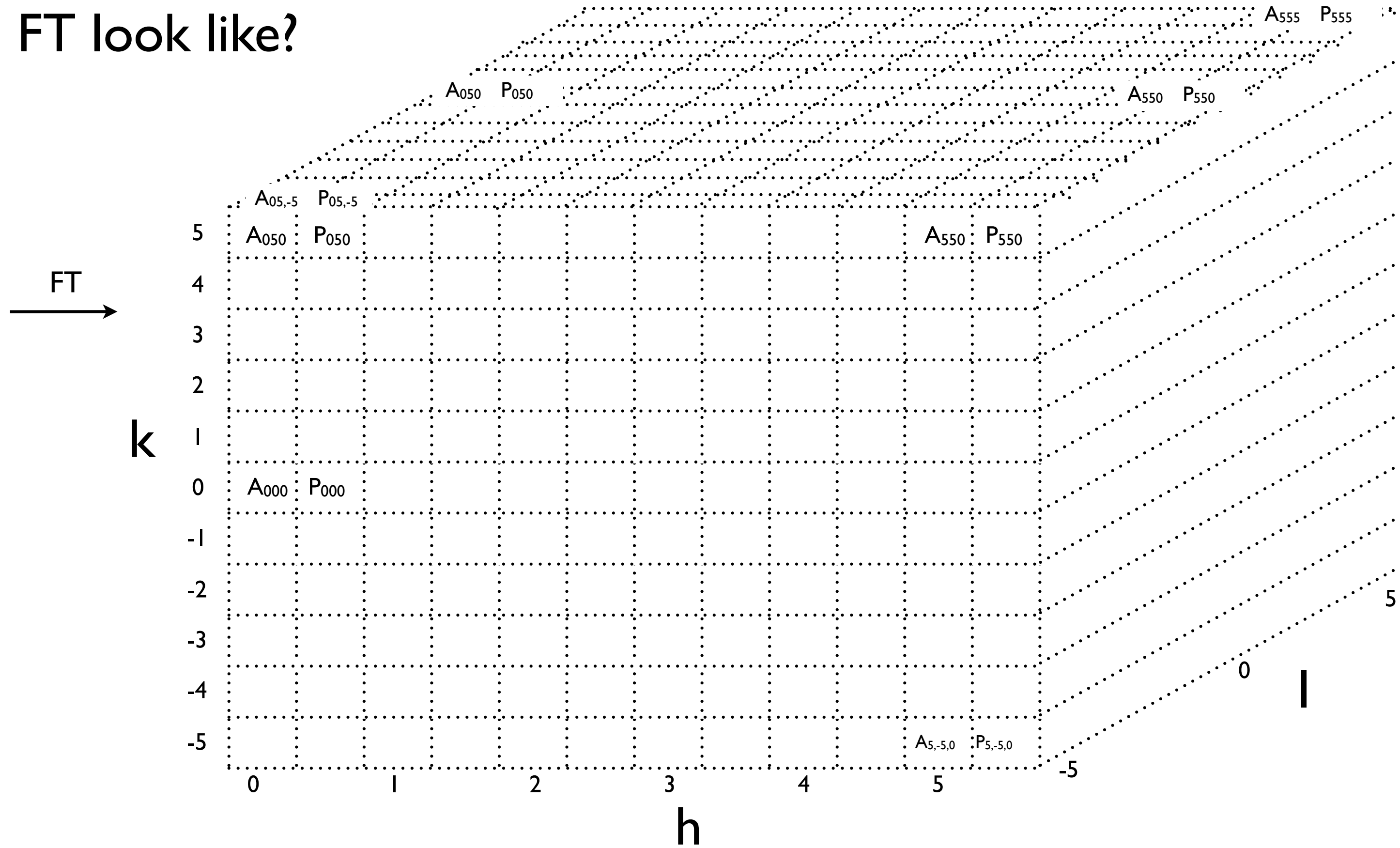
- In the Fourier transform of a real image, how much of reciprocal space (positive and negative values of "h" and "k") is unique?
- If an image "I" is the sum of several component images, what is the relationship of its Fourier transform to the Fourier transforms of the component images?
- What part of a Fourier transform is not displayed in a power spectrum?
- What does the "resolution" of a particular pixel in reciprocal space refer to?
- What is a "low pass" filter? "High pass"? "Band pass"?

In X-ray crystallography,
3-D microscopy, and 3-D NMR
we deal with 3-D images and transforms

What does a 3-D FT look like?



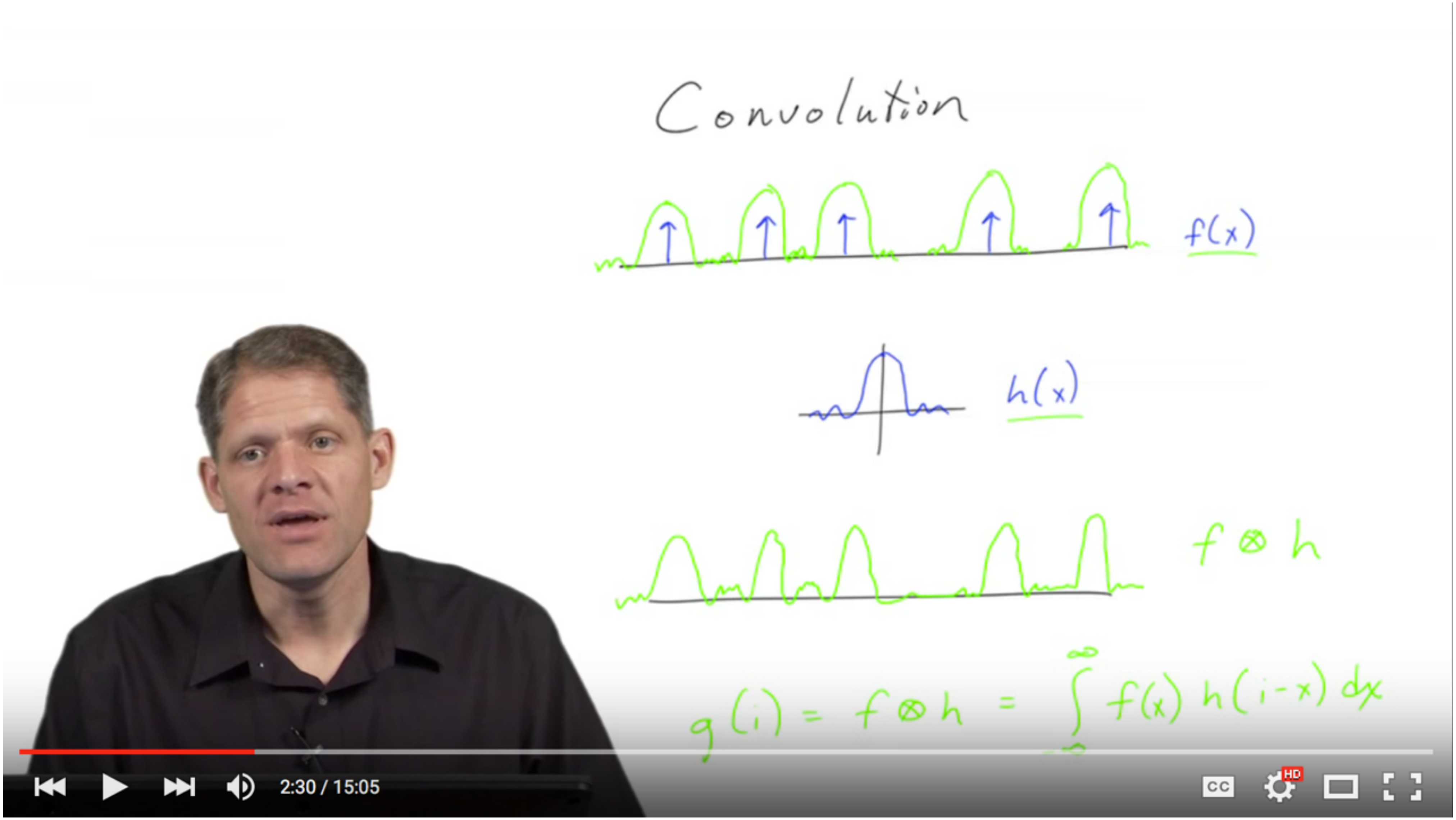
N^3 numbers



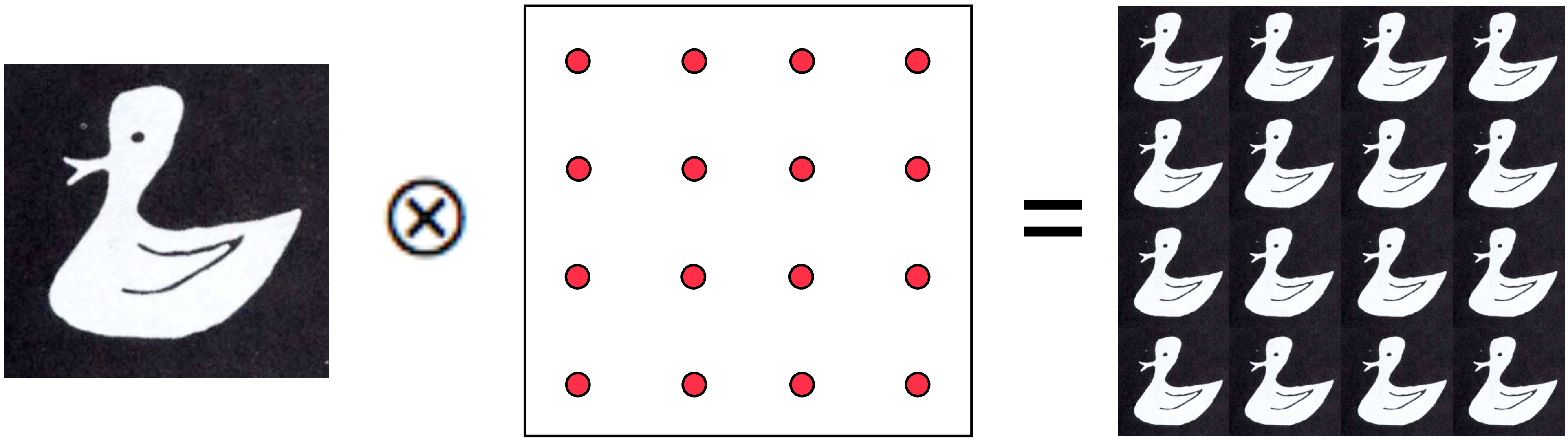
~N^3 numbers

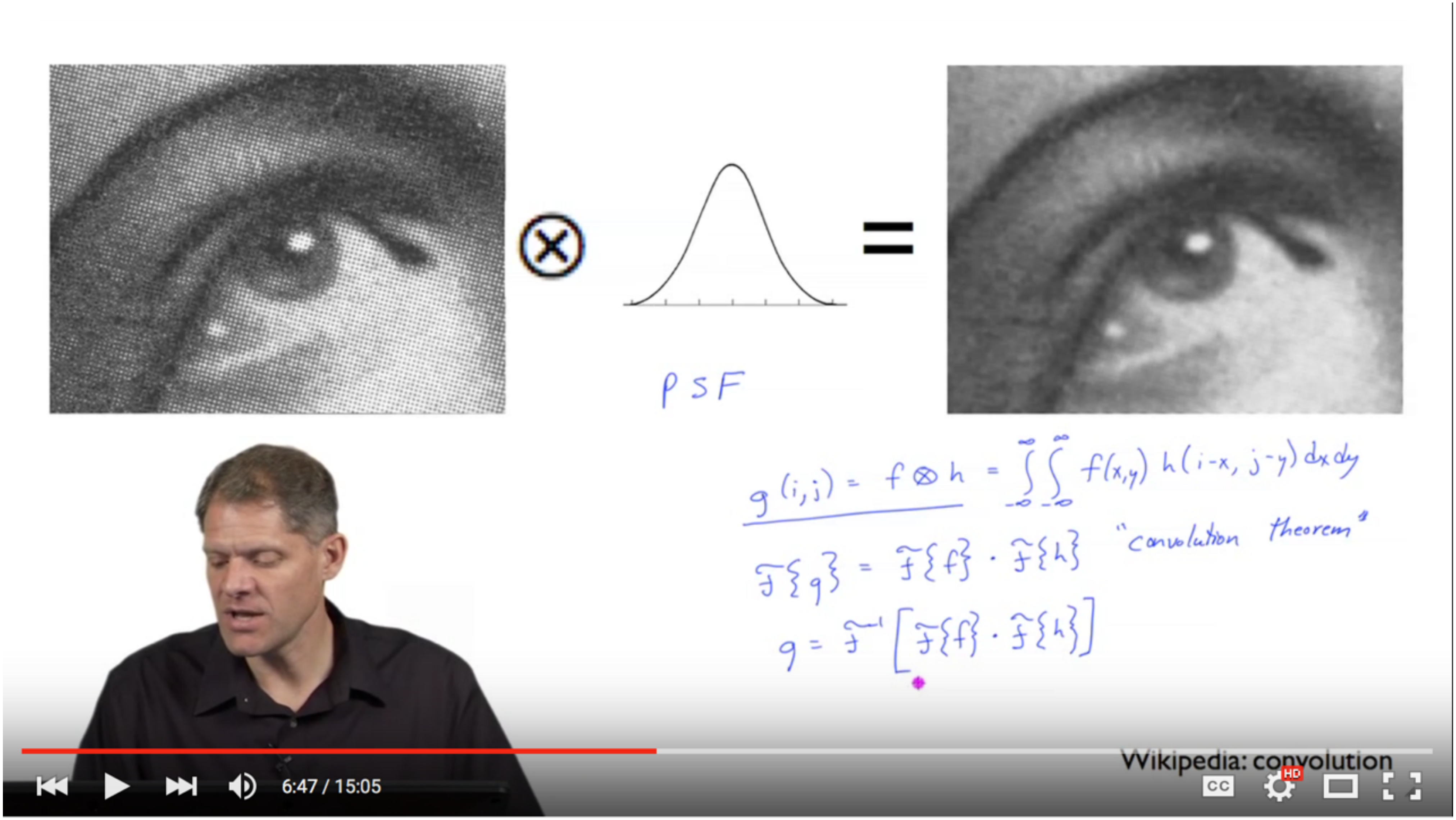
Three-dimensional waves and transforms Concept check questions:

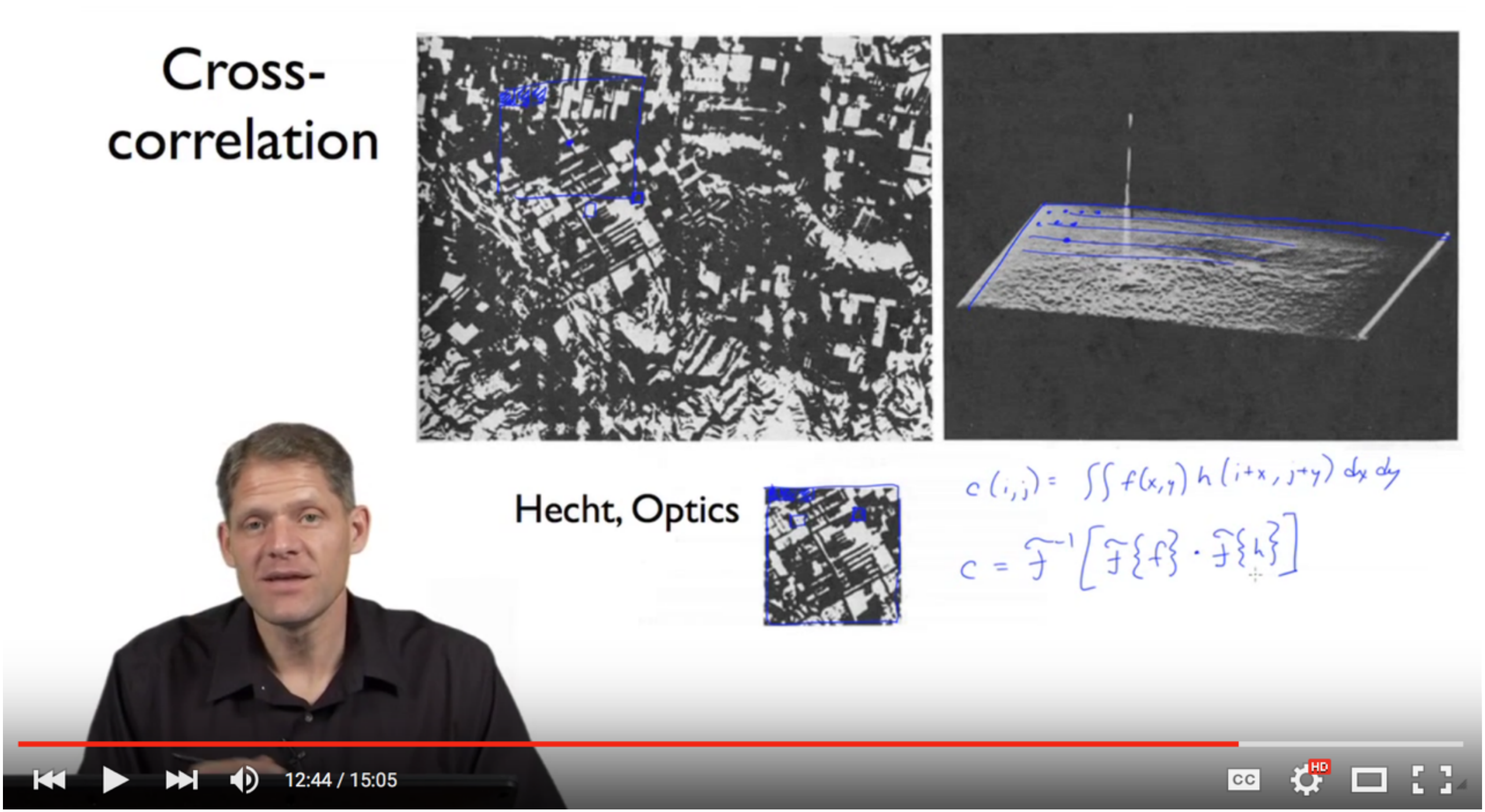
- What does a three-dimensional sine wave look like?
- What does the third "Miller" index "l" represent?

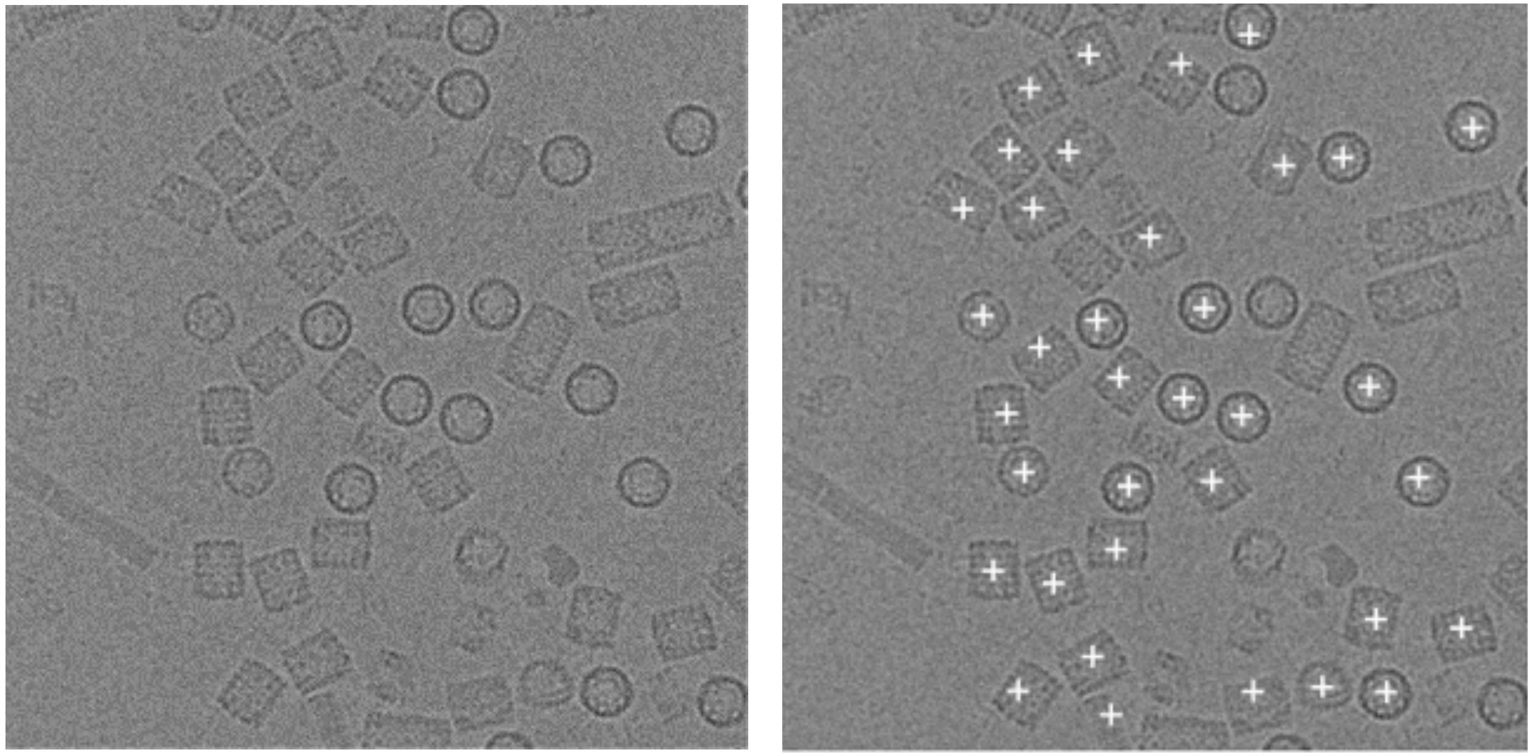

Convolution
f(x)
h(x)
f ⊗ h
g(i) = f ⊗ h = ∫ f(x) h(i-x) dx
2:30 / 15:05

Convolution




PSF
g(i,j) = f ⊗ h = ∫∫ f(x,y) h(i-x, j-y) dx dy
ℱ{g} = ℱ{f} · ℱ{h}
"convolution theorem"
g = ℱ⁻¹[ℱ{f} · ℱ{h}]
Wikipedia: convolution
6:47 / 15:05
CC
HD


Cross-correlation
Hecht, Optics
$c(i,j) = \iint f(x,y)\, h(i+x, j+y)\, dx\, dy$
$c = \mathcal{F}^{-1}\left[\mathcal{F}\{f\} \cdot \mathcal{F}\{h\}\right]$
12:44 / 15:05
CC
HD



Zhu et al., JSB 2004

Convolution and cross-correlation
Concept check questions:

- What is a “convolution”?
- What is the “convolution theorem”?
- What is a “point spread function”?
- What does convolution have to do with the structure of crystals?
- What is “cross-correlation”?
- How might cross-correlations be used in cryo-EM?