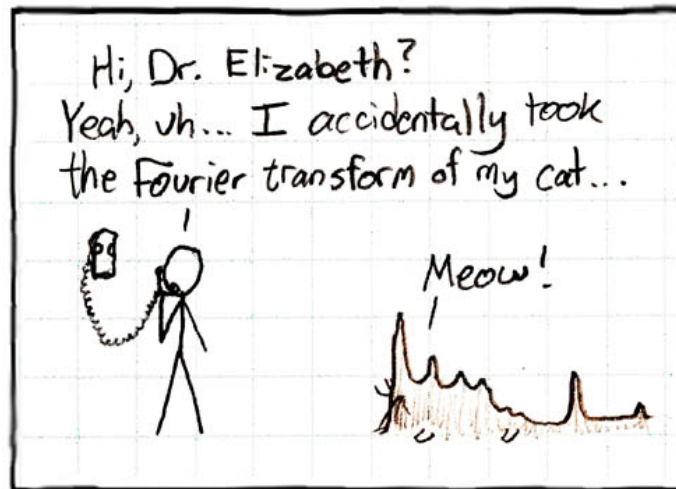


Fourier Transforms and Image Formation

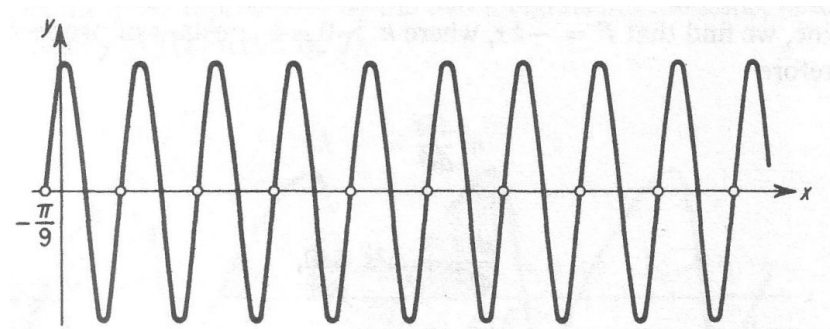


Essential Concepts

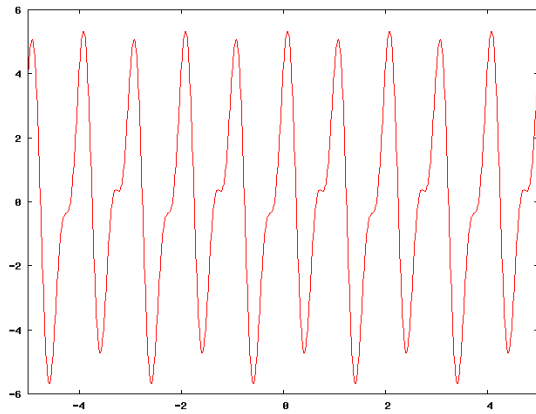
- Information from viewing FFT
- Four essential 1D Fourier transform mates
- Convolution theorem, correlation
- Sampling and Nyquist limit
- Projection theorem

Sine Wave

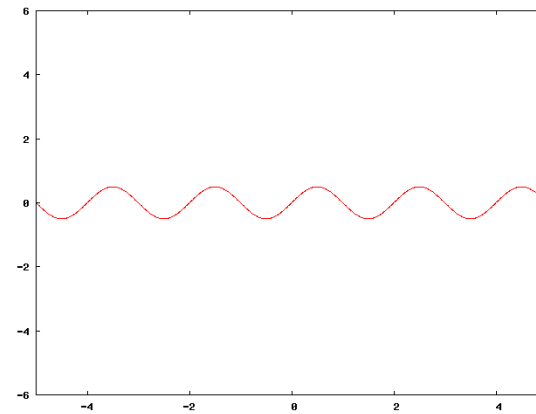
- $y = 2 \sin(3x + \frac{\pi}{3})$



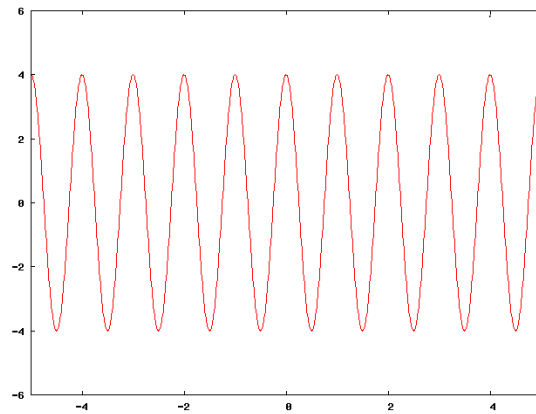
Fourier Series



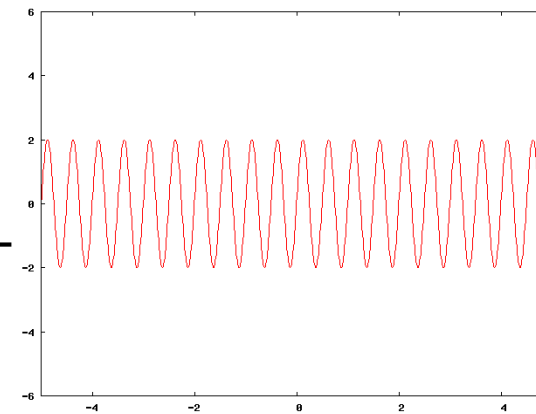
=



+

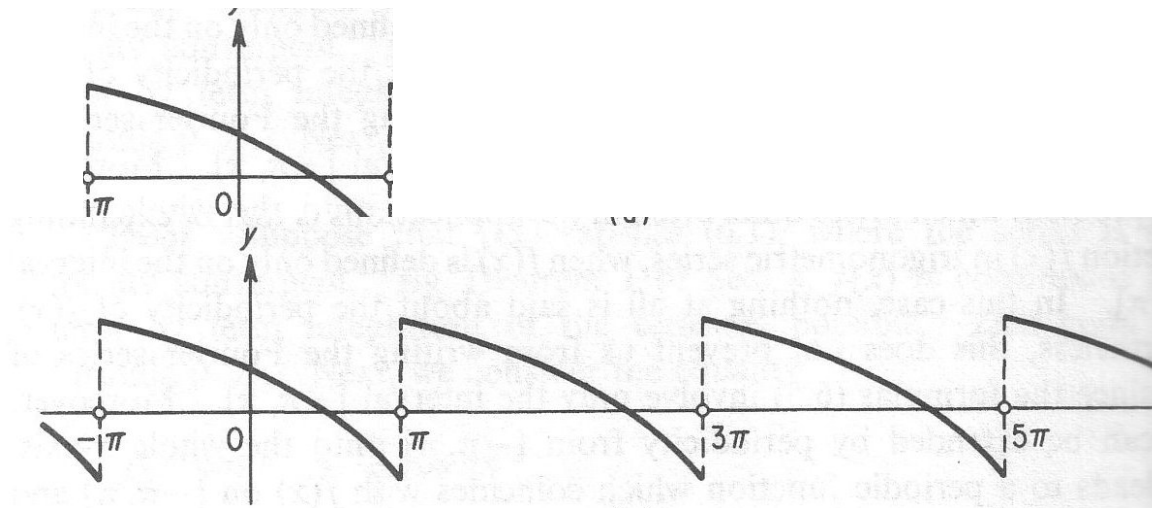


+



Fourier Series

- Non-periodic Functions
- For functions which are defined only on the interval $[-\pi, \pi]$, we extend the function by periodicity onto the whole x-axis:



Conventions

- **Image domain**

- Real space
- $f(x,y)$
- $f(r,\theta)$
- $f(t)$

- **Fourier Domain**

- Fourier Space
- Inverse space
- Reciprocal space
- Diffraction space
- $F(X,Y)$, $F(k_x,k_y)$
- $F(k,\Theta)$
- $H(\omega)$

Important Transform Pairs

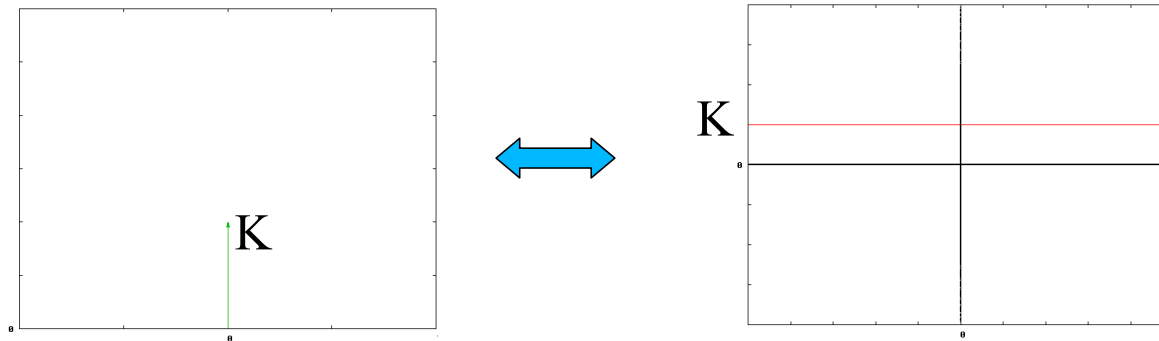
- Delta
- Top-hat
- Comb
- Gaussian

Fourier transform of a delta function

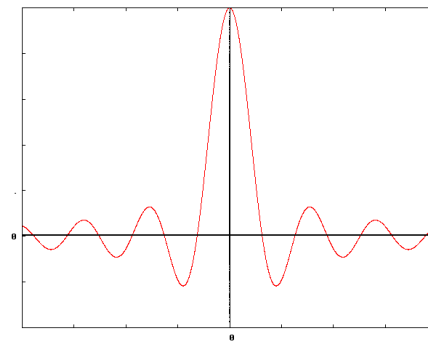
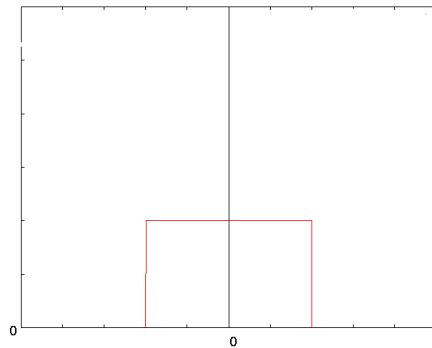
$$h(t) = K\delta(t)$$

$$H(f) = \int_{-\infty}^{\infty} K\delta(t)e^{-2\pi ift} dt$$

$$H(f) = K$$



Top-hat function

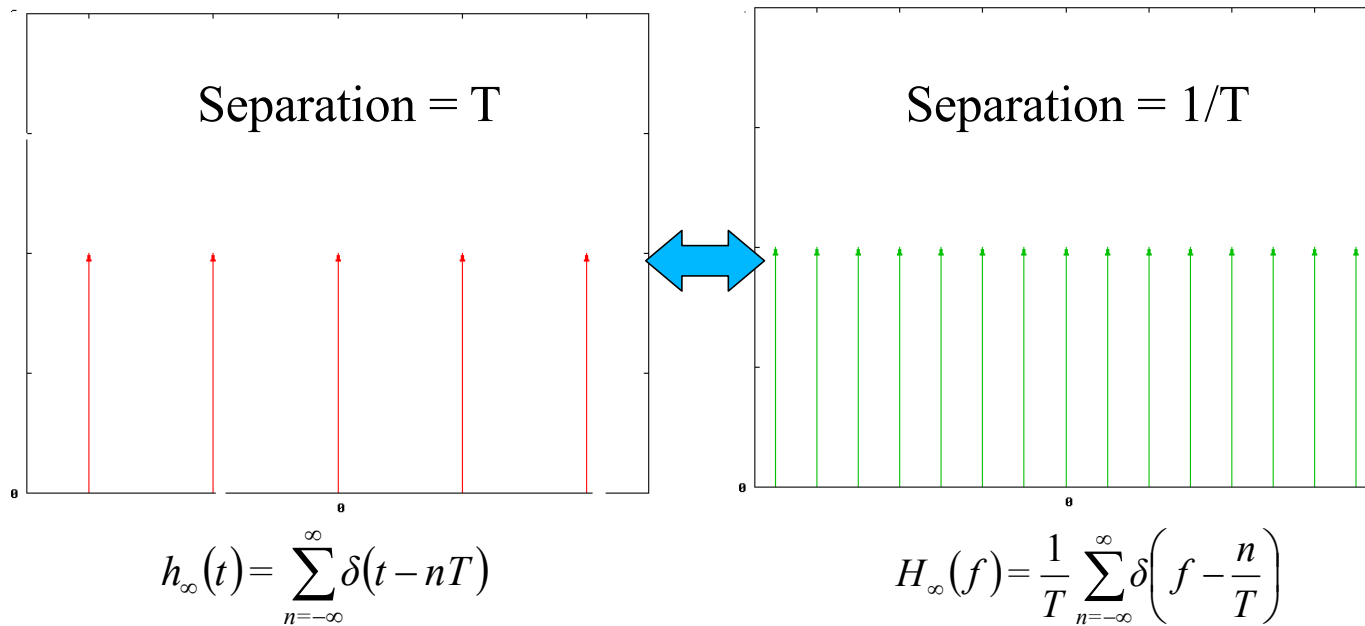


$$H(X) = \frac{\sin \pi X}{\pi X}$$

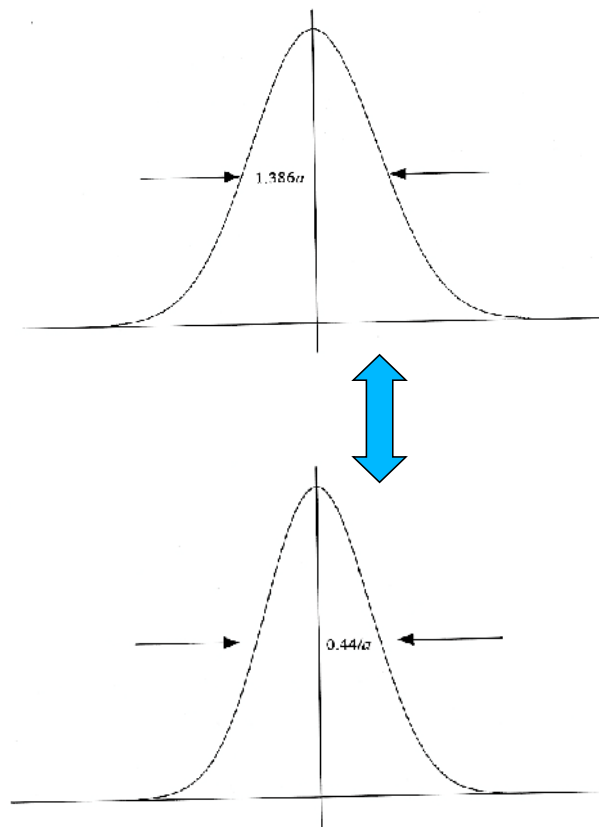
sinc function

Comb function

- Infinite points on comb



Gaussian Function



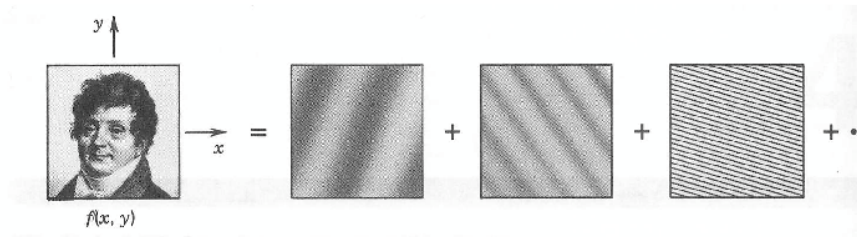
width= a

width= $1/a$

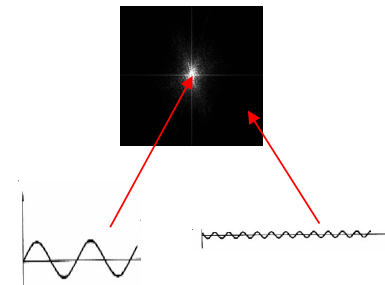
Images: Extending transforms into 2d

- Consider images as a 2 dimensional function of x and y , where the value of $f(x,y)$ is represented as brightness

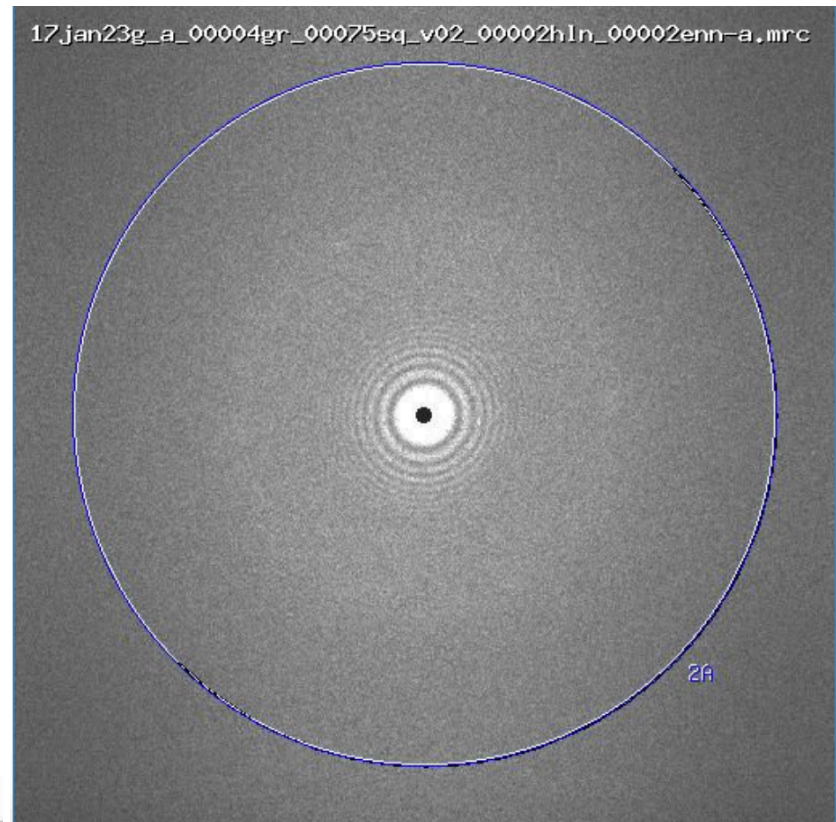
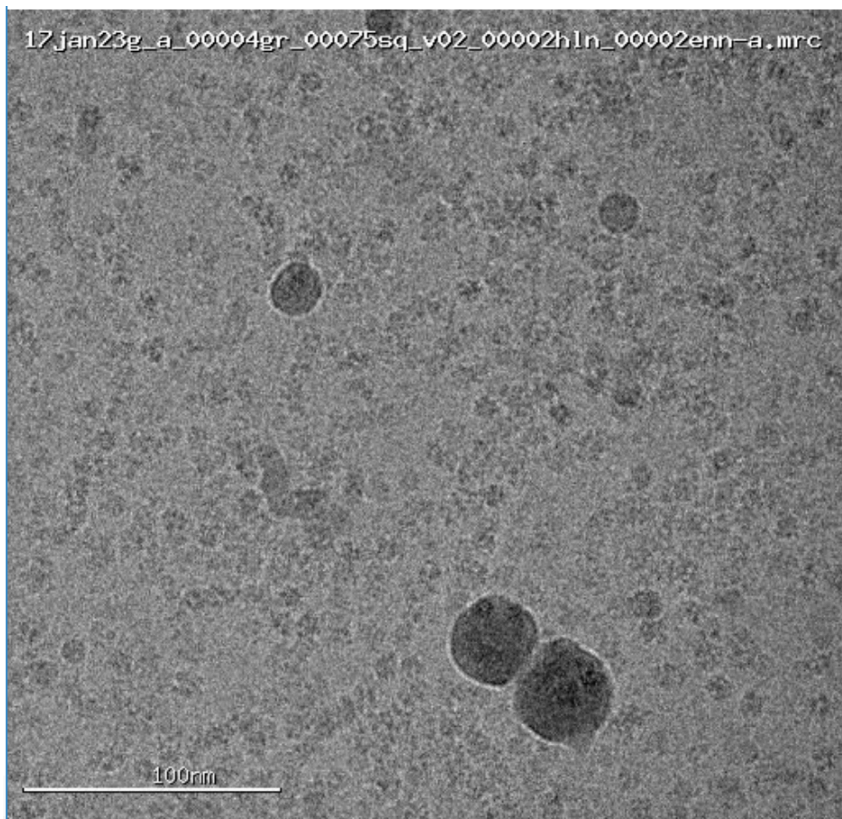
2D Fourier transform



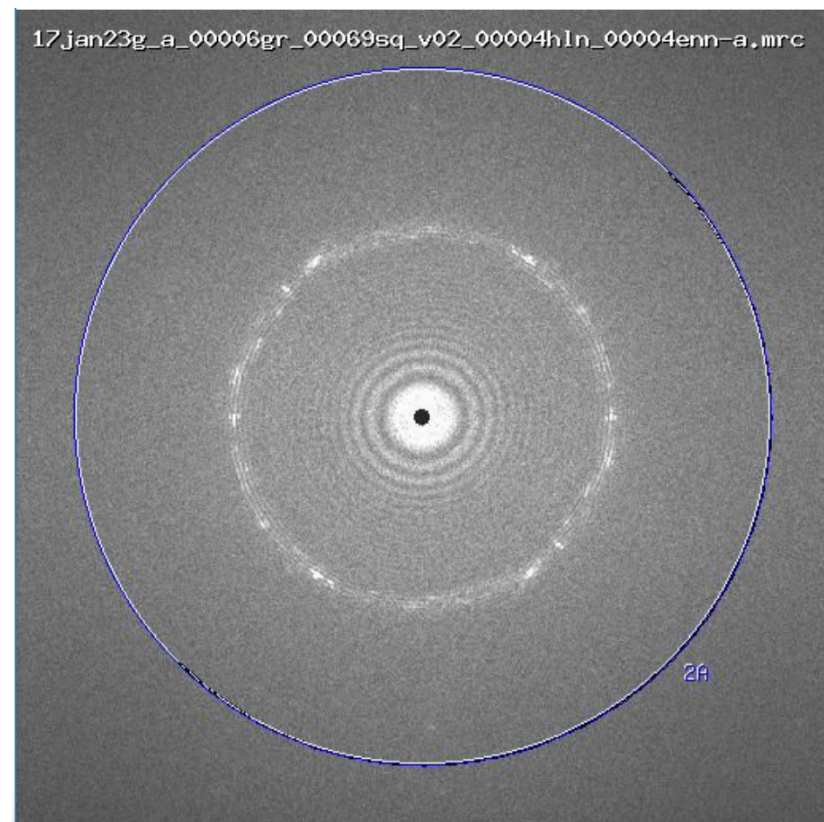
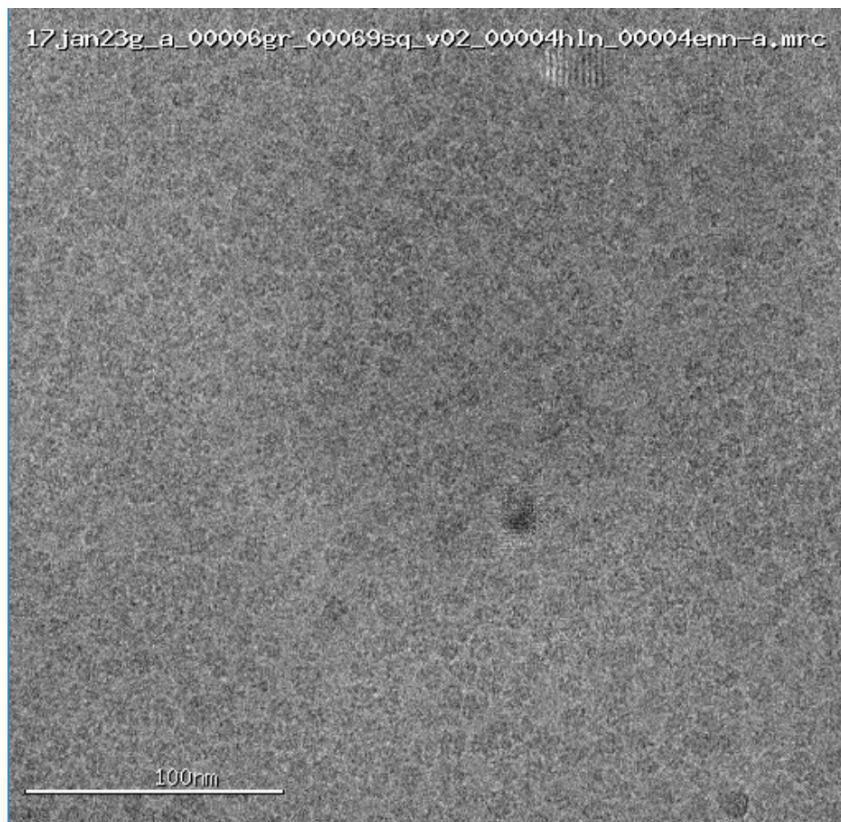
$$F(K_x, K_y) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x, y) \exp(i(K_x x + K_y y)) dx dy$$



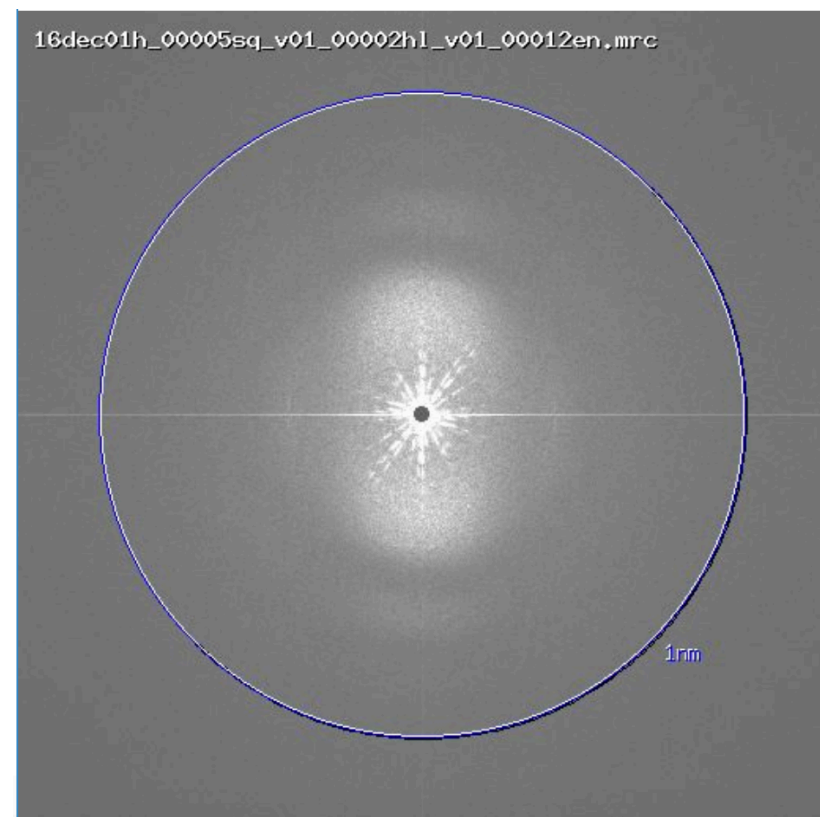
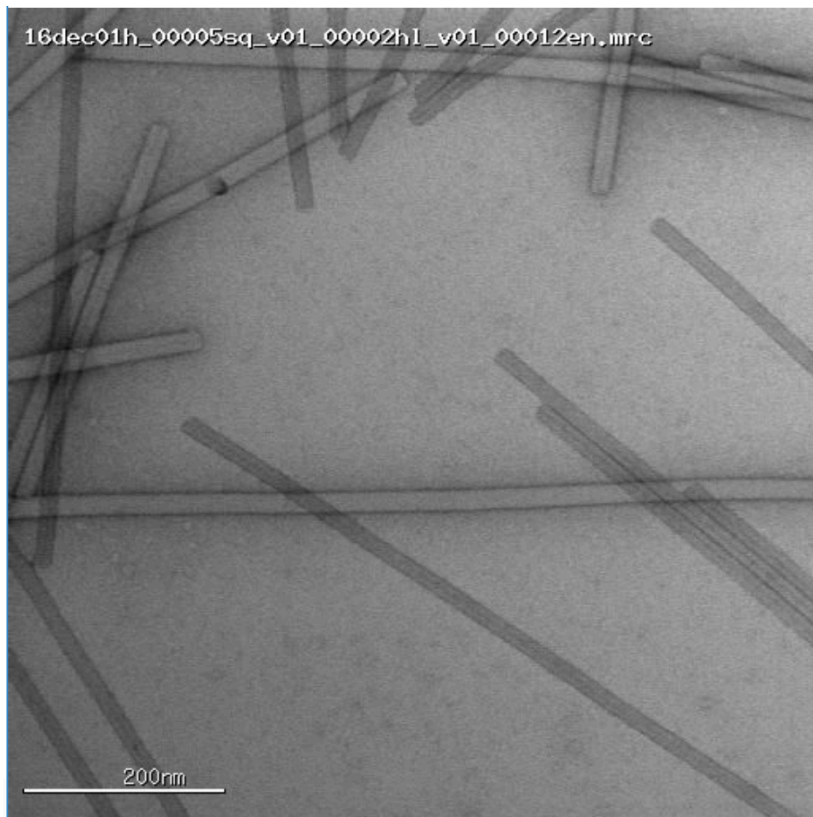
Information from visualizing FFT



Information from visualizing FFT



Information from visualizing FFT



Importance of Phase and Amplitude

1



Calculate FFT

Keep amplitude

2



Calculate FFT

Keep phase

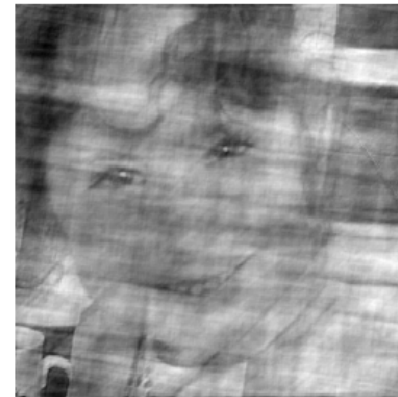
Importance of Phase and Amplitude

1



Amplitude of object 1
Phase of object 2

Inverse FT

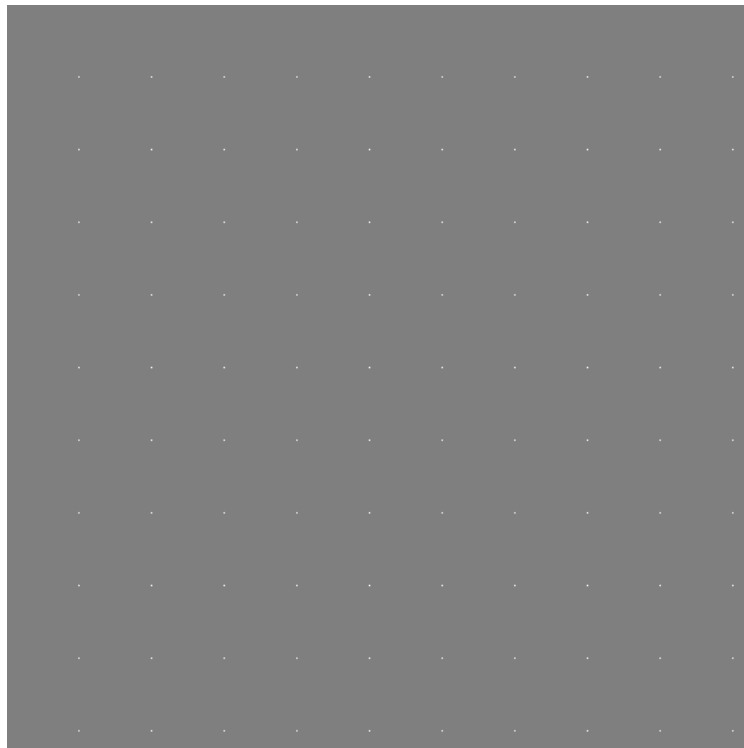


2



Reconstituted image is dominated by phase

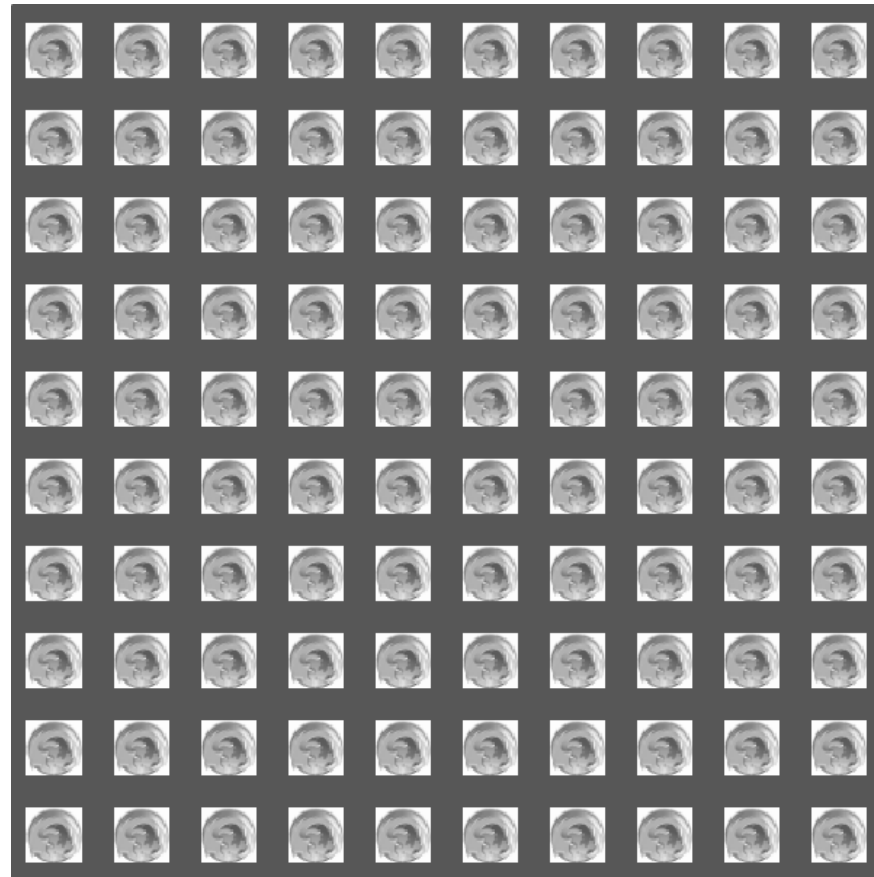
Convolution with set of delta functions



*

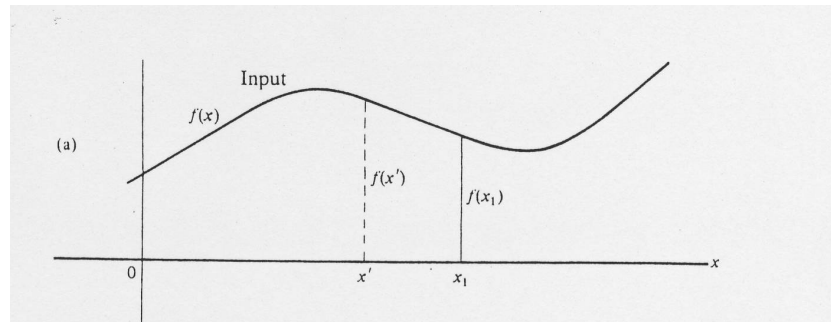


Convolution with set of delta functions



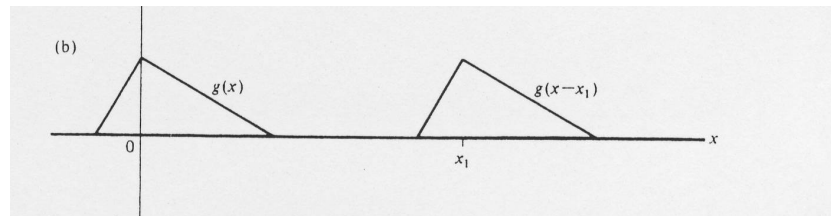
Convolution

Say we have a function $f(x)$



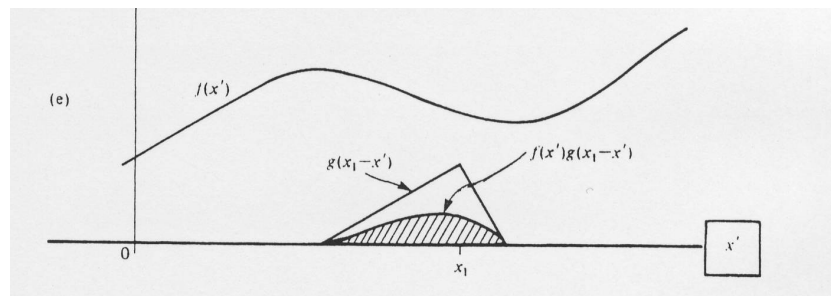
input to a device

and another function $g(x)$



scanning function

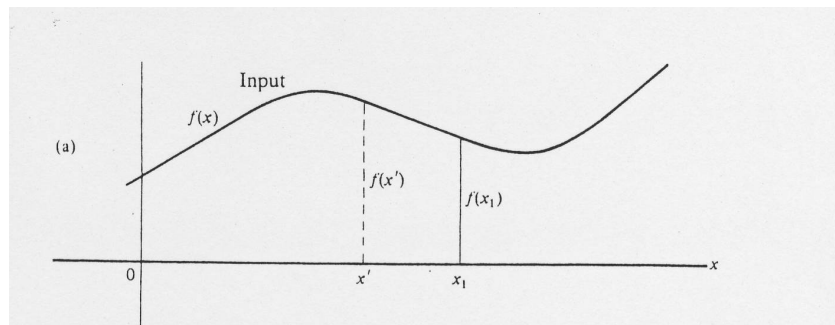
$g(x)$ is imperfect, and “smears” $f(x)$



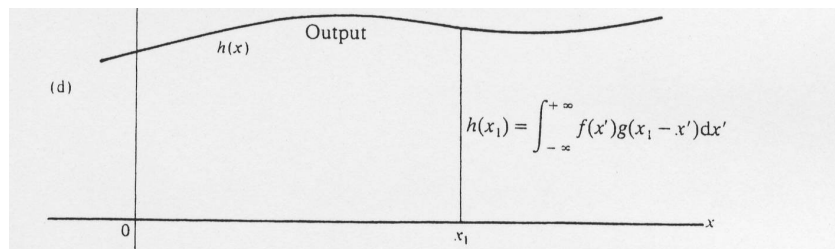
Slide the function $g(x)$ along the curve of $f(x)$

Point at x_1 is replaced by value of shaded integral

Convolution



Input



resultant output

Convolution Theorem

if $h(x) = f(x) * g(x)$

then $H(X) = F(X) \times G(X)$

Conversely,

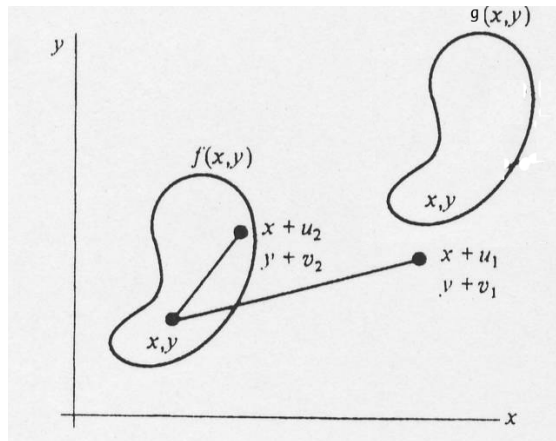
If $H(X) = F(X) * G(X)$

$$h(x) = f(x) \times g(x)$$

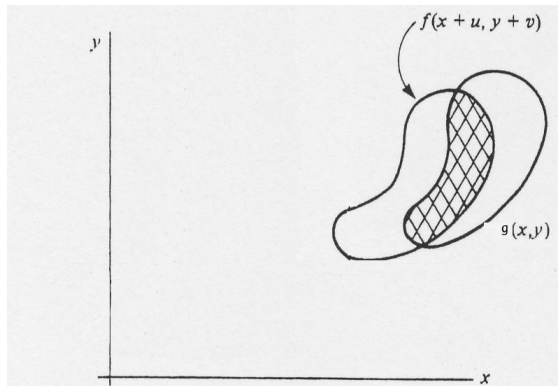
Convolution is easy to calculate:

take FT of each function, multiply, then take inverse FT

Correlation



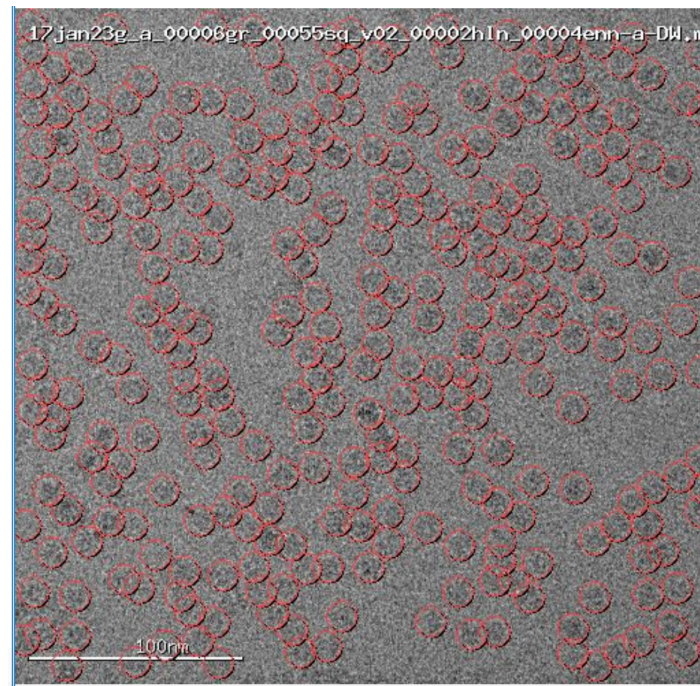
“slide” $f(x,y)$ over $g(x,y)$ and calculate overlap









formally, calculate a function P

$$P(x, y) = \iint_{-\infty}^{\infty} f(x', y') g(x' - x, y' - y) dx' dy'$$

Example: Particle Picking



	<input type="checkbox"/> Use Template 1		<input type="checkbox"/> Use Template 2
Template ID: 9 Diameter: 110 Å Pixel Size: 3.41962 Å	Rotation values (leave blank for no rotation): 0 Starting Angle 180 Ending Angle 30 Angular Increment	Template ID: 8 Diameter: 110 Å Pixel Size: 3.41962 Å	Rotation values (leave blank for no rotation): 0 Starting Angle 180 Ending Angle 30 Angular Increment
	<input type="checkbox"/> Use Template 3		<input type="checkbox"/> Use Template 4
Template ID: 7 Diameter: 110 Å Pixel Size: 3.41962 Å	Rotation values (leave blank for no rotation): 0 Starting Angle 180 Ending Angle 30 Angular Increment	Template ID: 6 Diameter: 110 Å Pixel Size: 3.41962 Å	Rotation values (leave blank for no rotation): 0 Starting Angle 180 Ending Angle 30 Angular Increment
	<input type="checkbox"/> Use Template 5		<input type="checkbox"/> Use Template 6
	Rotation values (leave blank for no rotation): 0 Starting Angle 120 Ending Angle 30 Angular Increment		Rotation values (leave blank for no rotation): 0 Starting Angle 180 Ending Angle 30 Angular Increment

Correlation and Convolution

$$h(x) = \int_{-\infty}^{\infty} f(x')g(x - x')dx \quad \text{Convolution}$$

$$p(x) = \int_{-\infty}^{\infty} f(x')g(x' - x)dx \quad \text{Correlation}$$

Convolution Theorem

$$h(x) = \text{FT}^{-1} \{F(X)G(X)\}$$

$$p(x) = \text{FT}^{-1} \{F(X)G^*(X)\}$$

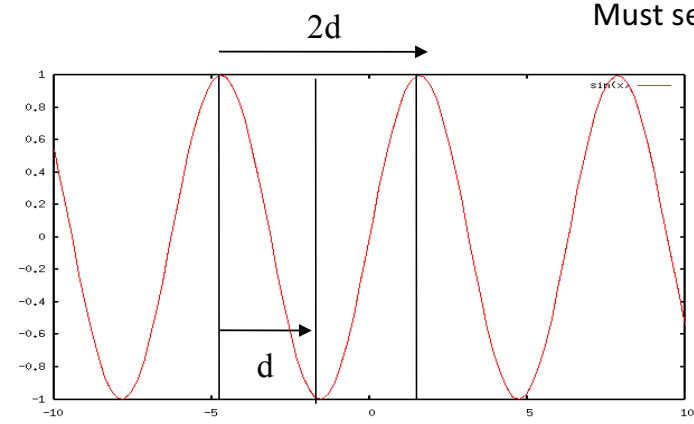
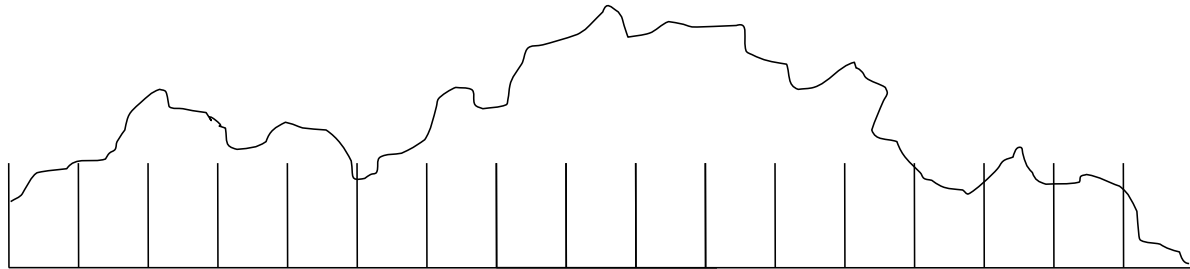
$G^*(X)$: complex conjugate of $G(X)$

Complex conjugate:

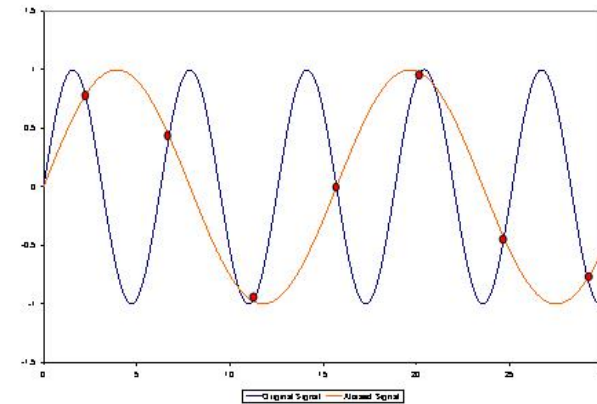
if $x = a + ib$, $x^* = a - ib$

Image sampling (for digital FT)

Shannon-Nyquist sampling limit:
Finest spatial period must be sampled $>2x$
Otherwise \rightarrow aliasing

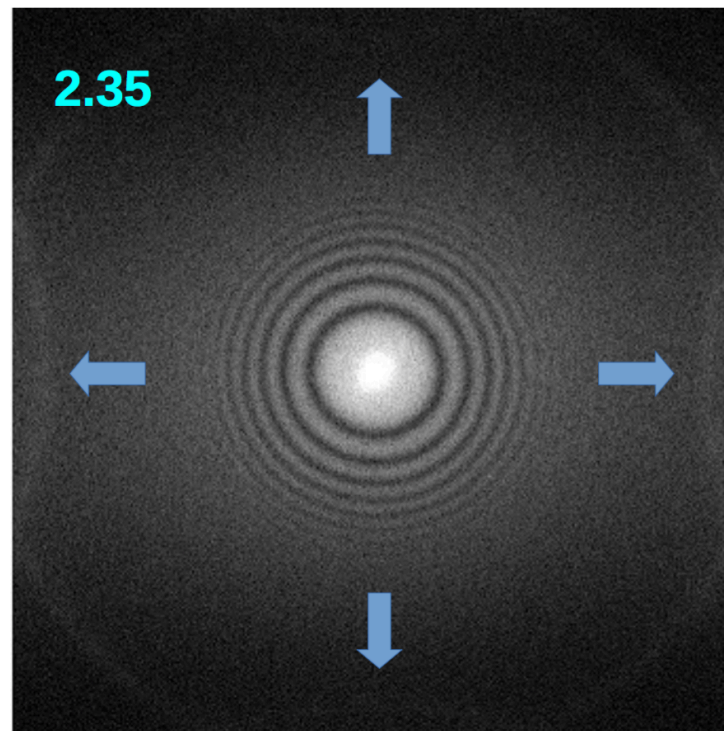


A minimally sampled image



Undersampled

30K: Gold Aliases Back into Image

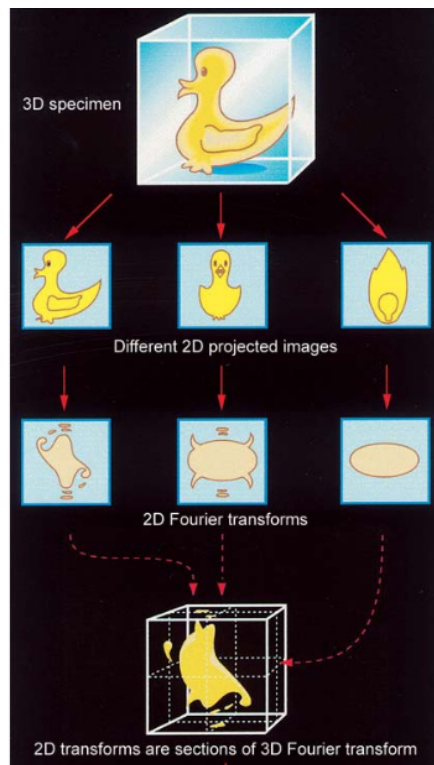


Pixel Size: 1.2 Å

Aliasing

- By sampling our function (image) at scanning frequency s , we are essentially multiplying by a set of delta functions with spacing s .
- Therefore in Fourier space, we are convoluting with a set of delta functions with spacing $1/s$

Projection Theorem (Central Slice Theorem)



From Baker and Henderson (2012), International Tables of Crystallography Vol. F, Ch. 19.6, pp. 593-614.

Fourier Inversion



Questions

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?

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?



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?

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"?

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?

Details

Fourier Series

- Final Fourier series expansion (after removing 2π):

- $$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} (a_k \cos kx + b_k \sin kx)$$

Terms a_k and b_k :

$$a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx$$

$$a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos kx \, dx$$

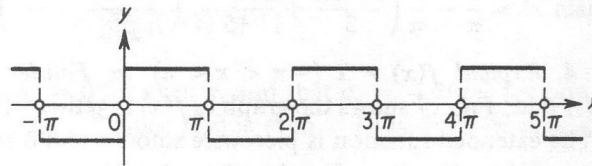
$$b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin kx \, dx$$

Fourier Series

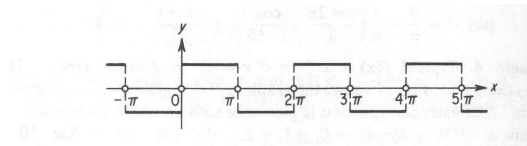
- Example: Determine the terms for the Fourier series expansion of
- $f(x) = -1, -\pi < x < 0$
- $f(x) = 0, x = (0, -\pi, \pi)$
- $f(x) = 1, 0 < x < \pi$

Reference:

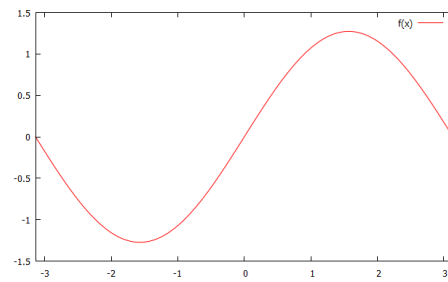
Fourier Series by Georgi P Tolstov
Translated by Richard A Silverman
Dover Publications Inc :
New York (1972)



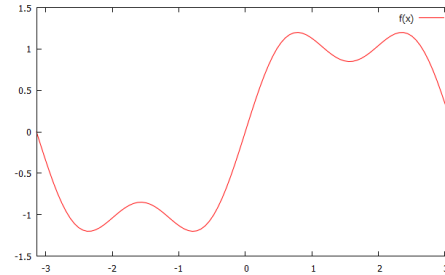
Fourier Series



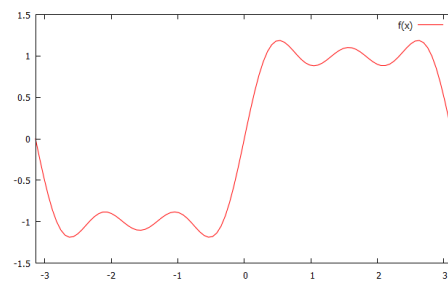
$$(f(x) = \frac{4}{\pi} (\sin x + \sin \frac{3x}{3} + \sin \frac{5x}{5} + \dots))$$



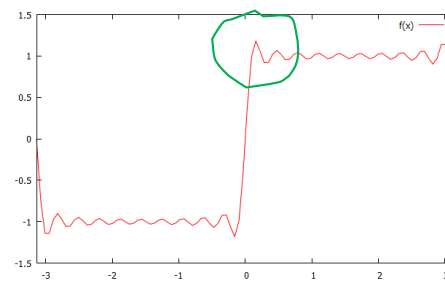
1 term



2 terms



3 terms



10 terms

Fourier Series: complex form

- From the Euler equation

- $e^{i\varphi} = \cos\varphi + i \sin\varphi$

- Can derive

- $\cos kx = \frac{e^{ikx} + e^{-ikx}}{2}$

- $\sin kx = i \frac{-e^{ikx} + e^{-ikx}}{2}$

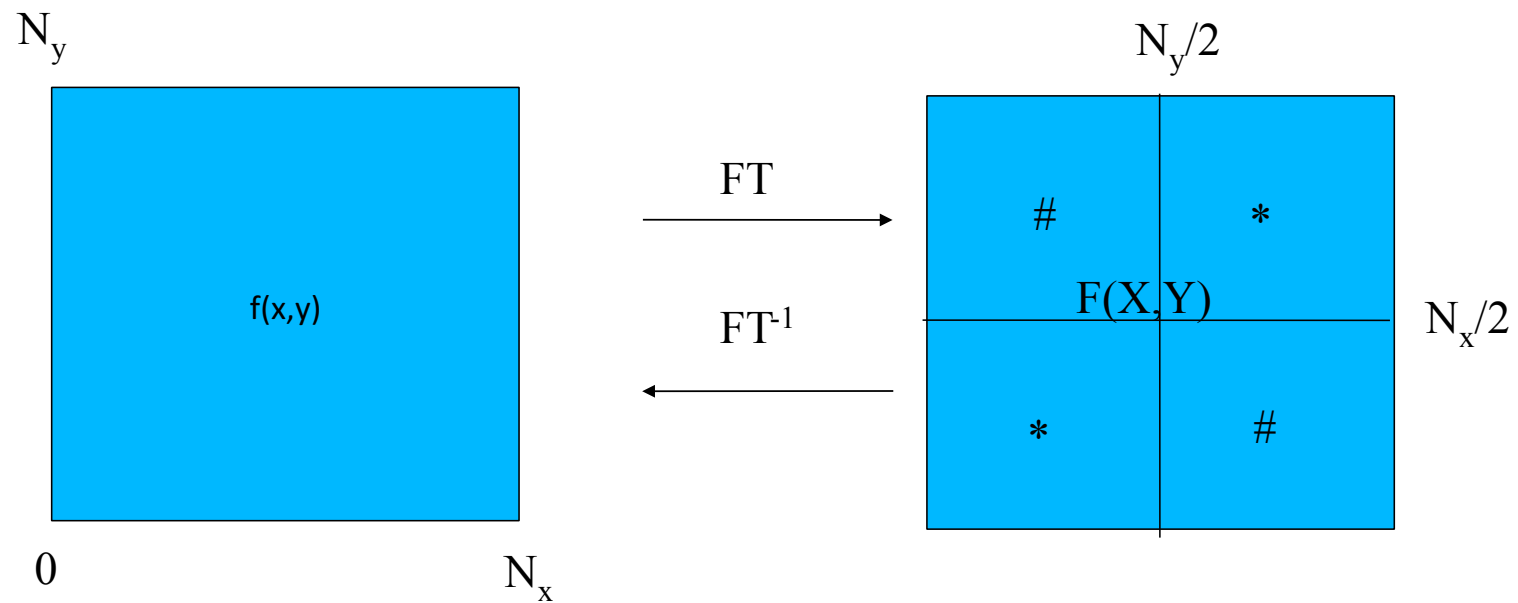
Fourier Transforms

- Take the limit of the series as period $l \rightarrow \infty$: (and much manipulation)
- $F(X) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i X x} dx$
- The inverse transform is:
- $f(x) = \int_{-\infty}^{\infty} F(X) e^{2\pi i x X} dX$
- The two equations are mates, and let you convert from real space to frequency space and back

Fourier Transforms of Images

- Computationally, images are a discrete matrix of points, and so the computer actually calculates the discrete Fourier transform (DFT)
- We are back to sums instead of integrals
- The Fast Fourier transform (FFT) is efficient: on order $n \log(n)$ rather than n^2 (Cooley and Tukey, 1965; Gauss 1805)
- Originally for n of power of 2, it can be calculated for all n , though power of 2 is simpler
- Generally only the amplitude is displayed

Fourier transform is an invertible operator

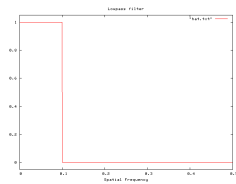


$*$, $\#$ - Friedel mates

Fourier Filters

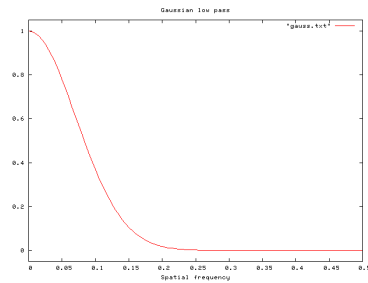
- Low pass filters
 - Restrict data to low frequency components
 - blurs out features (filter out high frequency noise)
- High pass filters
 - Restrict data to high frequency components
 - Eliminate gradients in images
- Band pass filters
 - Restrict data to a band of frequencies
- Band stop filters
 - suppress a band of frequencies

Low-pass filter



“ringing” effects caused by sharp mask

Gaussian Low-pass filter



Continuous or smoother mask prevents ringing

$$e^{-\frac{X^2}{2 \times RAD^2}}$$

Convolution

- If we have 2 functions $f(x)$ and $g(x)$
- The **convolution** of $f(x)$ with $g(x)$ is defined as
- $$h(x) = \int_{-\infty}^{\infty} f(x')g(x - x')dx'$$
- $$h(x) = f(x) * g(x)$$
- Reverse one function, offset it by x' (starting at $-\infty$), multiply by second function, and measure area under resultant curve. Slide from $-\infty$ to ∞ .

Further Reading

- Atlas of Optical Transforms by G. Harburn, C.A. Taylor, T.R. Welberry. Cornell University Press: Ithica, New York (1975)
- The Fourier Transform and its Applications, 2nd Edition by Ronald L. Bracewell. Mcgraw Hill Book Company: New York (1978)
- Fourier Optics: An Introduction (2nd Edition) by E.G. Steward. Dover Publications Inc.: Mineola, New York (2004)
- Fourier Series by Georgi P Tolstov (Translated by Richard A Silverman). Dover Publications Inc : New York (1972)