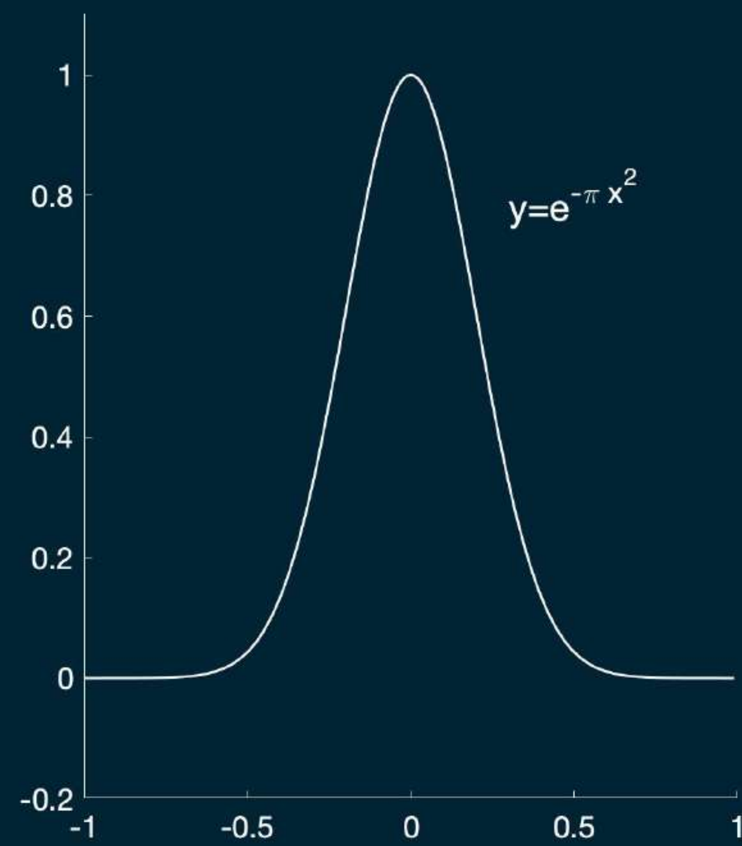
Cryo-EM Principles

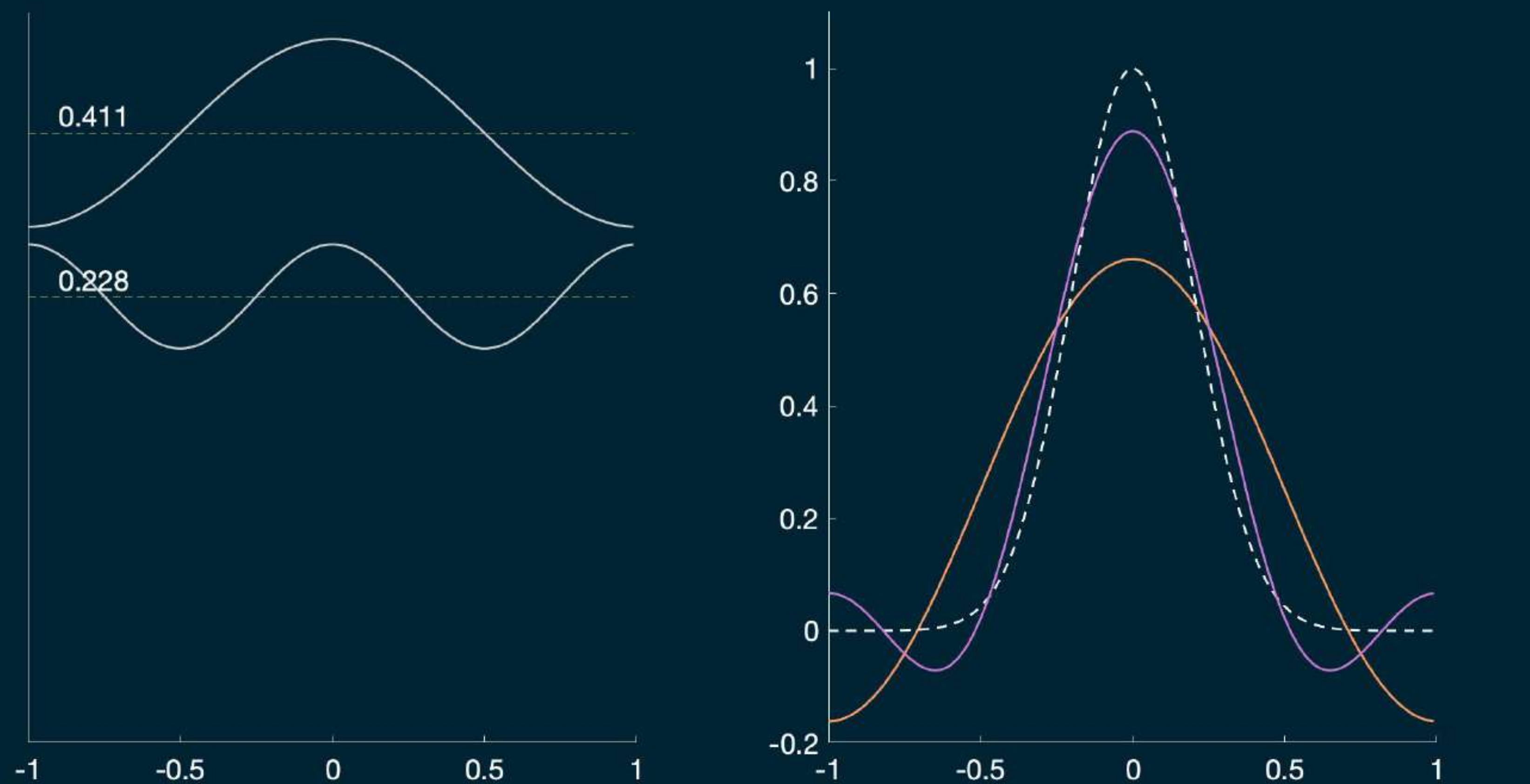
The Fourier Transform in One and More Dimensions

Fred Sigworth
Yale University

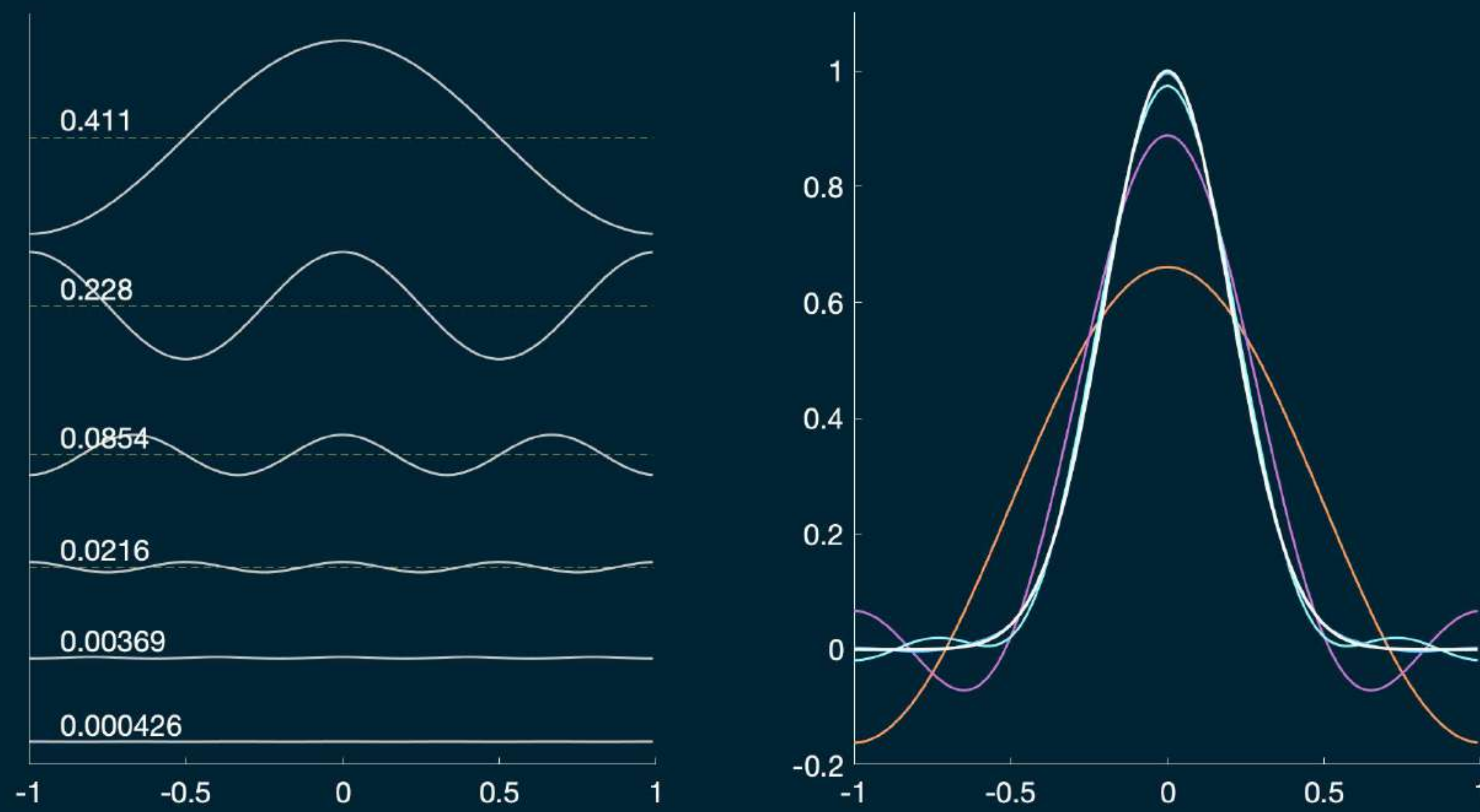
Fourier reconstruction of a Gaussian function



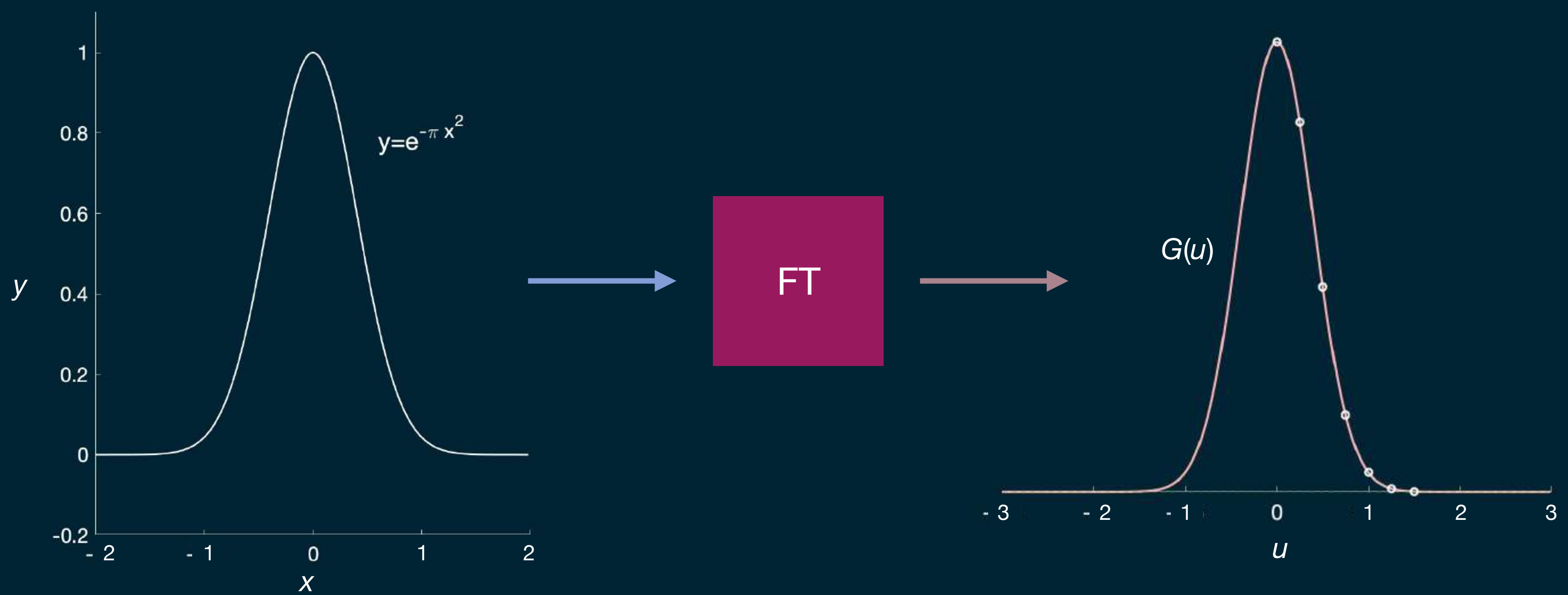
2 terms



“Converged” at 6 terms



The Fourier Transform gives us the coefficients



The formulas

Fourier transform

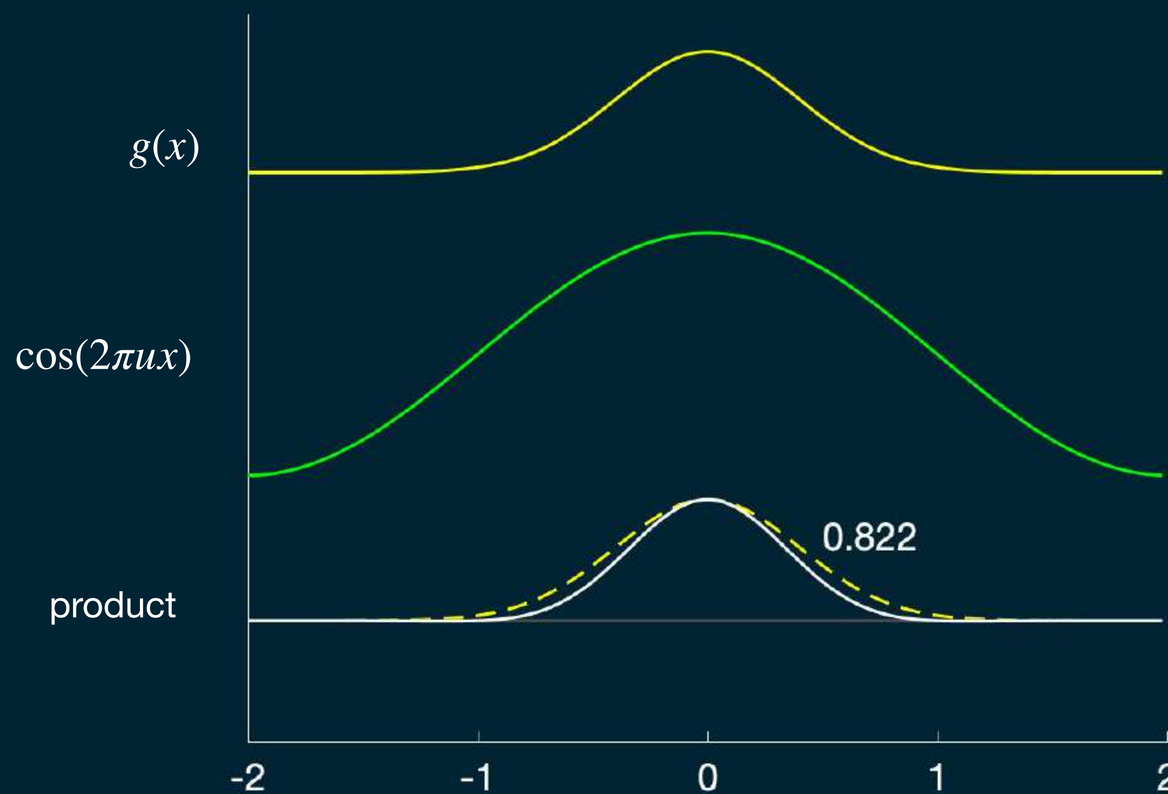
$$G(u) = \int g(x) e^{-i2\pi ux} dx$$

Example: $g(x) = e^{-\pi x^2}$

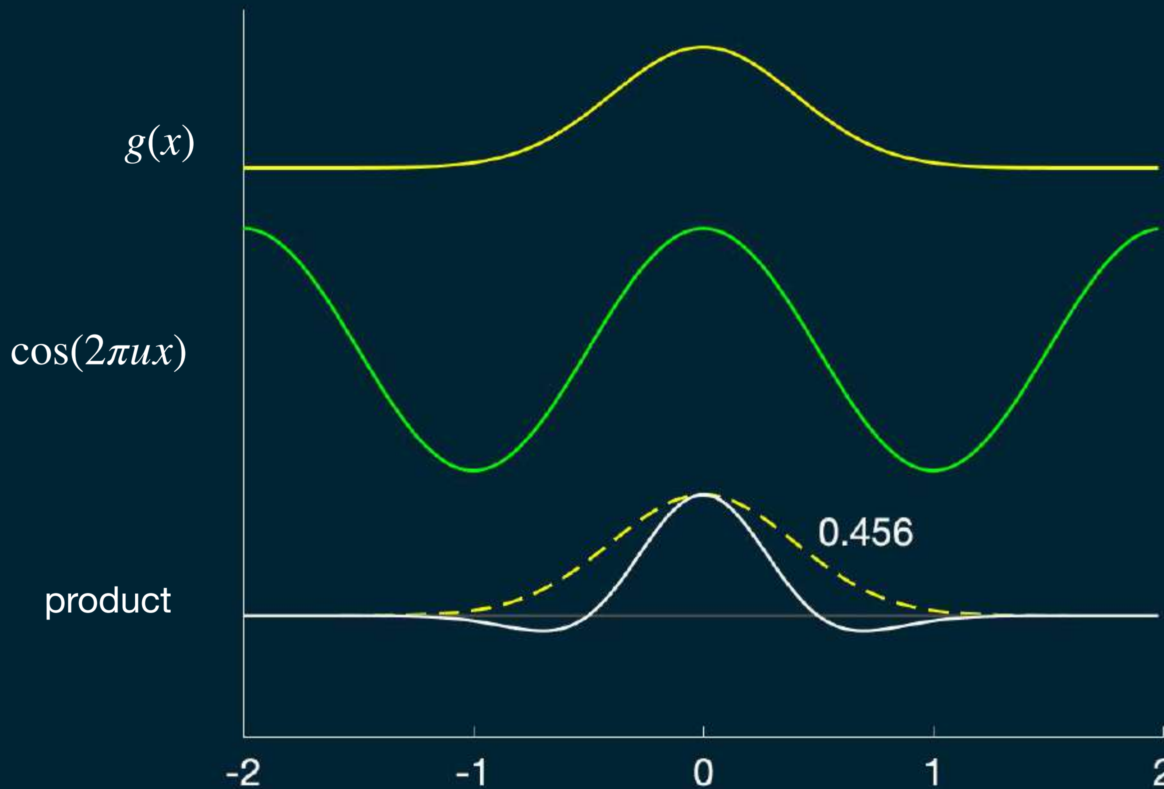
Inverse Fourier transform

$$g(x) = \int G(u) e^{+i2\pi ux} du$$

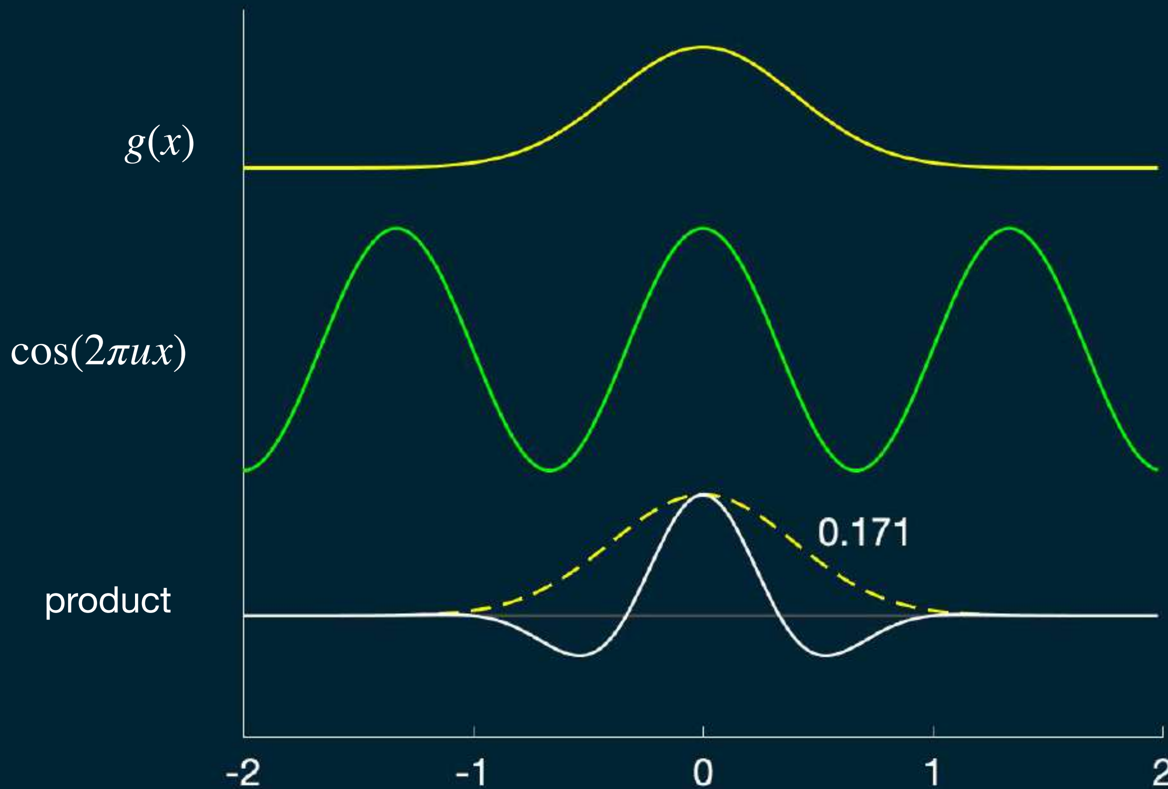
Cumputing $G(u)$ at $u = 1$



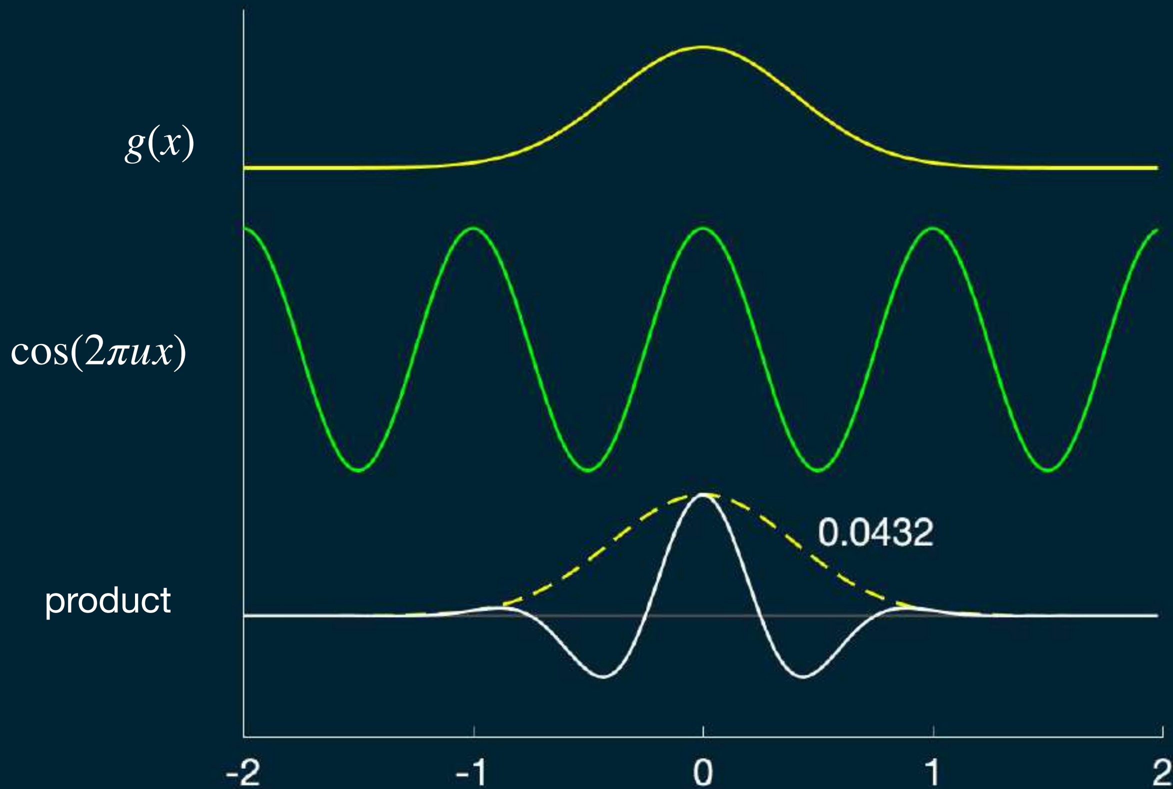
u=2



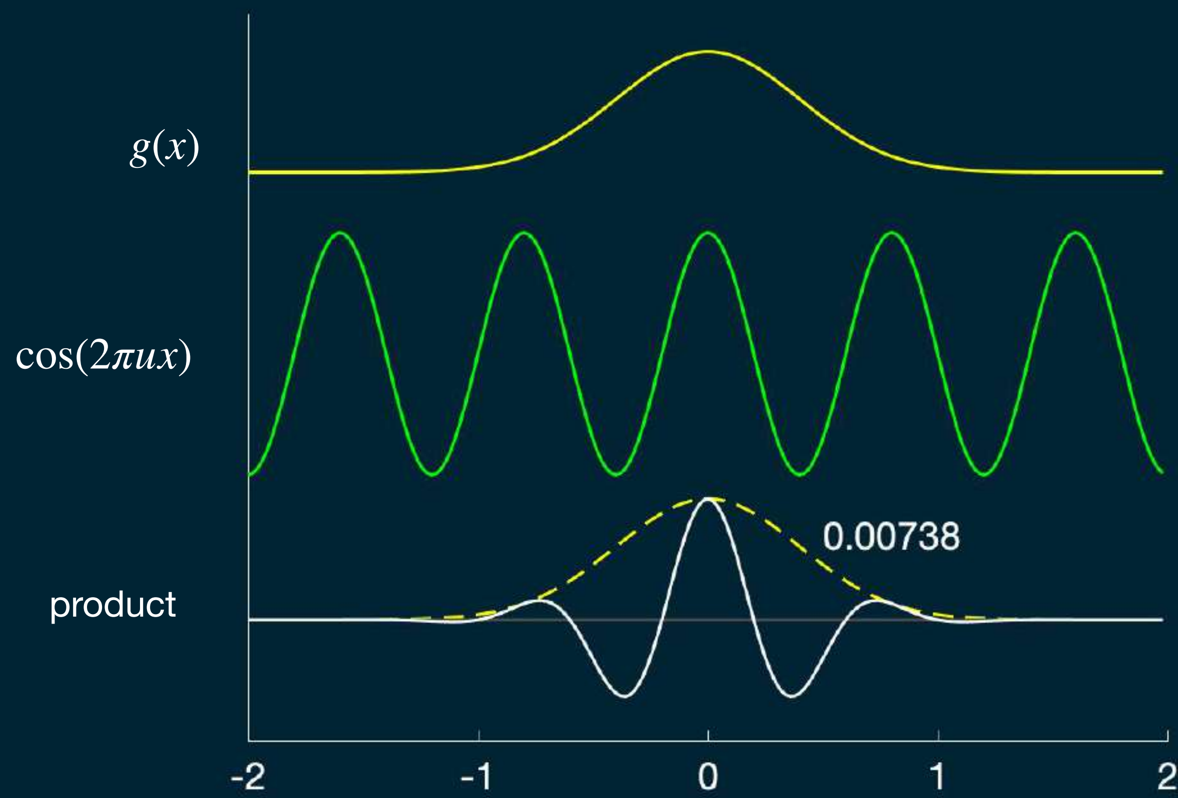
u=3



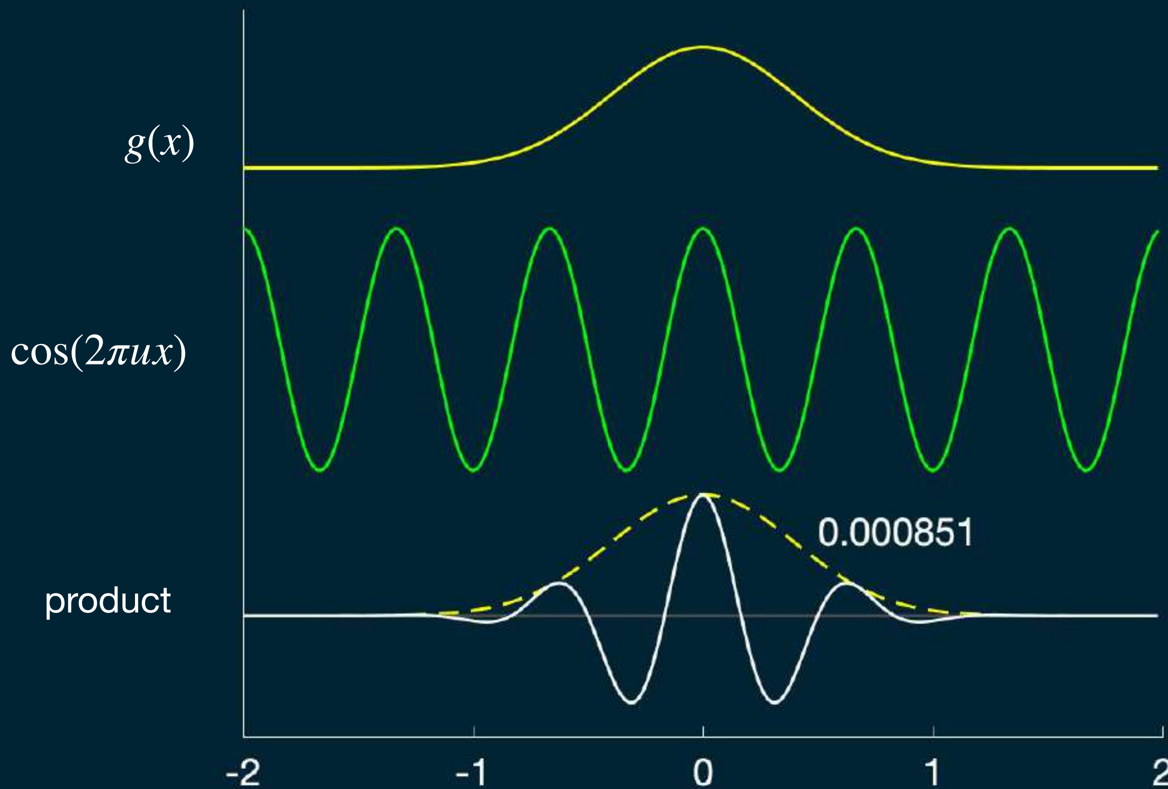
u=4



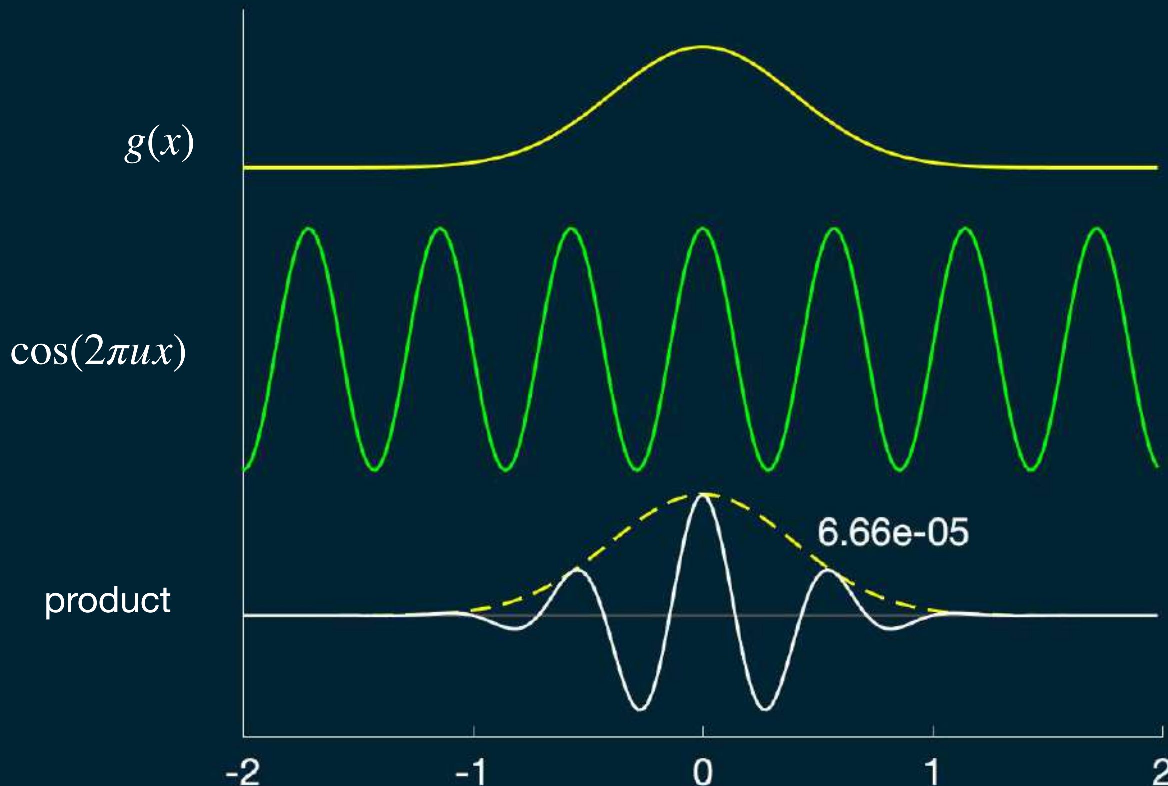
u=5



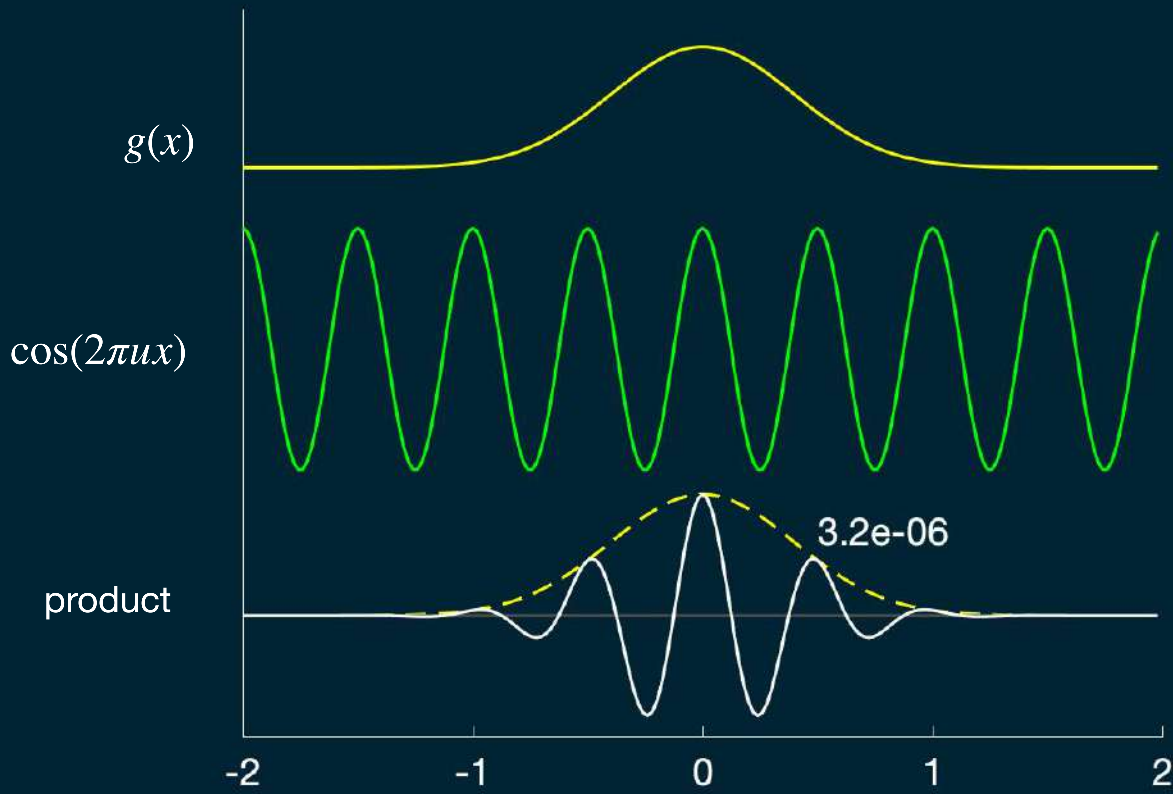
u=6



u=7



At $u = 8$, $G(u)$ is really small.



The Fourier transform of $e^{-\pi x^2}$ is $e^{-\pi u^2}$

$$G(u) = \int_{-\infty}^{\infty} e^{-\pi x^2} e^{-i2\pi ux}\, dx$$

$$= \int_{-\infty}^{\infty} e^{-\pi(x^2 + i2ux)}\, dx$$

This integral can be evaluated by completing the square in the exponent,

$$G(u) = \int_{-\infty}^{\infty} e^{-\pi(x^2 + i2ux - u^2)} dx \cdot e^{-\pi u^2}$$

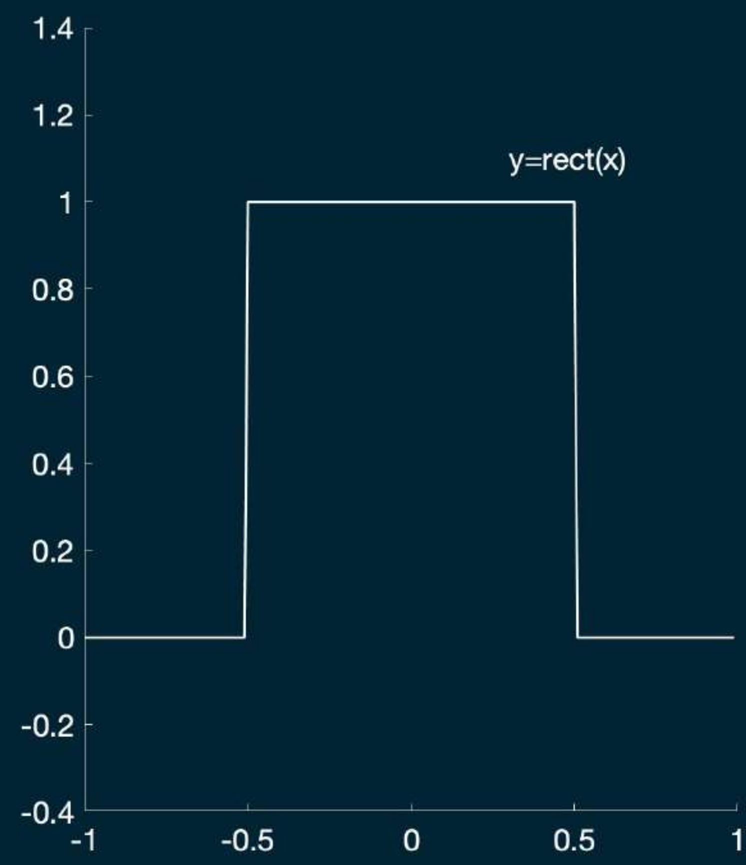
$$= \int_{-\infty}^{\infty} e^{-\pi(x+iu)^2} dx\; e^{-\pi u^2}$$

This integral = 1

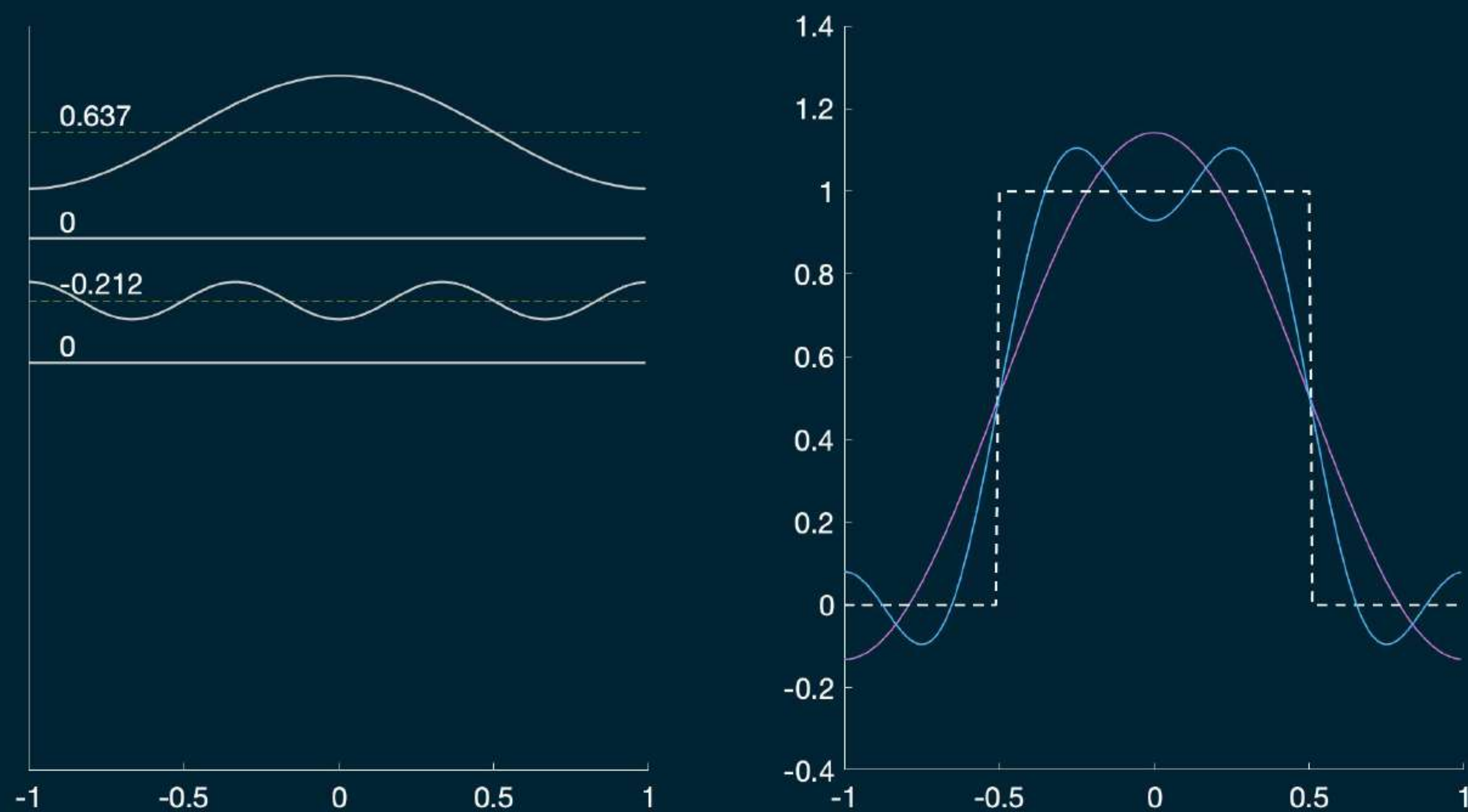
The final result is that

$$G(u) = e^{-\pi u^2}$$

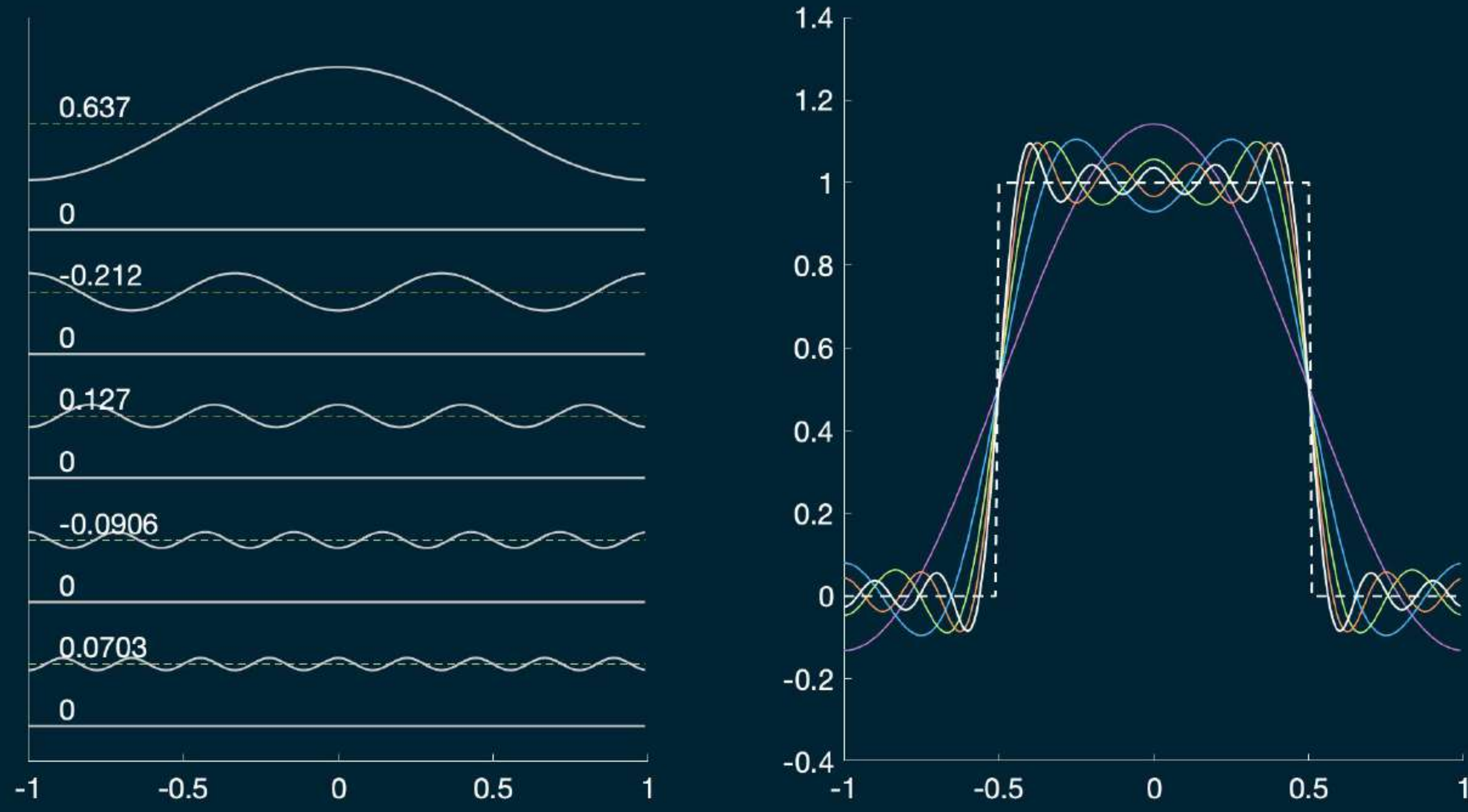
Fourier reconstruction of a rectangular function



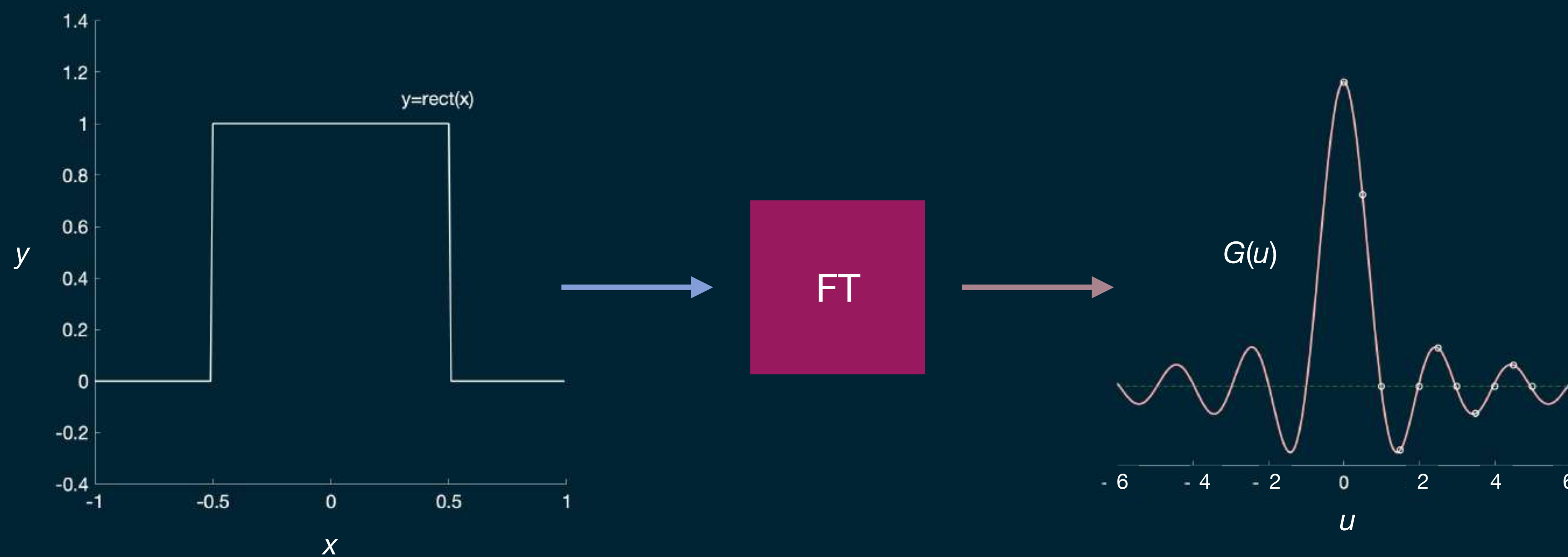
4 terms



Nowhere near convergence at 10 terms



The Fourier Transform of rect(*x*) is sinc(*u*)

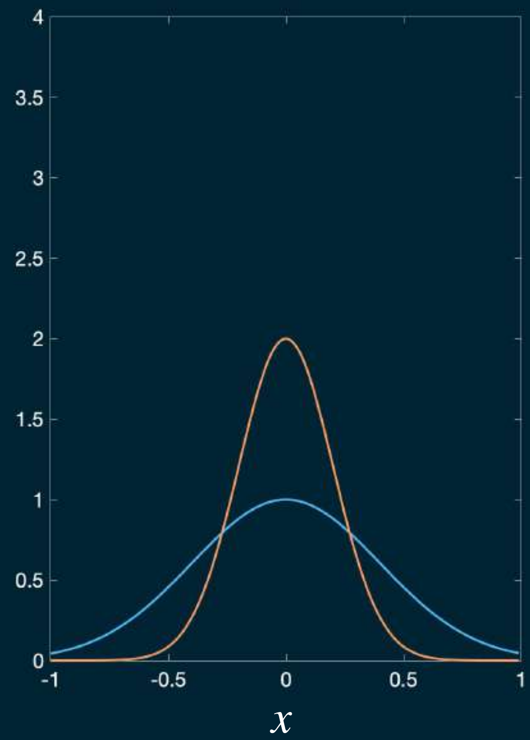


$$\mathrm{rect}(\mathrm{x}) \rightarrow \frac{\sin(\pi \mathrm{u})}{\pi \mathrm{u}}$$

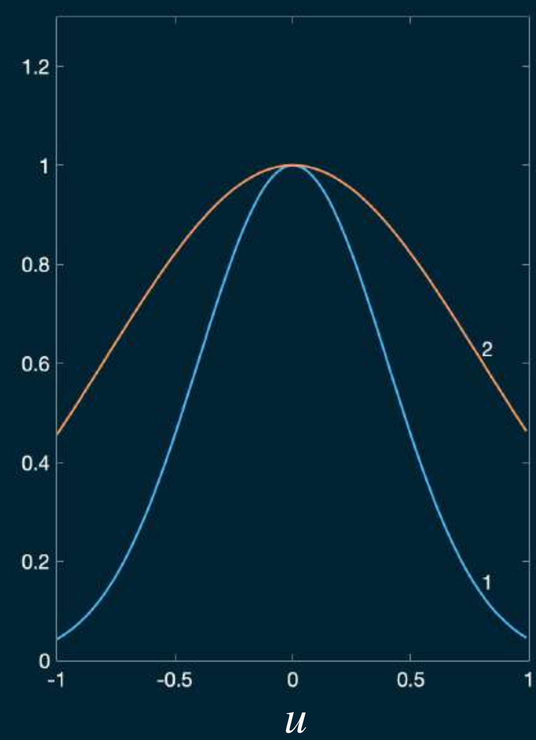
$\frac{\sin(\pi u)}{\pi u}$ is also known as: $\mathrm{sinc}(u)$

Reciprocal scaling of FT pairs

$$g(x) = ae^{-\pi(ax)^2}$$



$$G(u) = e^{-\pi(u/a)^2}$$



The scale property

If $g(x) = e^{-\pi x^2} \rightarrow G(u) = e^{-\pi u^2}$

what is the FT of $g_a(x) = ae^{-\pi(ax)^2}$?

The FT is:

$$G_a(u) = \int ae^{-\pi(ax)^2}e^{-i2\pi ux}dx.$$

Let $x' = ax$ and $x = x'/a$:

$$G_a(u) = \int e^{-\pi x'^2}e^{-i2\pi ux'/a}dx$$

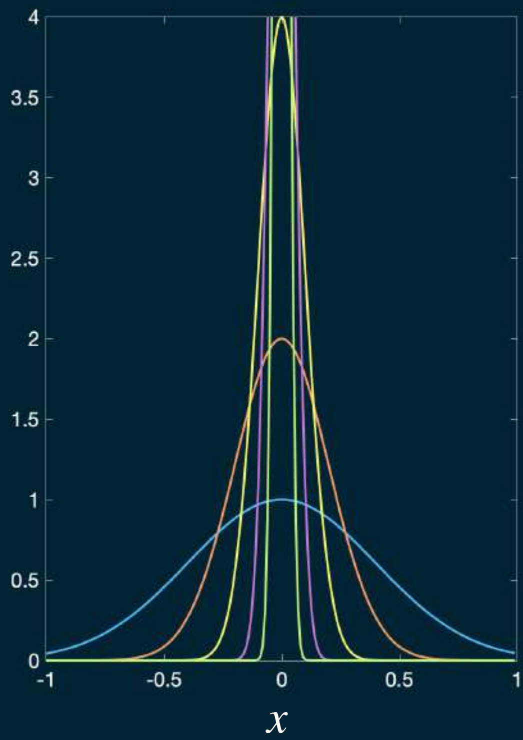
$$= G(u/a)$$

In general,

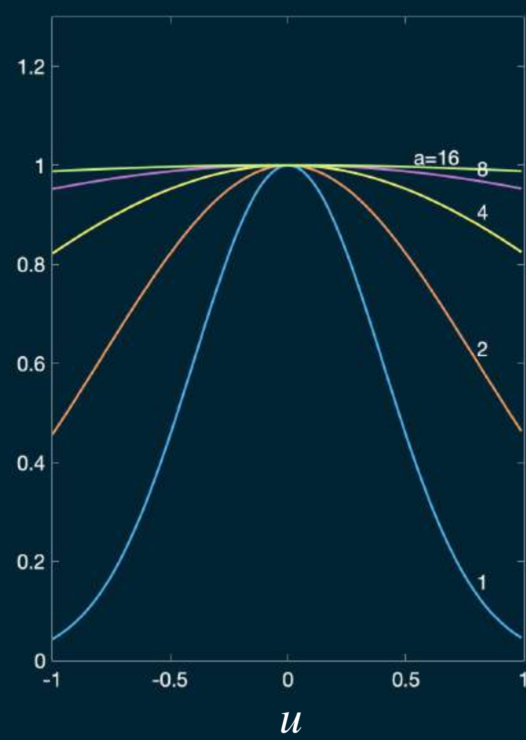
$$ag(ax) \rightarrow G(u/a)$$

Reciprocal scaling of FT pairs

$$g(x) = ae^{-\pi(ax)^2}$$



$$G(u) = e^{-\pi(u/a)^2}$$



Scale property

$$ag(ax) \rightarrow G(u/a)$$

Delta function

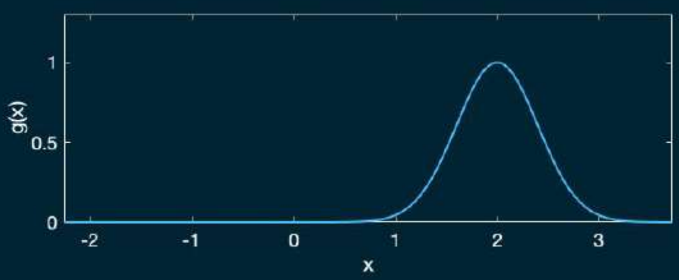
$$\delta(x) = \lim_{a \to \infty} ae^{-\pi(ax)^2}$$

FT Pair

$$\delta(x) \rightarrow 1$$

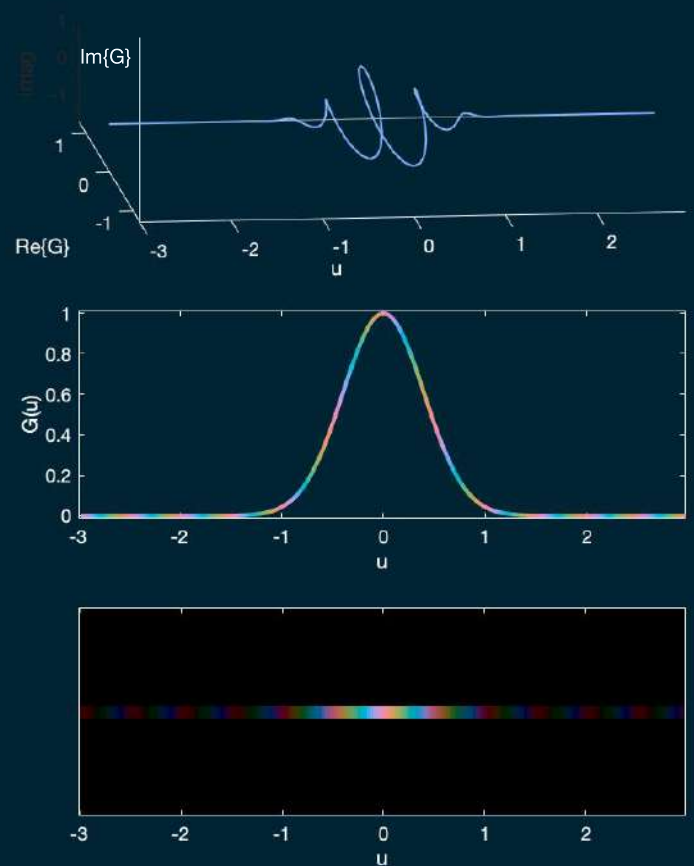
The shift property

$$g(x) = e^{-\pi(x-b)^2}$$



$$G(u) = e^{-\pi u^2} e^{-i2\pi ub}$$

...three visualizations:



The shift property

$$G(u) = \int e^{-\pi(x-b)^2} e^{-i2\pi ux} dx$$

Let

$$x' = x - b,$$

$$x = x + b, \text{ and}$$

$$e^{-i2\pi(x+b)} = e^{-i2\pi ux} e^{-i2\pi ub}.$$

Then

$$G(u) = e^{-i2\pi ub} \int e^{-\pi(x')^2} e^{-i2\pi ux'} dx'$$

In general,

$$g(x - b) \rightarrow G(u) e^{-i2\pi ub}$$

Convolution

$$f(x) = g * h = \int g(s)h(x-s)ds$$

Its FT is

$$F(u) = \iint g(s)h(x-s)e^{-i2\pi ux}ds\,dx.$$

Let

$$x' = x - s,$$

$$x = x' + s, \text{ and}$$

$$e^{-i2\pi(x'+s)} = e^{-i2\pi us}\,e^{-i2\pi ux'},$$

then

$$F(u) = \int g(s)e^{-i2\pi us}dx \int h(x')e^{-i2\pi ux'}dx'$$

Hence,

$$F(u) = G(u)H(u)$$

Fourier transform pairs

$$e^{-\pi x^2} \rightarrow e^{-\pi u^2}$$

$$\mathrm{rect(x)} \rightarrow \frac{\sin(\pi \mathrm{u})}{\pi \mathrm{u}}$$

$$\delta(x) \rightarrow 1$$

1D Fourier transform properties

$$g(x) + h(x) \rightarrow G(x) + H(x)$$ **Linearity**

$$ag(ax) \rightarrow G(u/a)$$ **Scale**

$$g(x-b) \rightarrow G(u)e^{-i2\pi ub}$$ **Shift**

$$g \star h \rightarrow G(u)H(u)$$ **Convolution**

Summary

Fourier transform

$$G(u) = \int g(x) e^{-i2\pi ux} dx$$

Inverse Fourier transform

$$g(x) = \int G(u) e^{+i2\pi ux} du$$

FT Pairs

$$e^{-\pi x^2} \rightarrow e^{-\pi u^2}$$

$$\mathrm{rect(x)} \rightarrow \frac{\sin(\pi \mathrm{u})}{\pi \mathrm{u}}$$

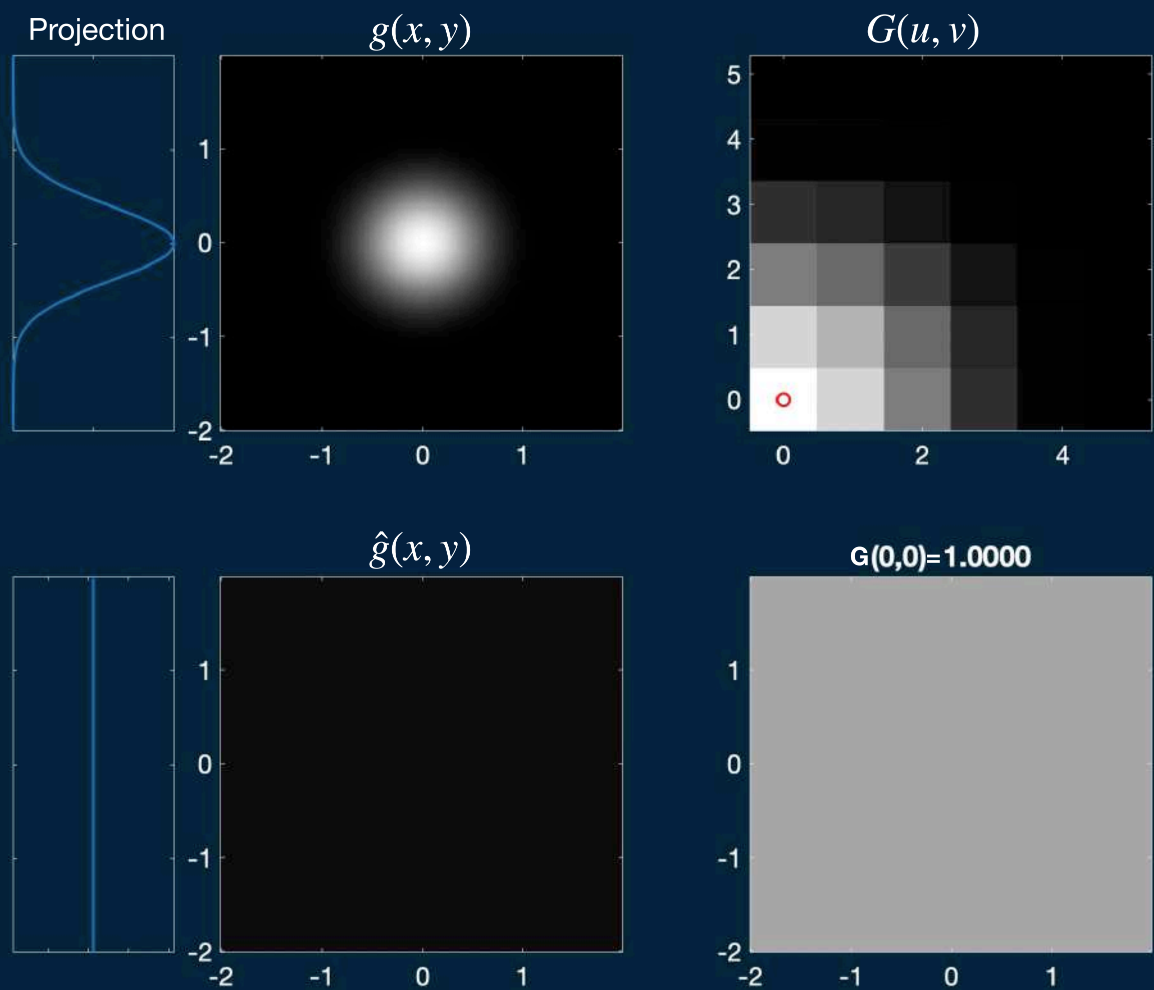
$$\delta(x) \rightarrow 1$$

FT Properties

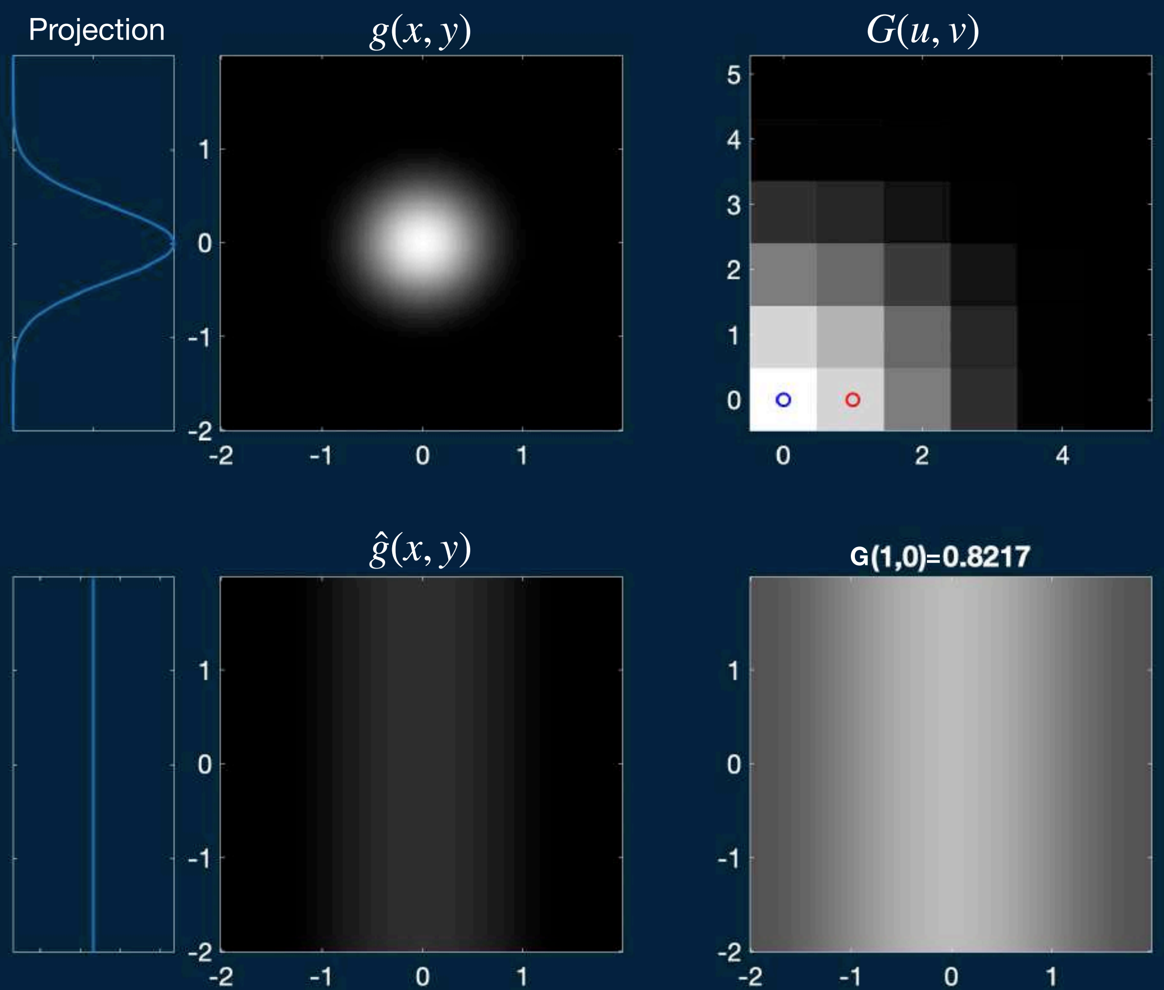
$g(x) + h(x) \rightarrow G(x) + H(x)$	Linearity
$ag(ax) \rightarrow G(u/a)$	Scale
$g(x-b) \rightarrow G(u)e^{-i2\pi ub}$	Shift

The Fourier transform in two dimensions

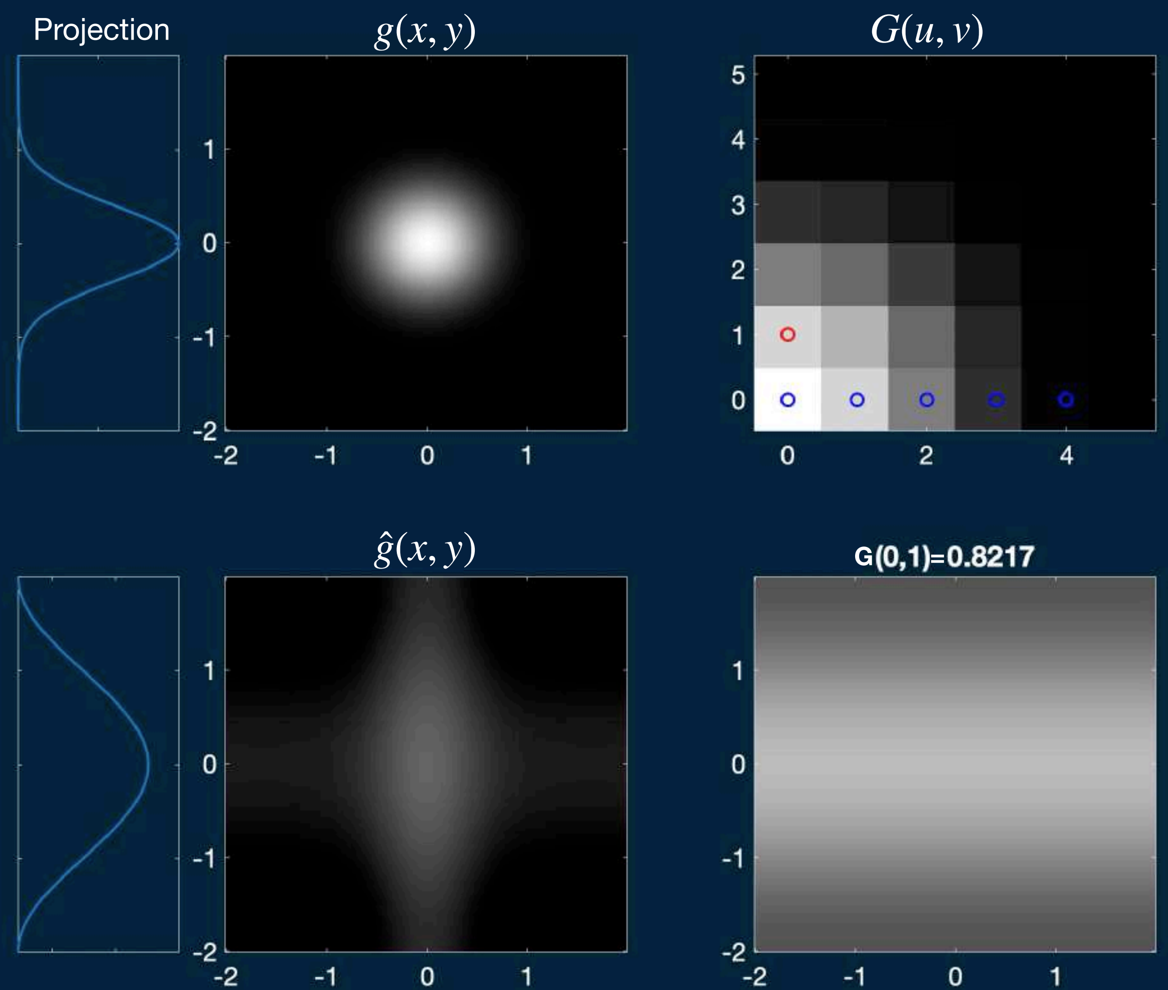
Fourier reconstruction of a 2D Gaussian function



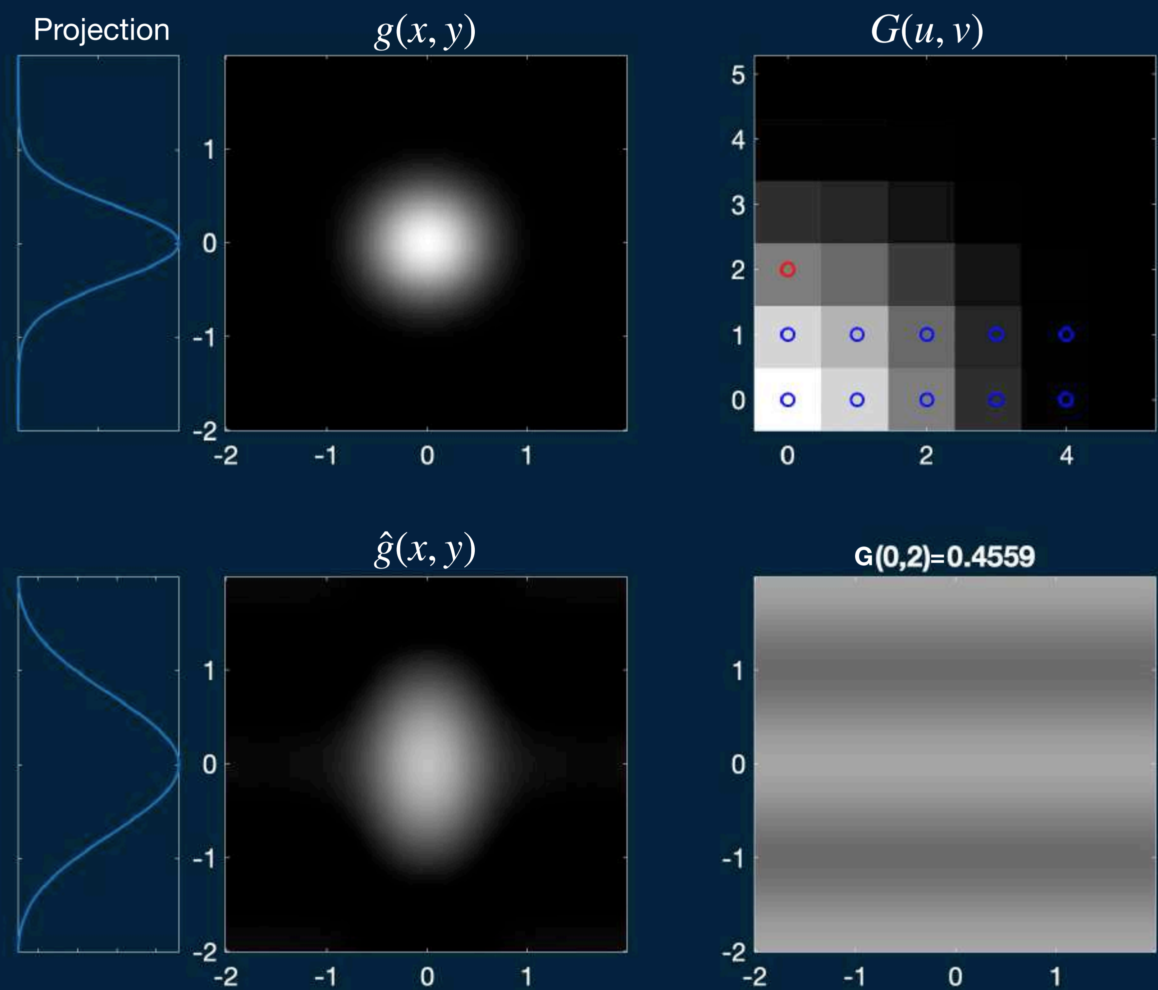
Fourier reconstruction of a 2D Gaussian function



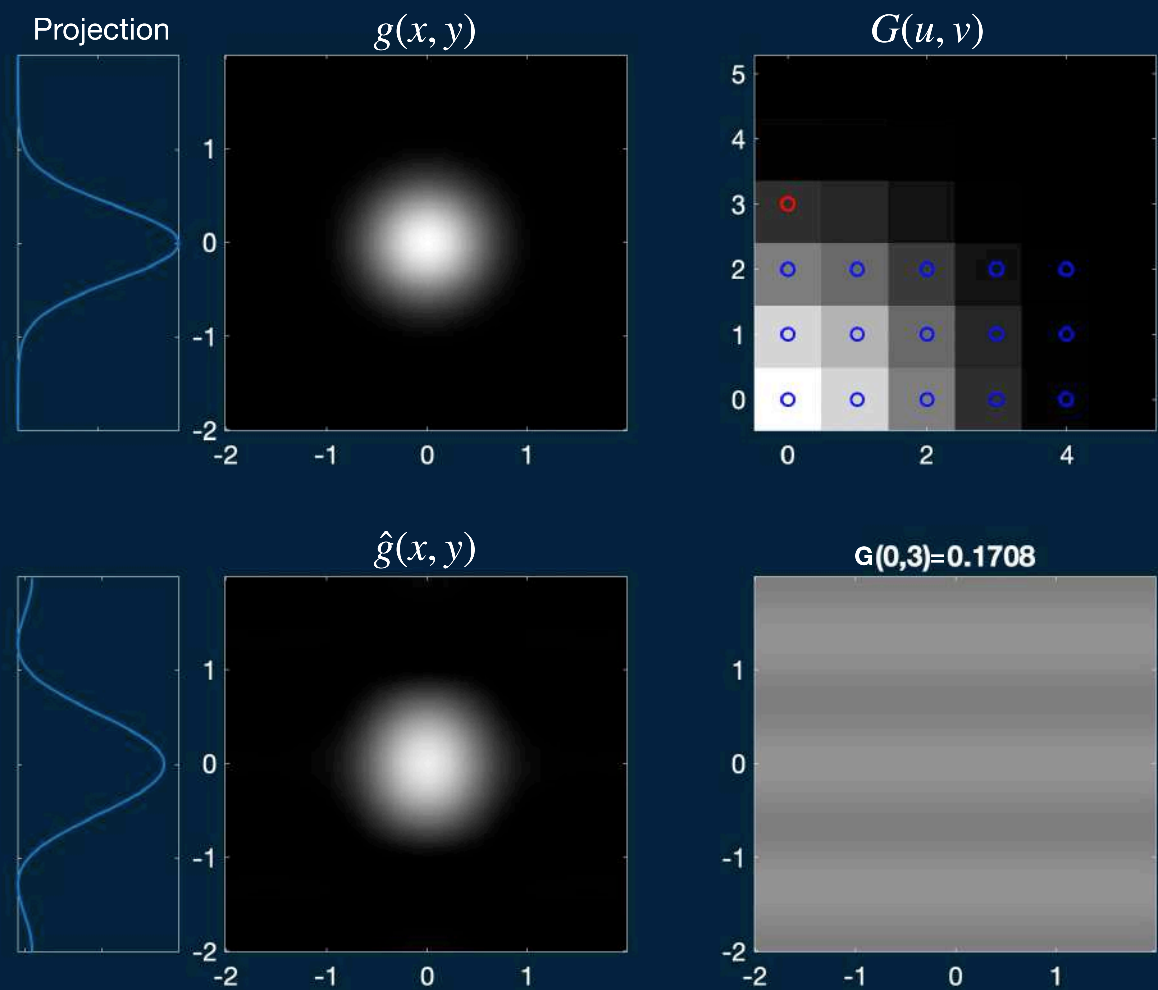
Fourier reconstruction of a 2D Gaussian function



Fourier reconstruction of a 2D Gaussian function



Fourier reconstruction of a 2D Gaussian function



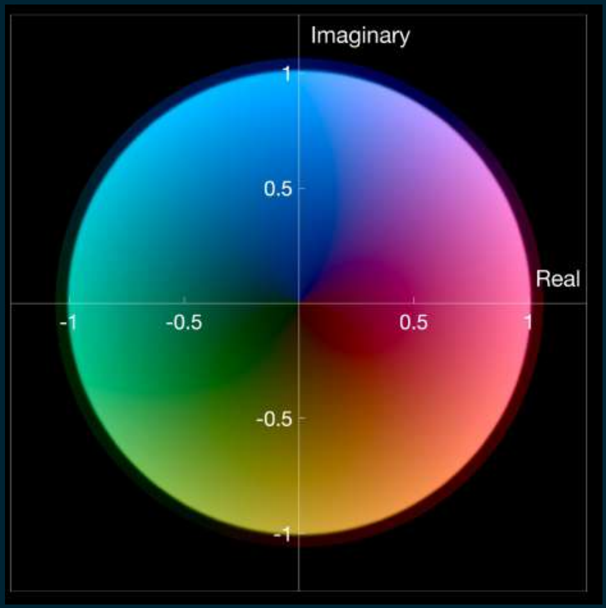
2D Fourier transform

$$G(u, v) = \int\int g(x, y)\, e^{-i2\pi(ux+vy)} dx\, dy$$

2D inverse Fourier transform

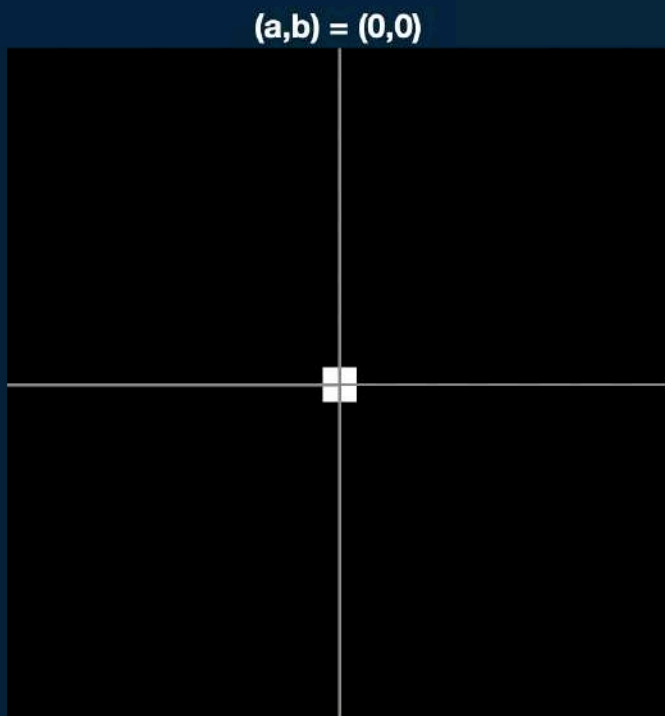
$$g(x, y) = \int\int G(u, v)\, e^{i2\pi(ux+vy)} du\, dv$$

Complex numbers

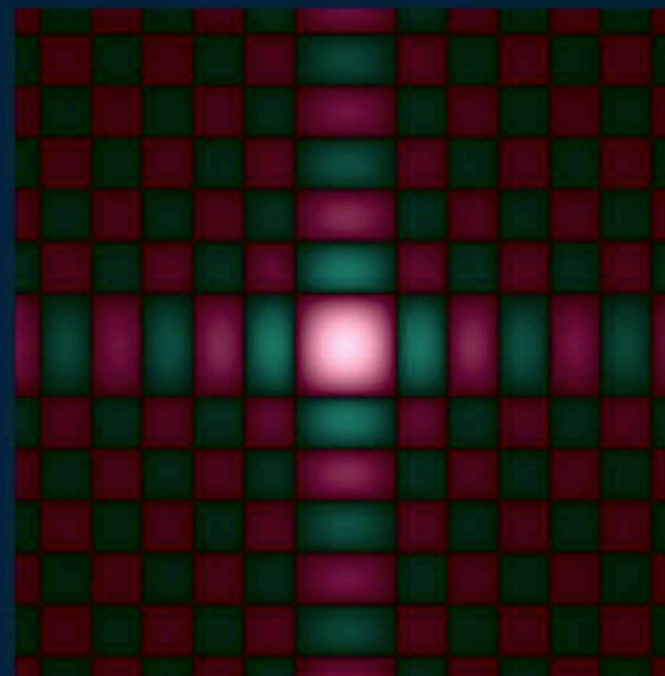


We'll represent complex numbers
using this scheme

FT of a square

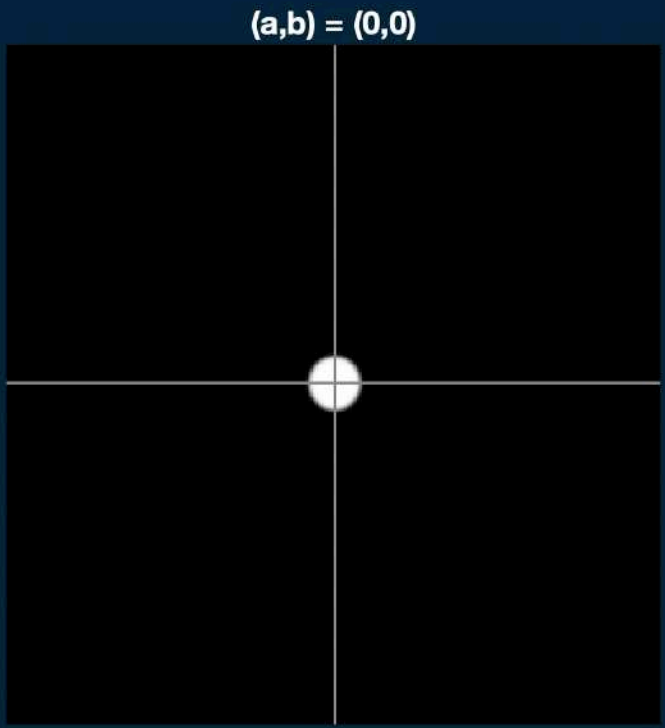


$$g = \mathrm{rect}(x)\,\mathrm{rect}(y)$$



$$G = \mathrm{sinc}(u)\,\mathrm{sinc}(v)$$

FT of a disc



$$g(x, y) = \mathrm{circ}(r)$$

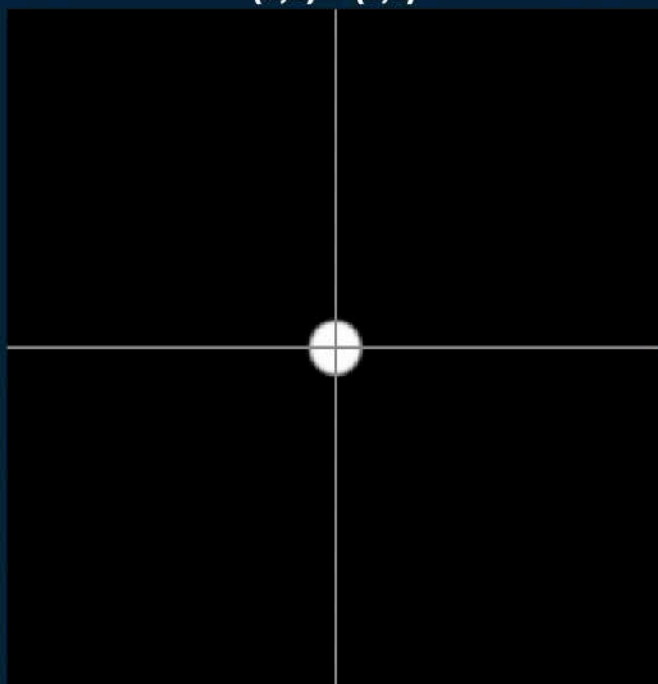
$$G(u, v) = \frac{J_1(2\pi\rho)}{\rho}$$

The shift property

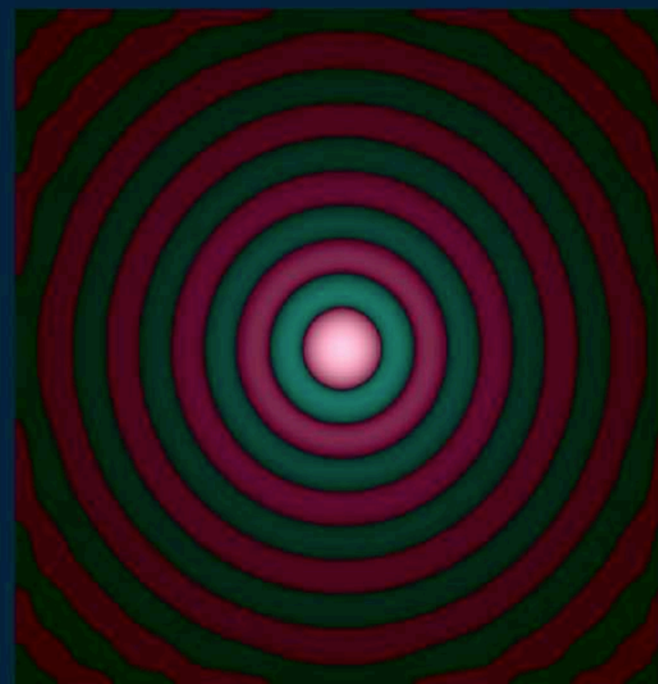
$$g(x - a, y - b) \rightarrow G(u, v)e^{-i2\pi(au+bv)}$$

2D Shift property

(a,b) = (0,0)

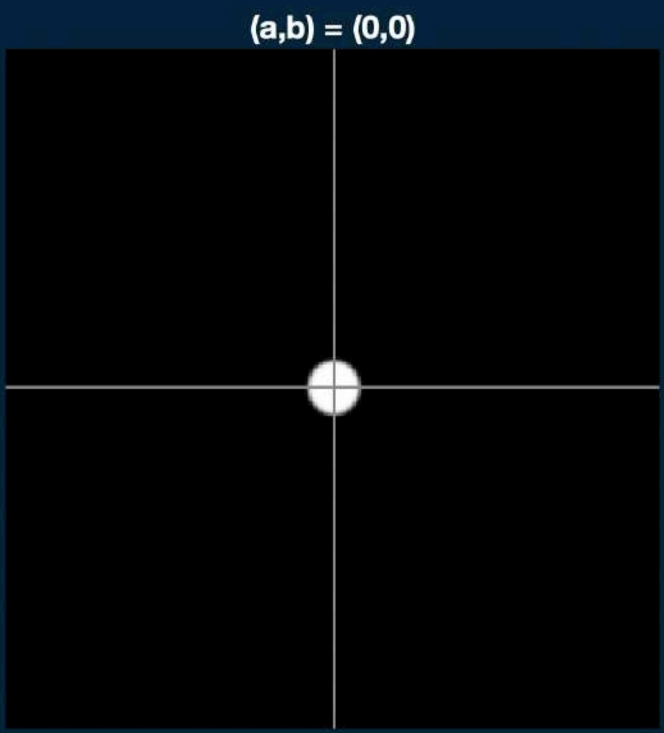


$g(x - a, y - b)$

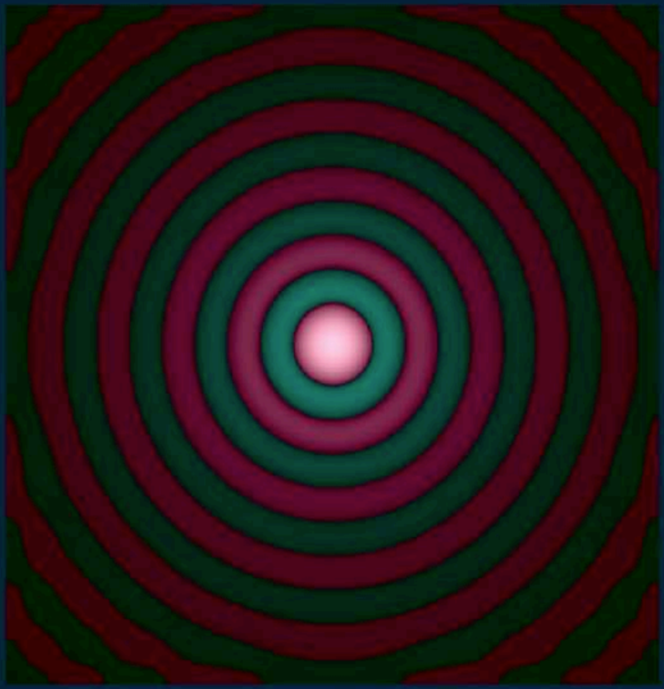


$G(u, v)e^{-i2\pi(au+bv)}$

2D Shift property



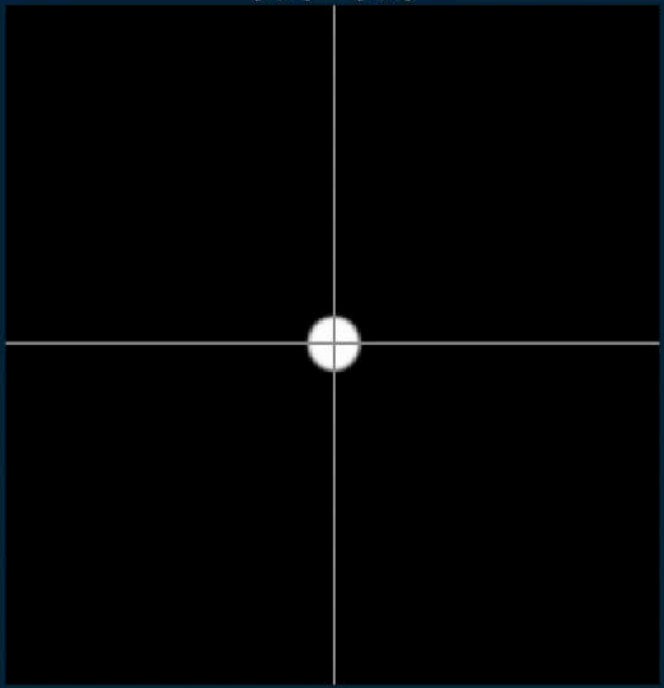
$g(x - a, y - b)$

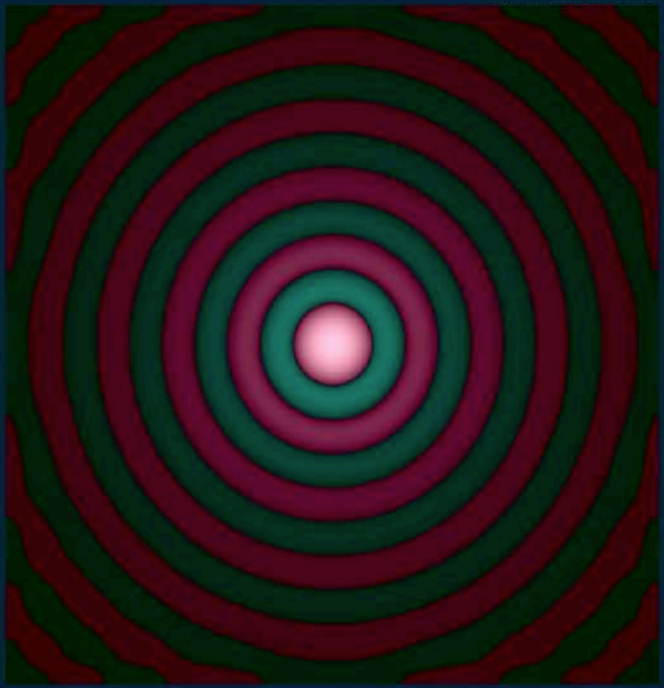


$G(u, v)e^{-i2\pi(au+bv)}$

2D Shift property

(a,b) = (0,0)

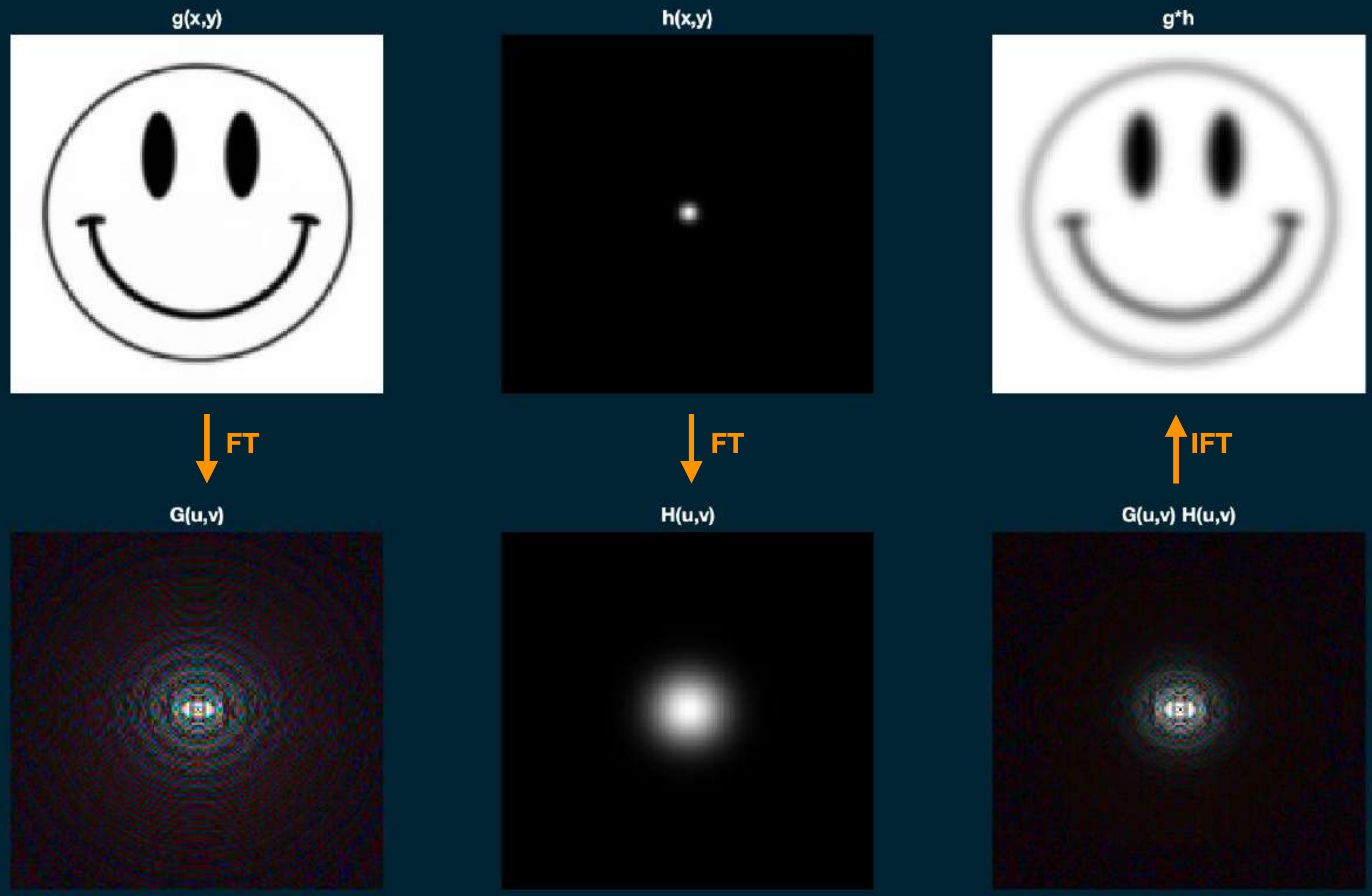




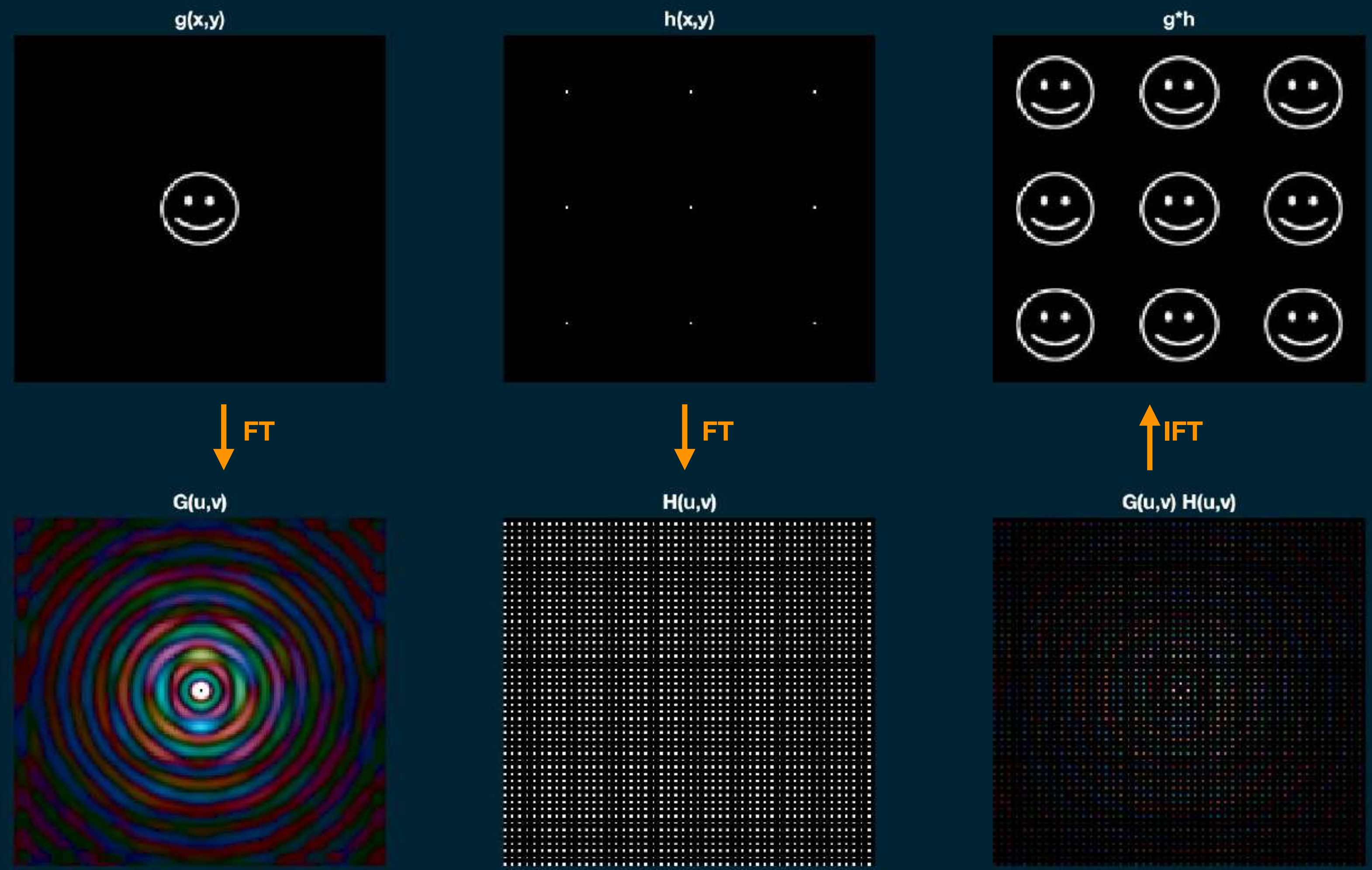
$$g(x - a, y - b)$$

$$G(u, v)e^{-i2\pi(au+bv)}$$

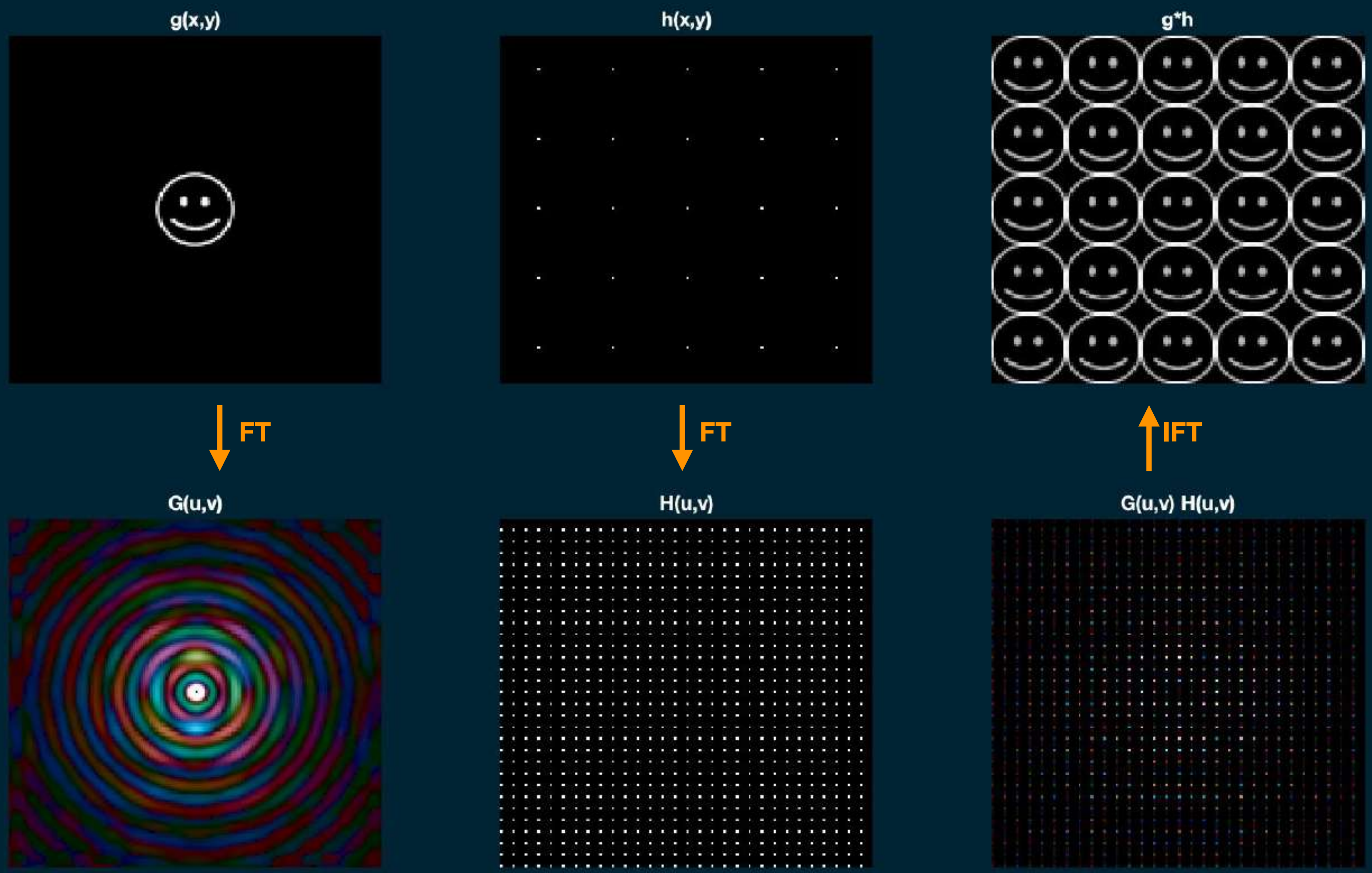
Convolution with a Gaussian



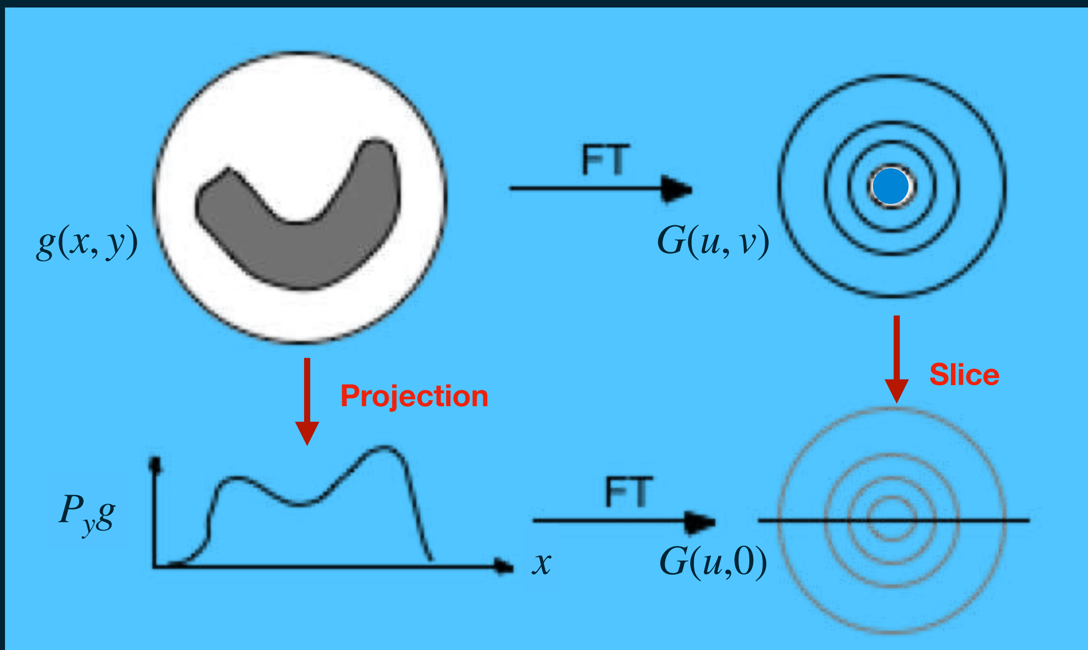
Convolution with a lattice



An undersampling lattice



The Fourier Slice Theorem

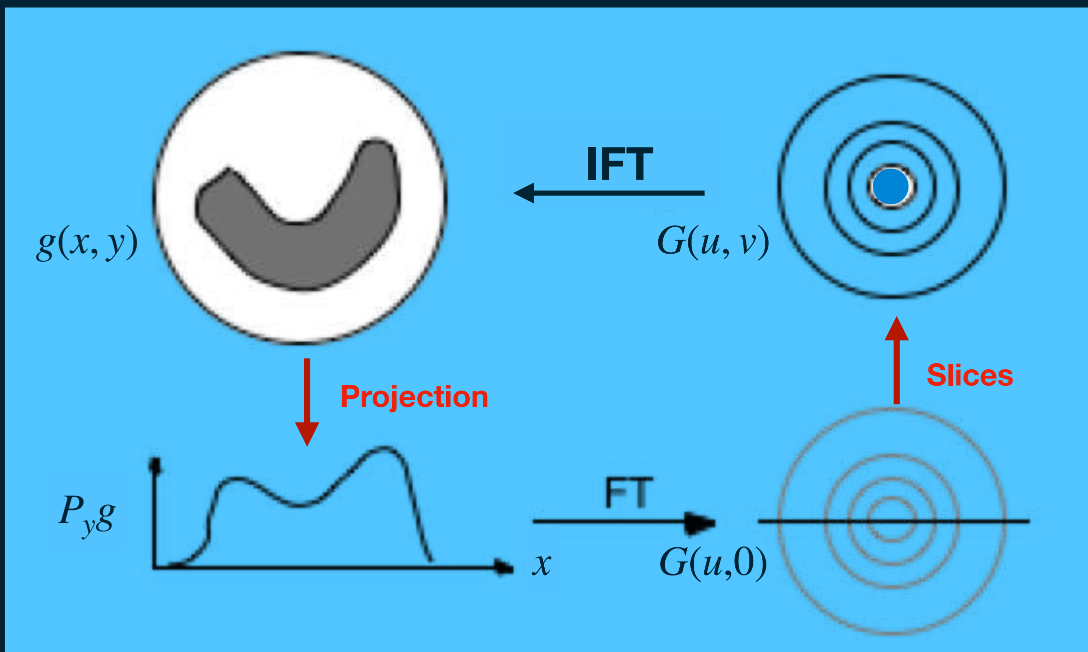


$$G(u, v) = \iint g(x, y) e^{-i2\pi(ux+vy)} dxdy$$

$$G(u,0) = \int \left(\int g(x, y) dy \right) e^{-i2\pi(ux)} dx$$
$$= \mathscr{F}\{P_y g\}$$

$$P_y g(x, y) = \int g(x, y) dy$$

Reconstruction using the Fourier Slice Theorem



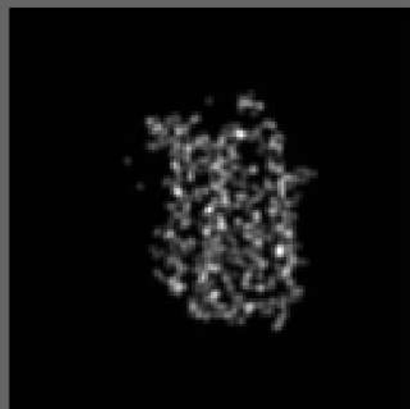
$$G(u, v) = \iint g(x, y) e^{-i2\pi(ux+vy)} dxdy$$

$$G(u,0) = \int \left(\int g(x, y) dy \right) e^{-i2\pi(ux)} dx$$
$$= \mathscr{F}\{P_y g\}$$

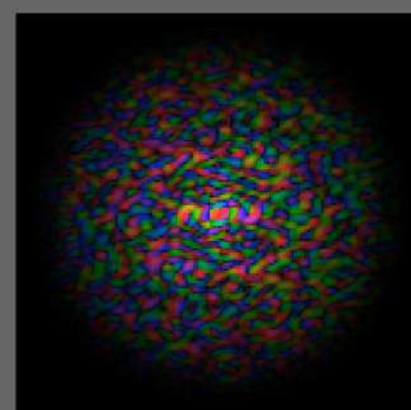
$$P_y g(x, y) = \int g(x, y) dy$$

The rotation property says:
If we can collect projections from all directions, we can construct all of $G(u, v)$

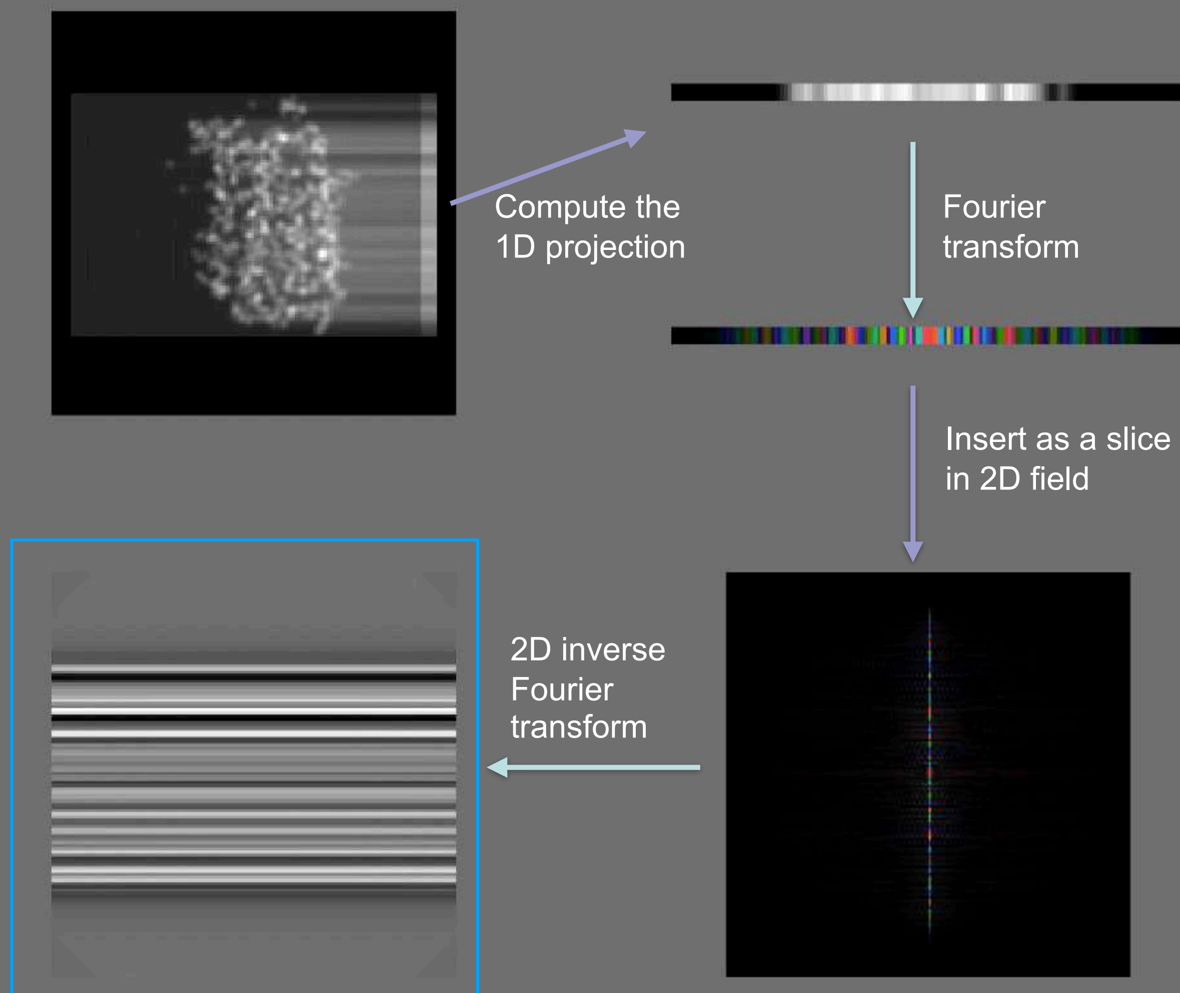
2D reconstruction using the slice theorem



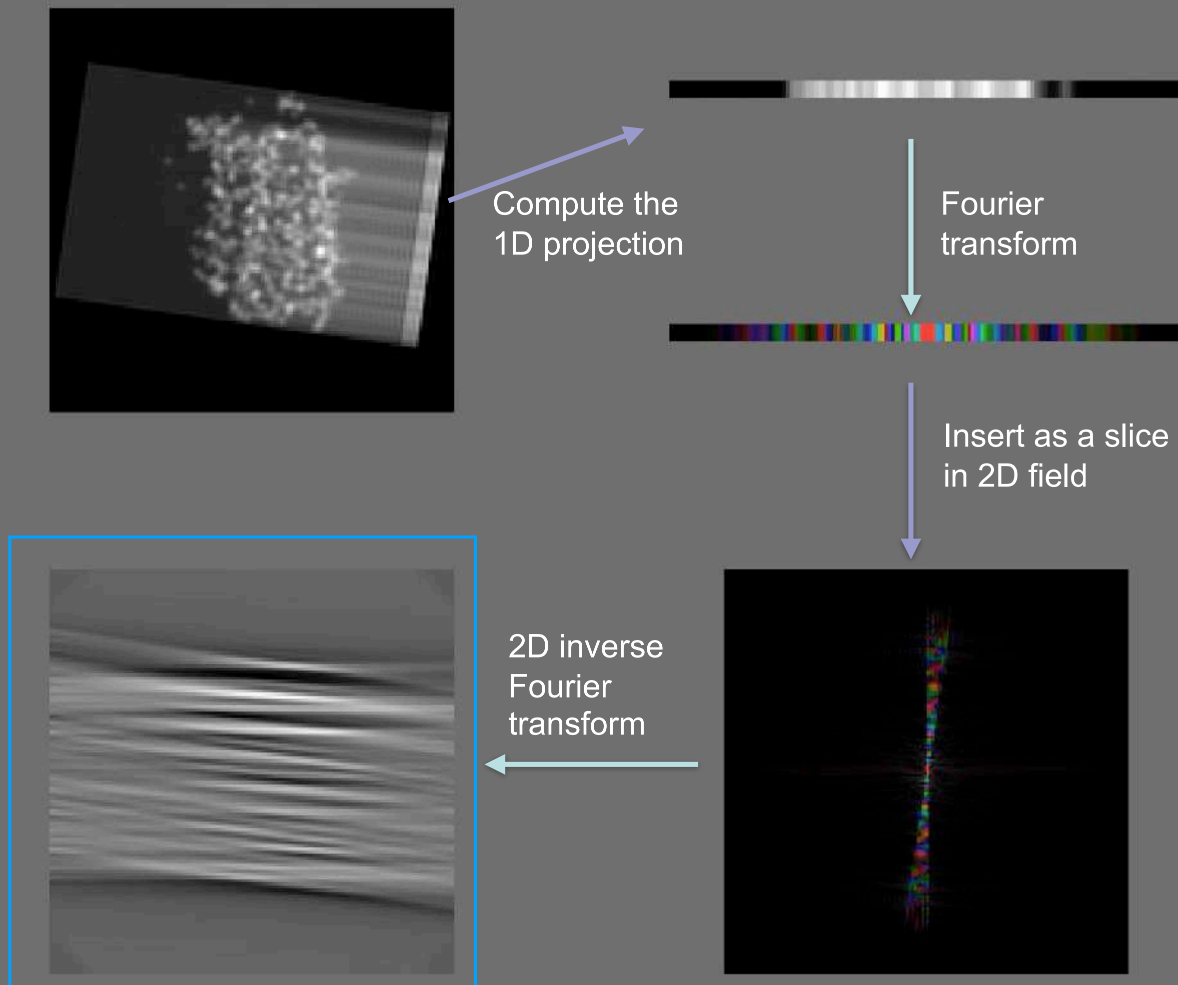
Fourier transform



2D reconstruction using the slice theorem



2D reconstruction using the slice theorem



The discrete FT is what is calculated on a computer

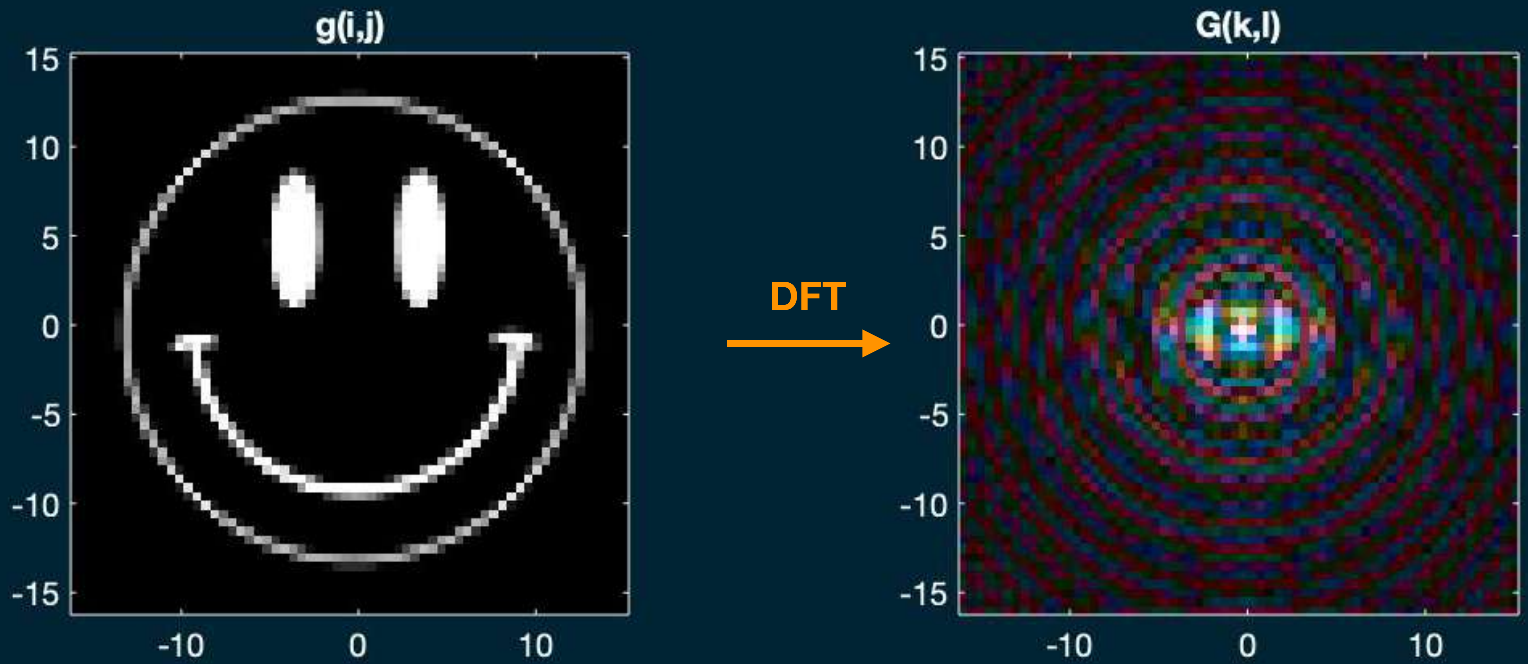
2D Fourier transform

$$G(u,v) = \int\int g(x,y)\, e^{-i2\pi(ux+vy)} dx\, dy$$

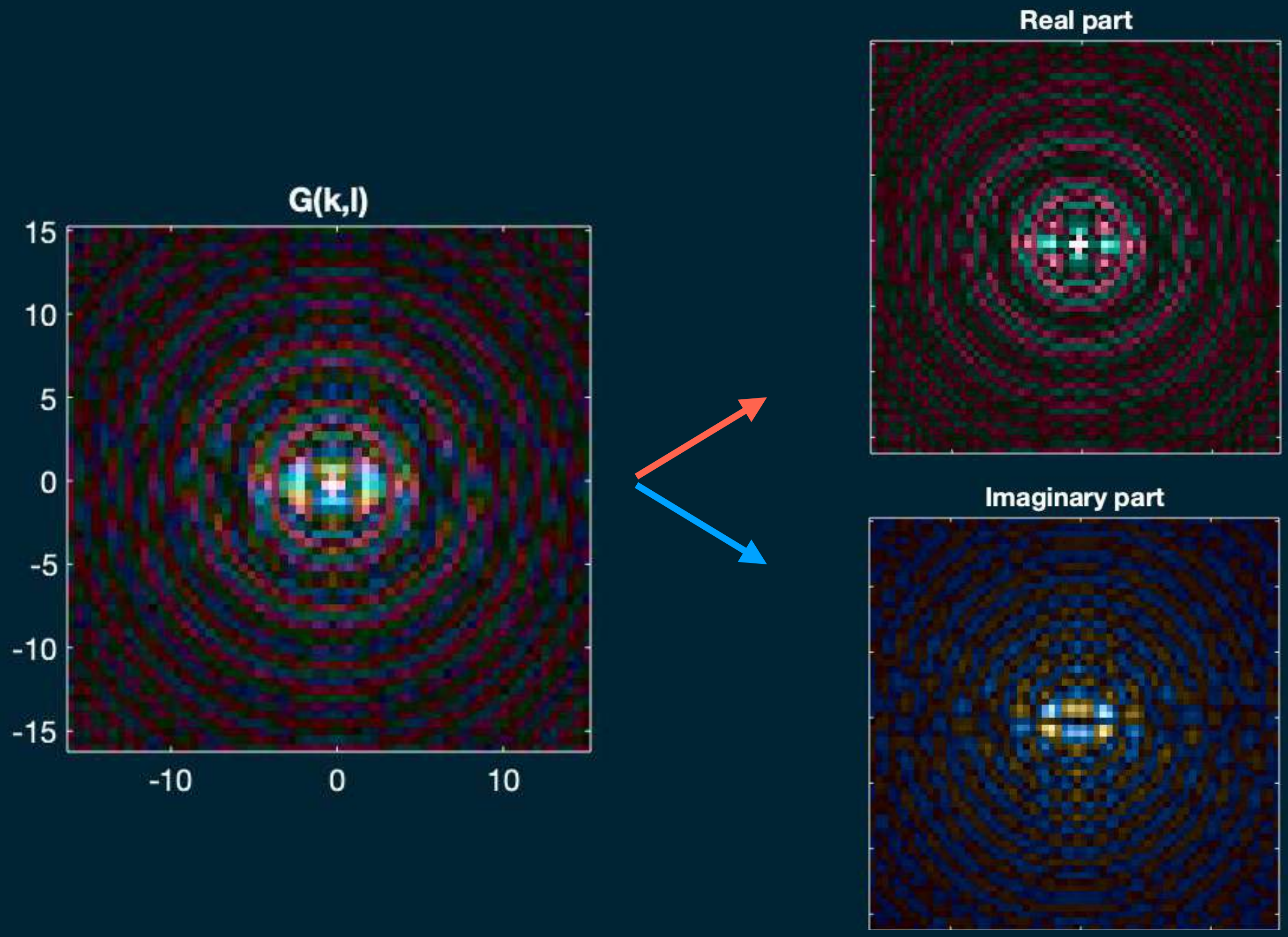
2D discrete Fourier transform

$$G(k,l) = \frac{1}{N} \sum_{i=-N/2}^{N/2-1} \sum_{j=-N/2}^{N/2-1} g(i,j)\, e^{-i2\pi(ik+jl)/N}$$

The DFT of a 32 x 32 pixel image has 32 x 32 complex pixel values



But the DFT of a real image has twofold redundancy



Summary of 2D Fourier transform

2DFT Pairs

$$e^{-\pi(x^2+y^2)} \rightarrow e^{-\pi(u^2+v^2)}$$

$$\text{rect}(x)\text{rect}(y) \rightarrow \text{sinc}(u)\text{sinc}(v)$$

$$\text{circ}(r) \rightarrow \frac{J_1(2\pi\rho)}{\rho}$$

$$\delta(x)\delta(y) \rightarrow 1$$

$$\text{III}(x, y) \rightarrow \text{III}(u, v)$$

$$\text{sinc}(u) = \frac{\sin(\pi u)}{\pi u}$$

2DFT Properties

$$ab\, g(ax, by) \rightarrow G(u/a, v/b)$$ Scale

$$g(x-a, y-b) \rightarrow G(u, v)e^{-i2\pi(au+bv)}$$ Shift

$$g(x', y') \rightarrow G(u', v')$$ Rotation

$$P_y\, g(x, y) \rightarrow G(u,0)$$ Projection

$$f \star g \rightarrow FG$$ Convolution

$$(x', y') = R_\theta(x, y)$$

$$(u', v') = R_\theta(u, v)$$

The 3D transform

3D Fourier transform

$$G(u, v, w) = \iiint g(x, y, z) e^{-i2\pi(ux+vy+wz)} dx\, dy\, dz$$

3D Inverse Fourier transform

$$g(x, y, z) = \iiint G(u, v, w) e^{+i2\pi(ux+vy+wz)} du\, dv\, dw$$