

Lecture 4a

Algorithms and Foundational Math

The contrast transfer function
and Fourier transforms

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I. Phase contrast and the contrast transfer function

1. Complex numbers: review
2. Defocus contrast and the CTF (simple version)
3. Image delocalization
4. Objective lens effects on the CTF

Why complex numbers?

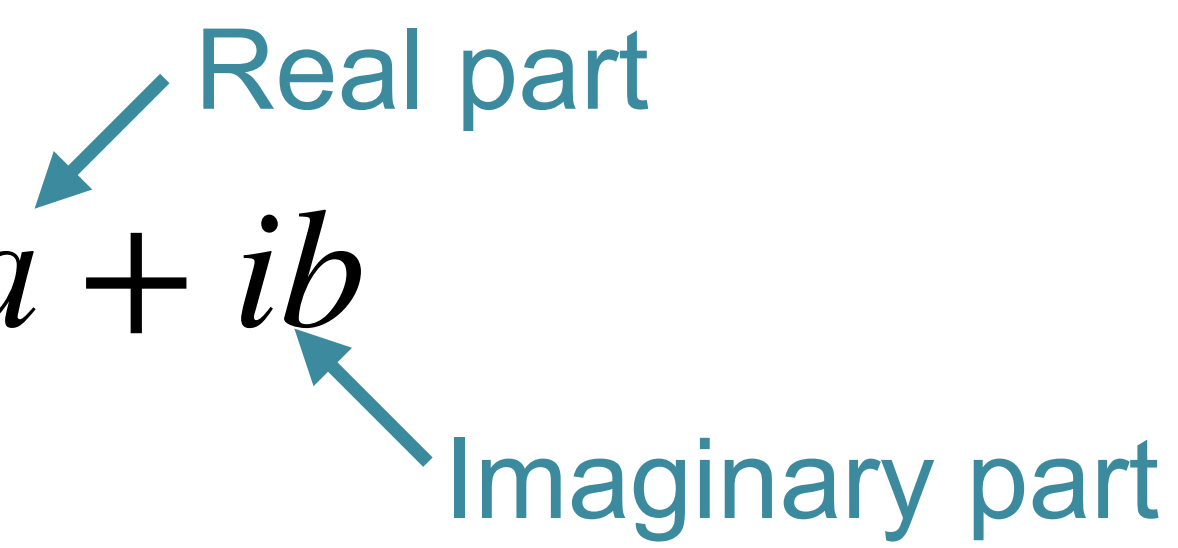
- They make the equations simpler
- Natural for Fourier transforms
- Give us the magnitude and phase of structure factors

i , the imaginary unit

The unit imaginary number

$$i = \sqrt{-1}$$

A complex number

$$z = a + ib$$


Real part

Imaginary part

You can do arithmetic with complex numbers

$$z = a + ib$$

$$w = c + id$$

Add $z + w = (a + c) + i(b + d)$

Multiply $zw = (ab - bd) + i(ad + bc)$

Real part $\operatorname{Re}(z) = a$

Imaginary part $\operatorname{Im}(z) = b$

Absolute value $|z| = \sqrt{a^2 + b^2}$

Conjugate $z^* = a - ib$

The exponential function e^x

$$e = 2.718\dots$$

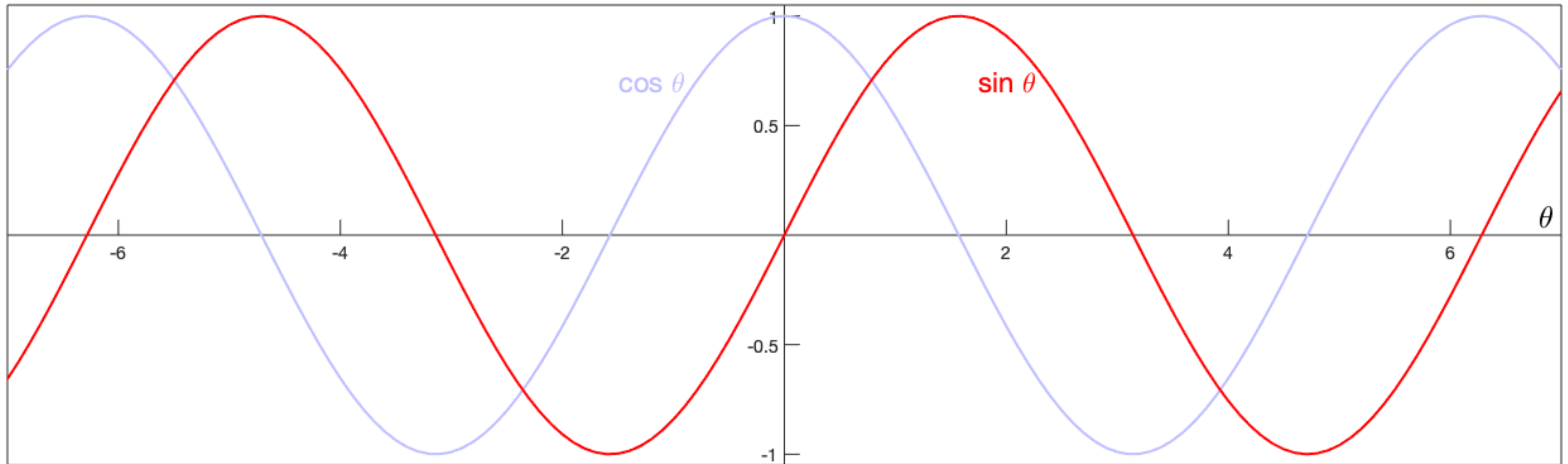
$$e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{2 \times 3} + \dots$$

A very important approximation

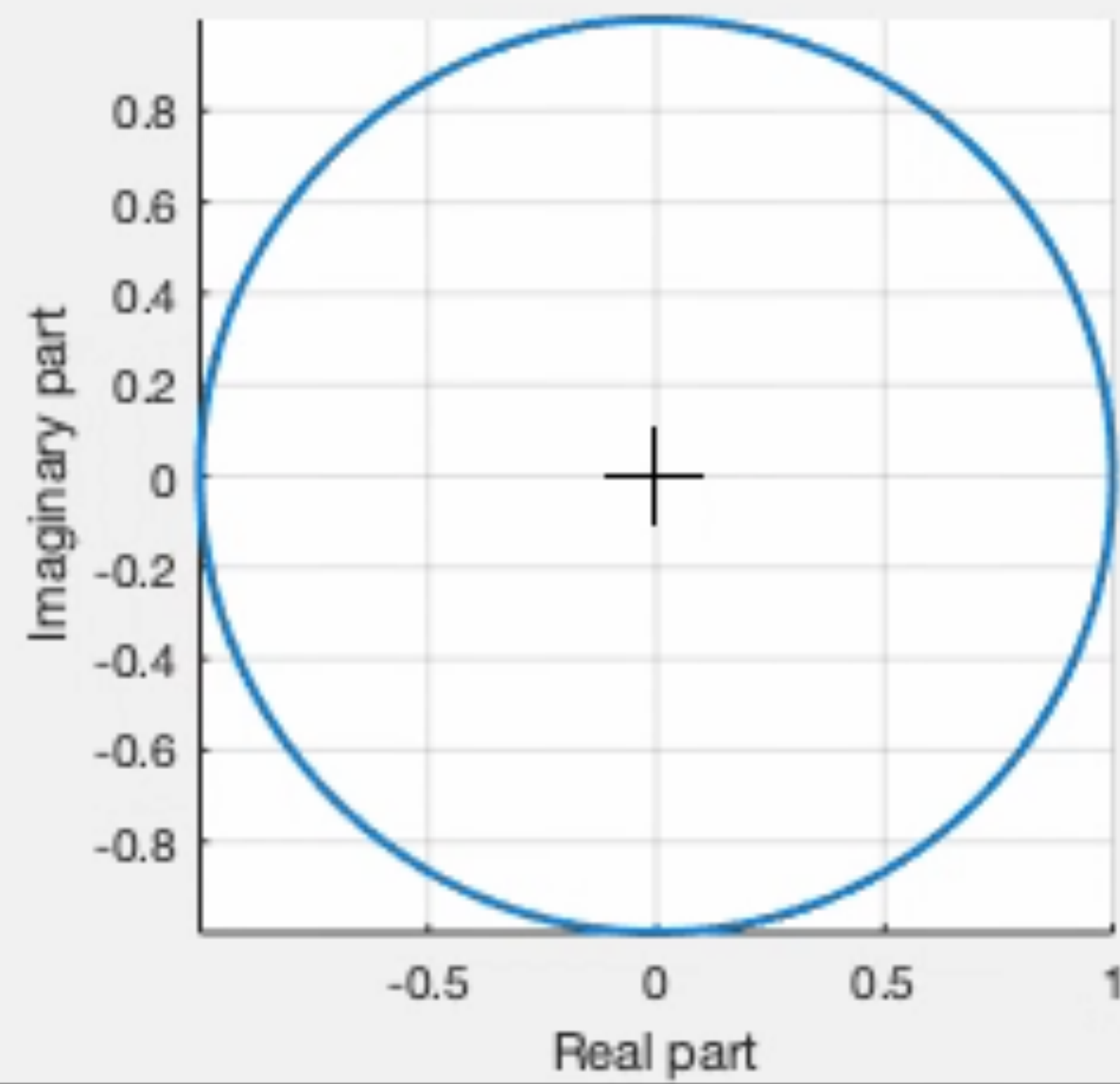
$$e^x \approx 1 + x, \quad x \ll 1$$

The complex exponential

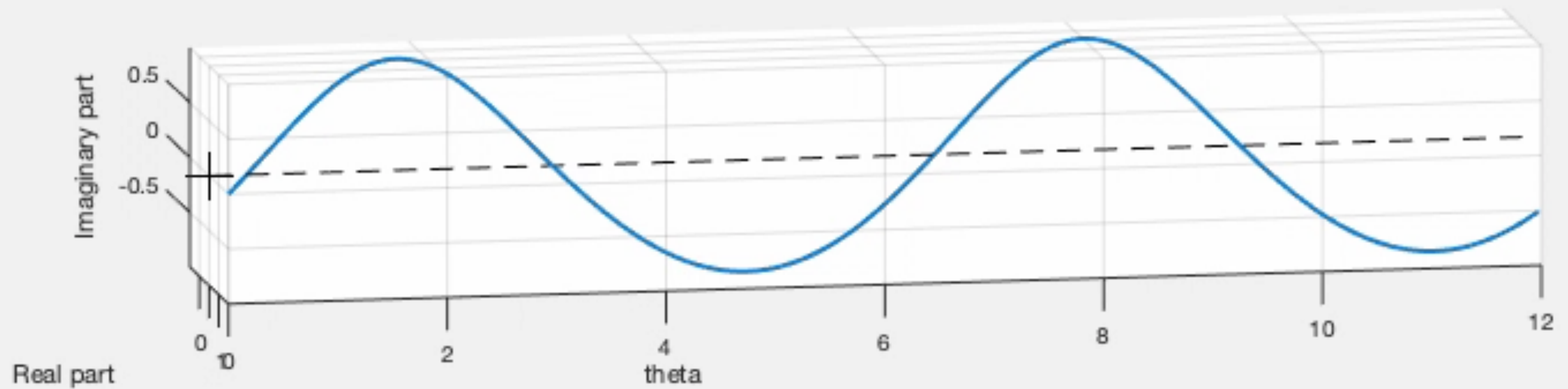
$$e^{i\theta} = \cos \theta + i \sin \theta$$



A plot of $e^{i\theta}$



A plot of $e^{i\theta}$



Any z can be represented as (a, b) or as (r, θ)

$$z = a + ib$$

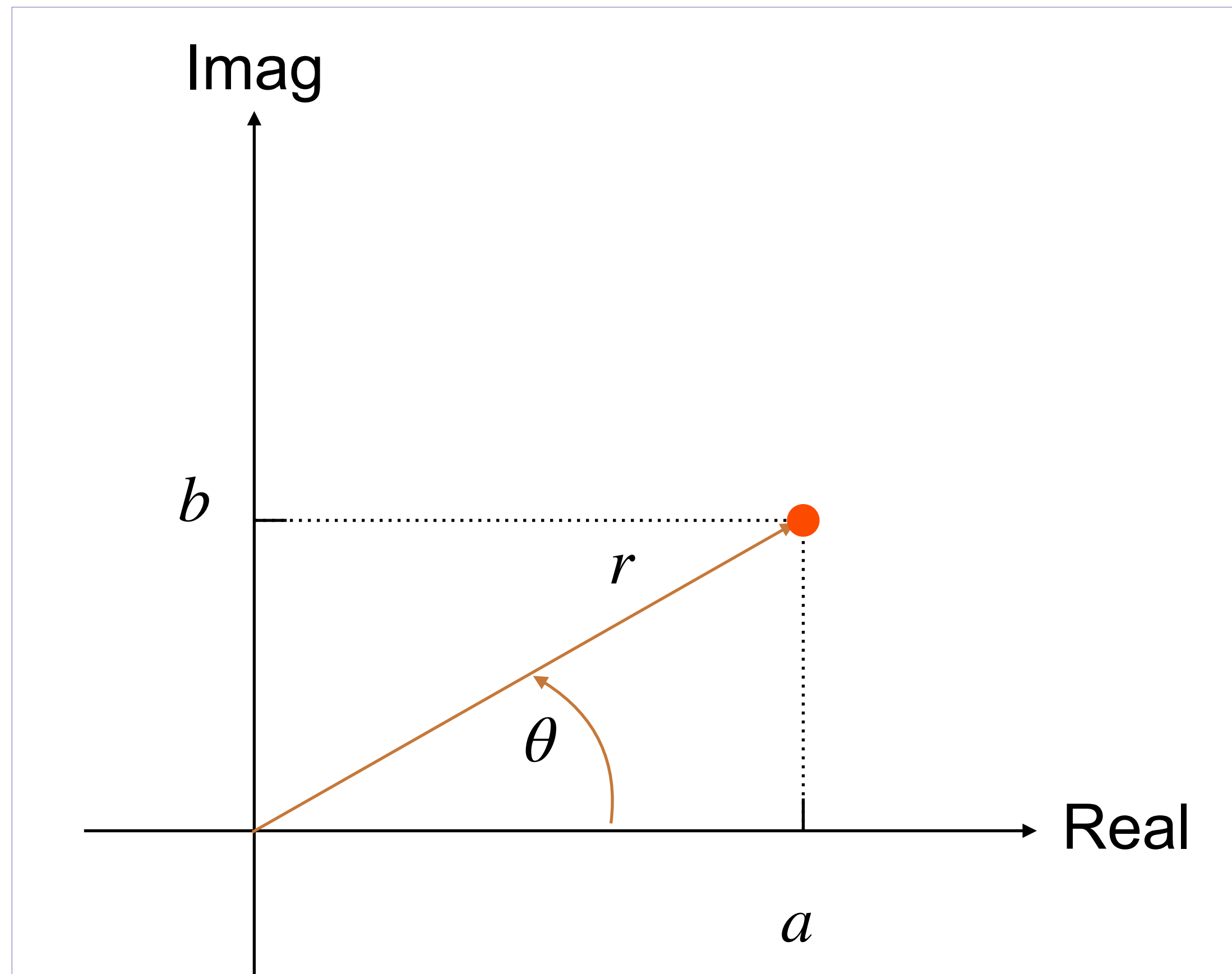
a is the real part

b is the imaginary part

$$z = re^{i\theta}$$

r is the magnitude

θ is the phase



Recall that

$$e^x e^y = e^{x+y}$$

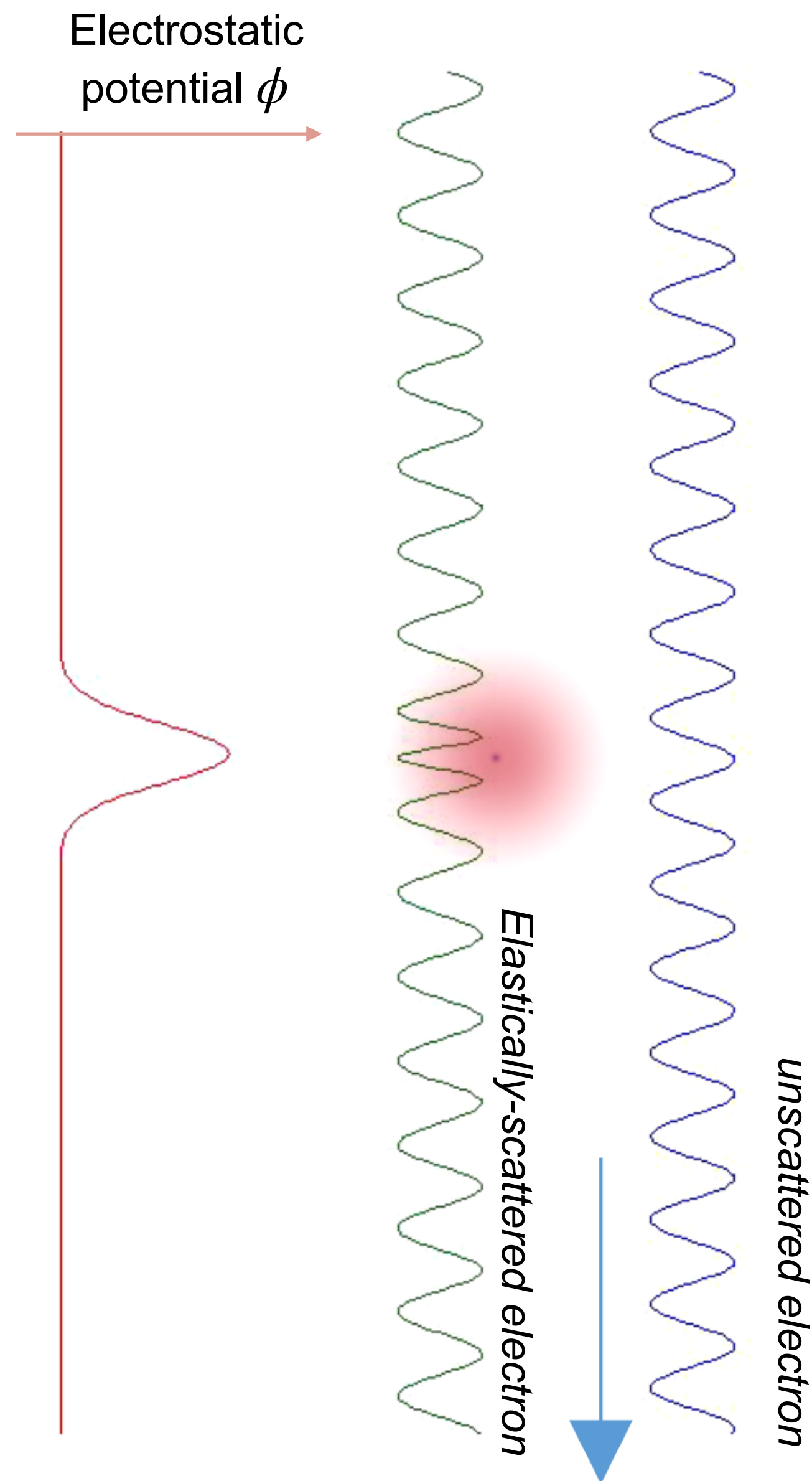
so, when you multiply
two complex numbers,
the phases add:

$$e^{i\theta_1} e^{i\theta_2} = e^{i(\theta_1 + \theta_2)}.$$

Phase contrast and the contrast transfer function

1. Complex numbers: review
2. Defocus contrast and the CTF (simple version)
3. Image delocalization
4. Objective lens effects on the CTF

Cryo-EM specimens are imaged by phase contrast



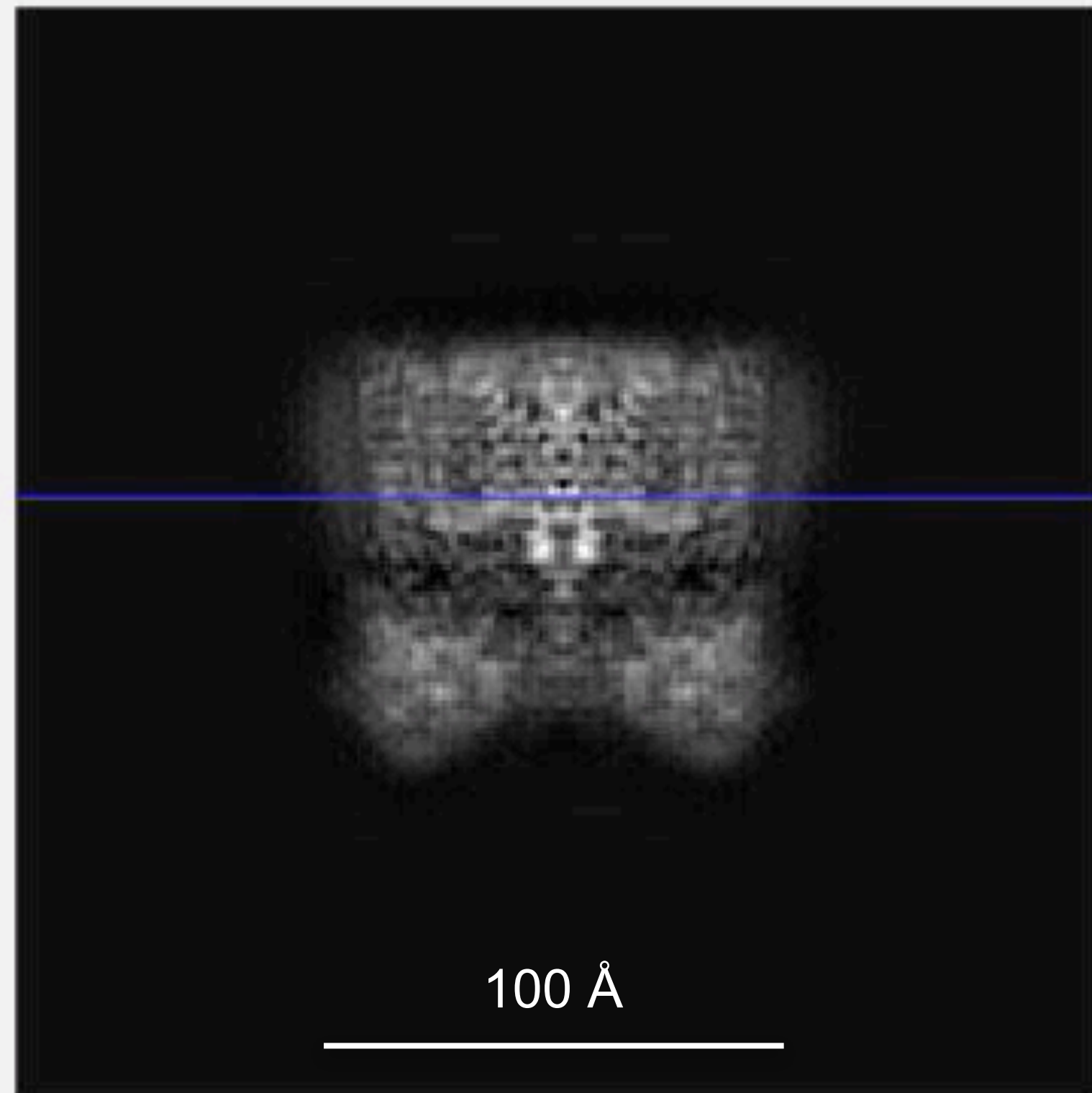
The imaging electrons are phase-shifted when passing near atomic nuclei or fixed charges.

The phase shift coefficient σ is about 0.5 milliradian per volt-angstrom of integrated potential.

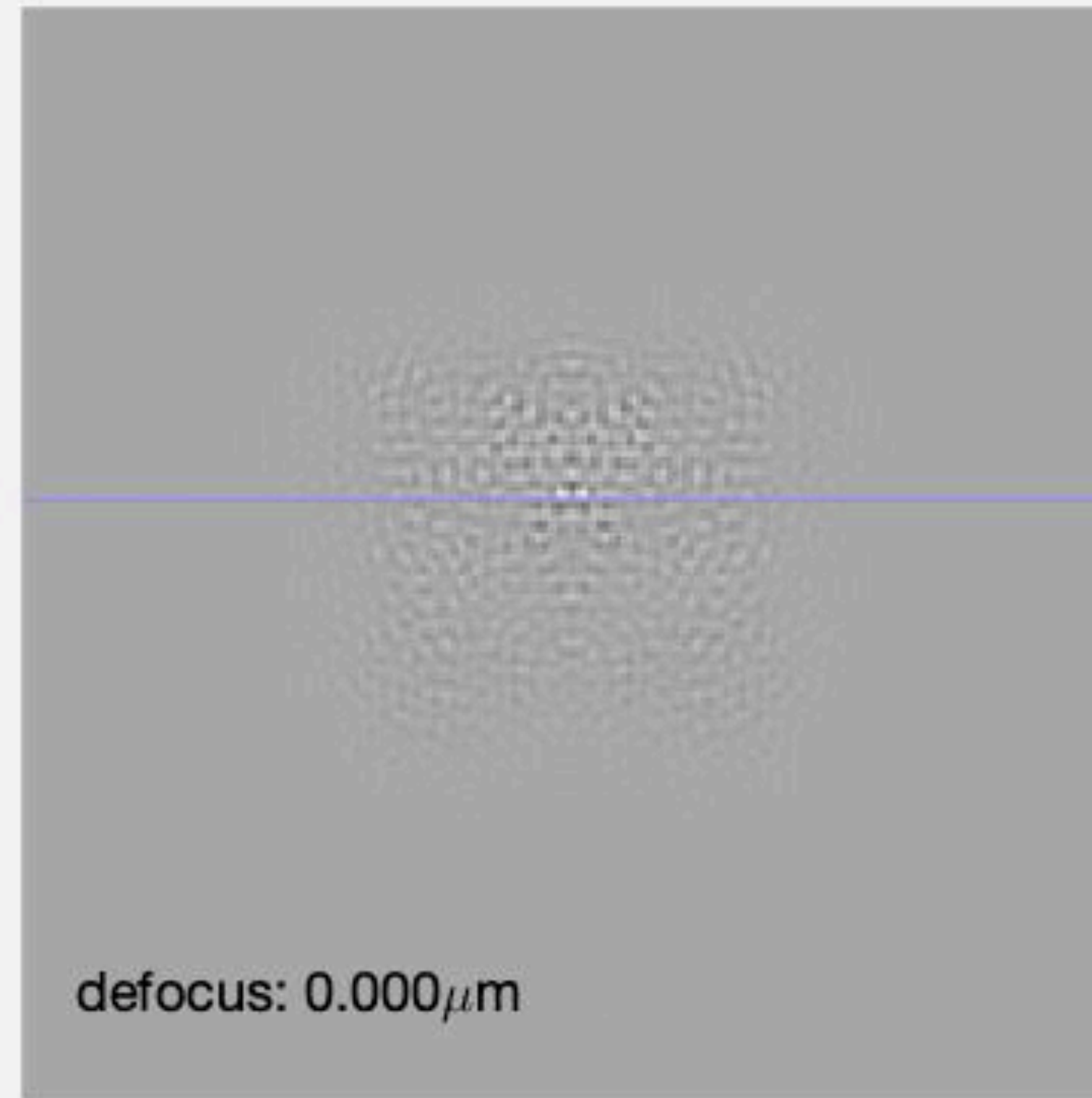
The phase shift near a single atom is ~ 1 milliradian.

Most cryo-EM data are acquired using defocus contrast

object



image



- At high defocus, high-resolution information in the image is strongly **delocalized**.
- Image processing can re-localize the signals, but at most **only about half of the theoretical contrast** is preserved by defocusing.

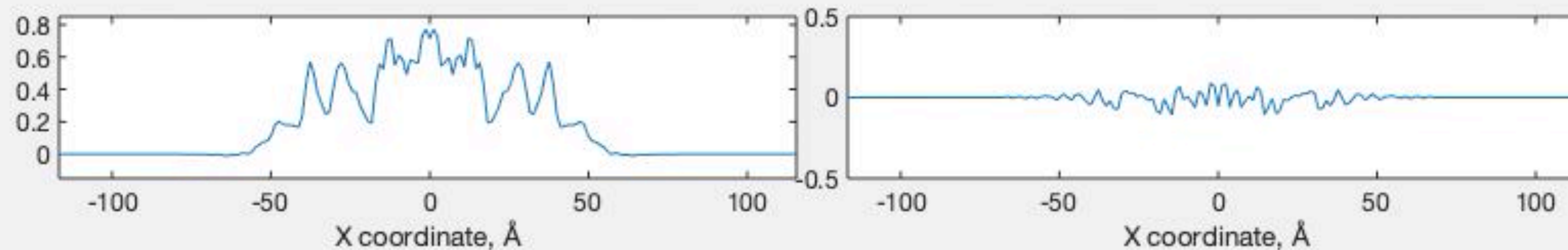
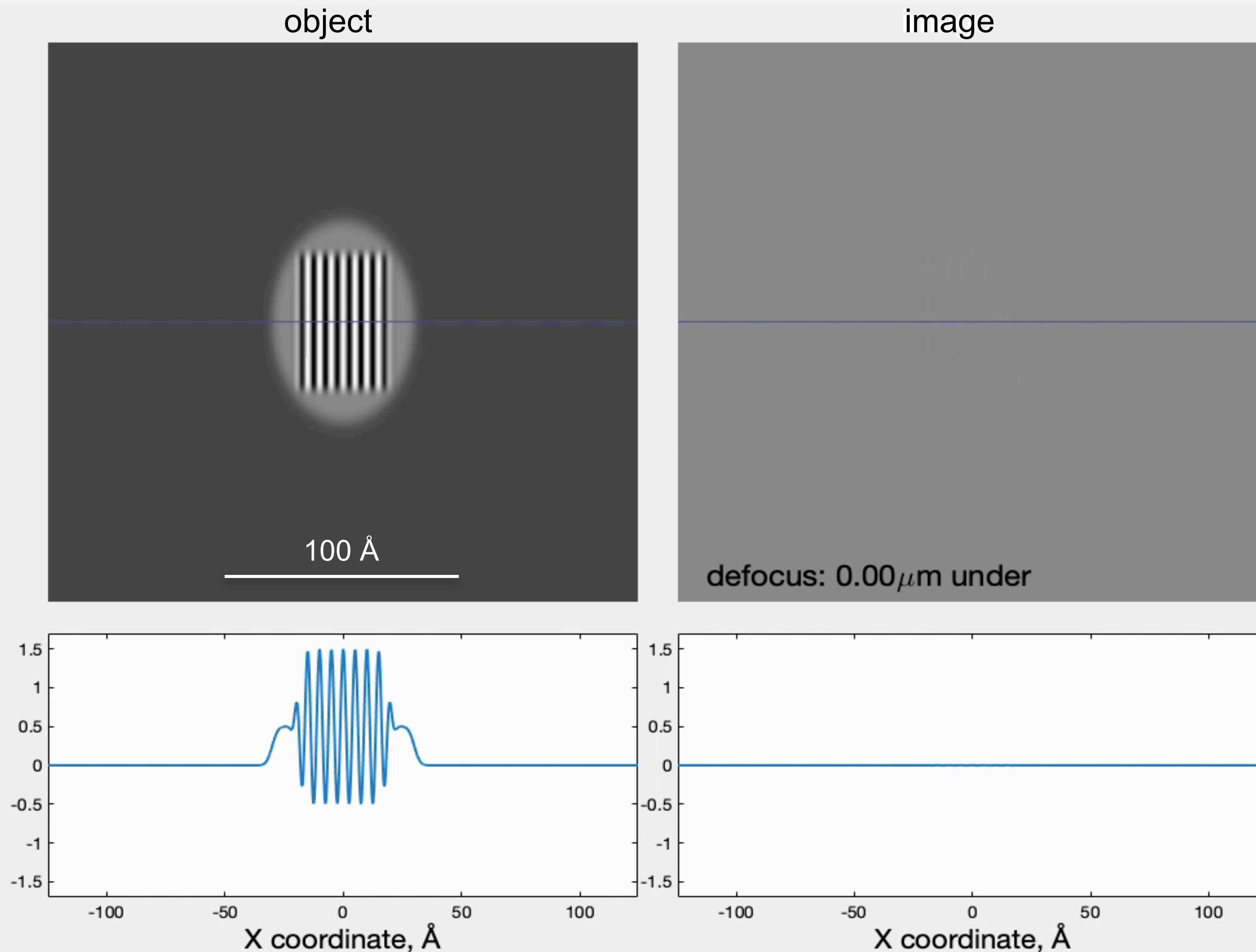


Image of an object with 5Å periodicity

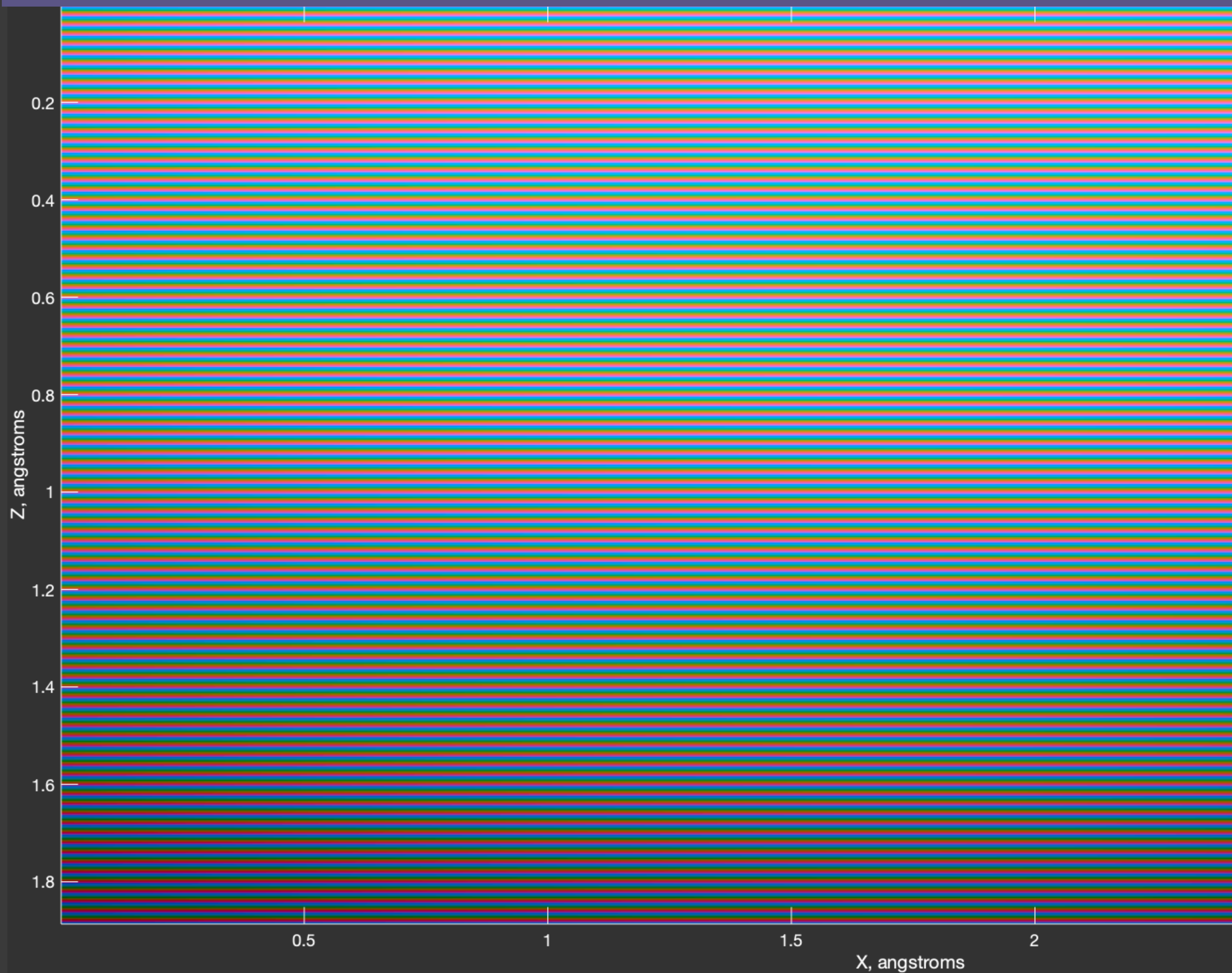


- At high defocus, high-resolution information in the image is strongly **delocalized**.
- Image processing can re-localize the signals, but at most **only about half of the theoretical contrast** is preserved by defocusing.

Defocus contrast in a nutshell

1. The contrast in the image of a grating object varies with the amount of defocus.
2. The grating object produces diffracted waves with shifting phase.
3. When the diffracted waves interfere with the undiffracted waves, we have contrast.

A snapshot of an electron wave



Energy (keV)	Wavelength (Å)	Velocity (fraction of c)
120	0.033	0.59
200	0.025	0.70
300	0.020	0.78

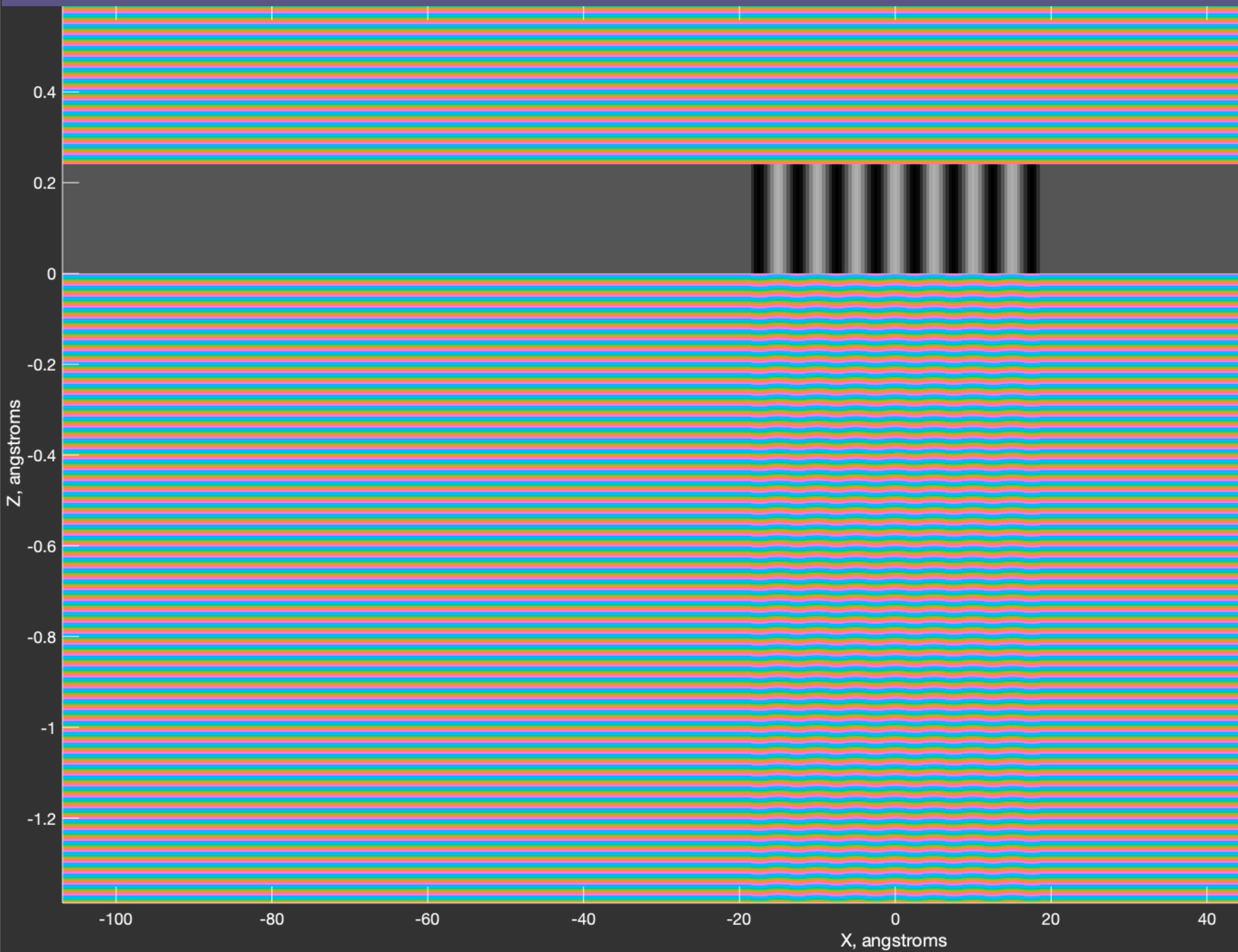
For an electron propagating in the z direction,
the time-independent wave function is

$$\Psi_0 = e^{ikz}$$

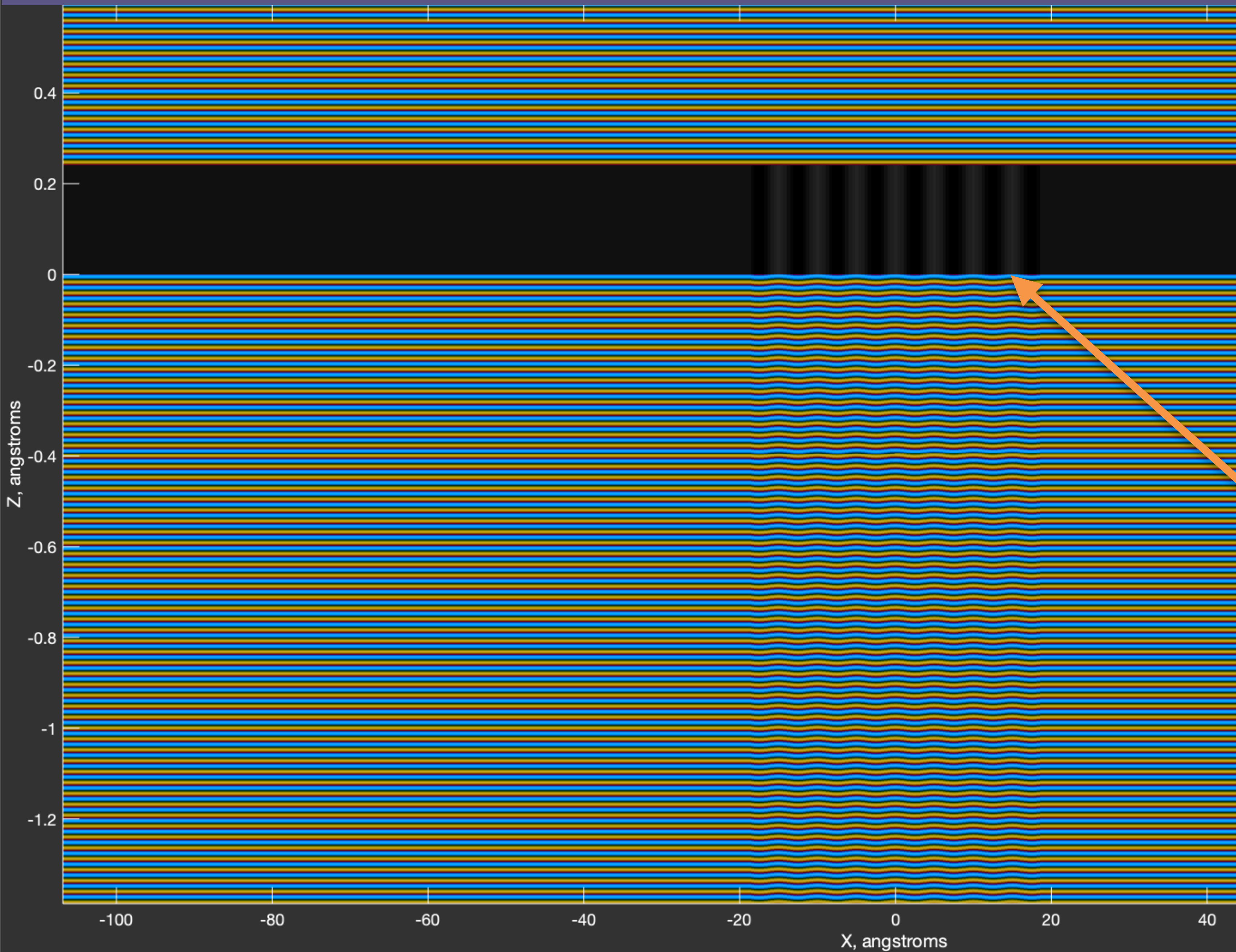
with

$$k = 2\pi/\lambda$$

Insert a phase-shifting object that perturbs the electron wave function



Insert a phase-shifting object that perturbs the electron wave function



The object is a grating,
 $\epsilon\phi(x) = \epsilon \cos(2\pi x/d)$.

Example:

$d = 5\text{\AA}$ and $\epsilon \ll 1$.

At $z = 0$,

$$\Psi = e^{i\epsilon\phi(x)}$$

The weak-phase approximation

- Just below the specimen, at $z = 0$, the electron wave function is $\Psi = e^{i\epsilon\phi(x)}$.
- Then, by the approximation $e^x \approx 1 + x$ we have just after the specimen

$$\Psi \approx 1 + i\epsilon\phi(x)$$

This is the **weak phase approximation**.

What are the two terms in the approximation?

- There is an **undiffracted wave**—essentially the same as the incident wave—of amplitude 1. We'll call this Ψ_0
- And there is a new wave combination of amplitude ϵ . In this example of a grating there are actually two **diffracted waves**, Ψ_+ and Ψ_-
- The full wavefunction is

$$\Psi = \Psi_0 + \Psi_+ + \Psi_-$$

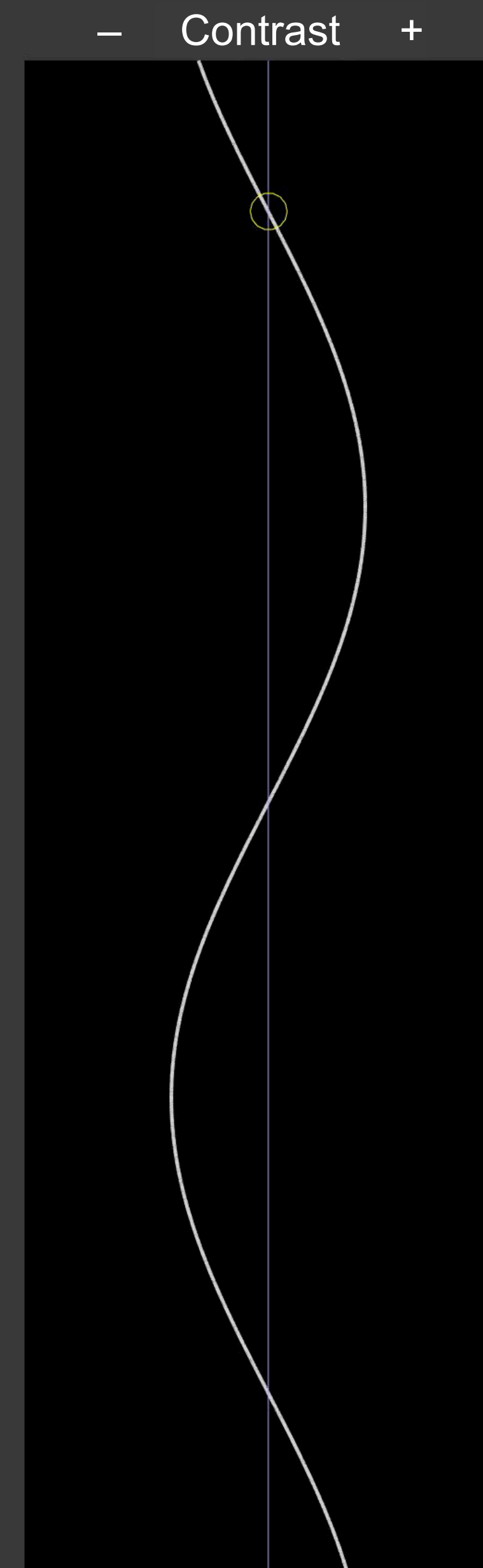
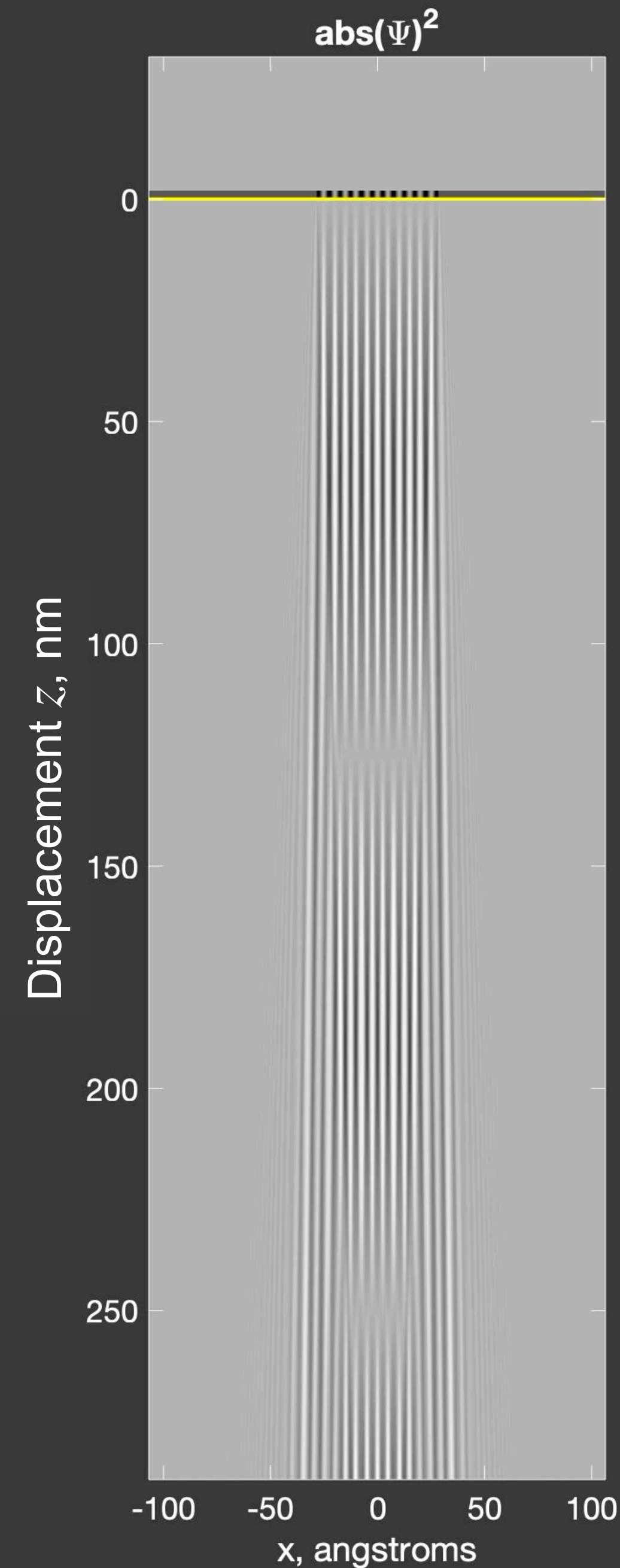
The contrast of a grating object varies with the distance below the object



Intensity at z

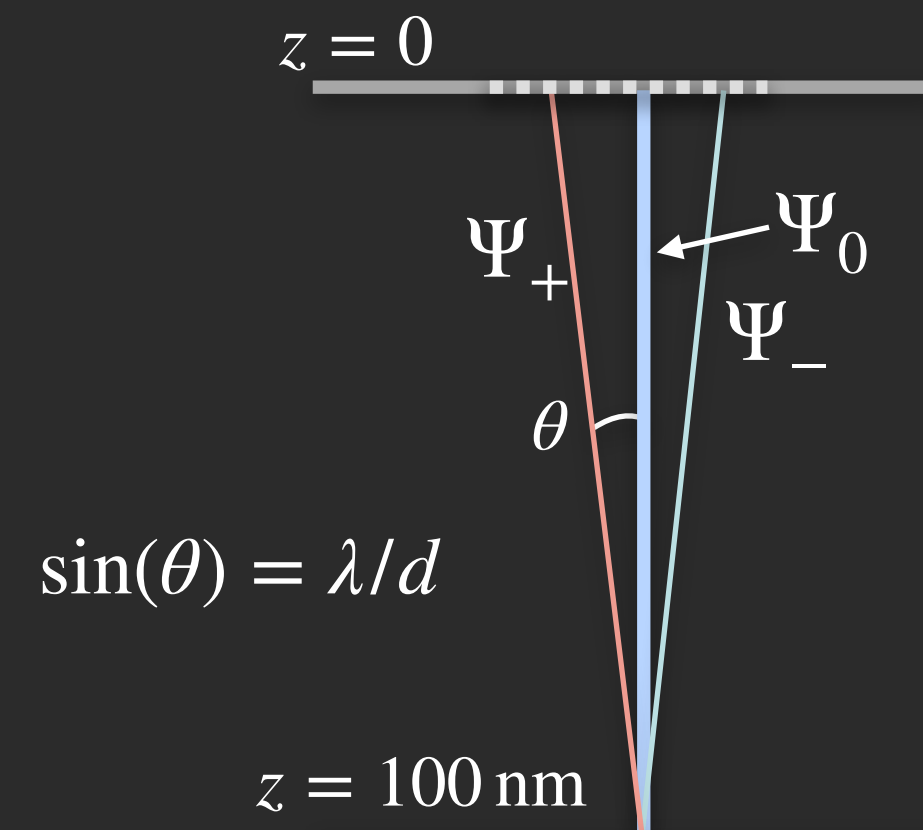
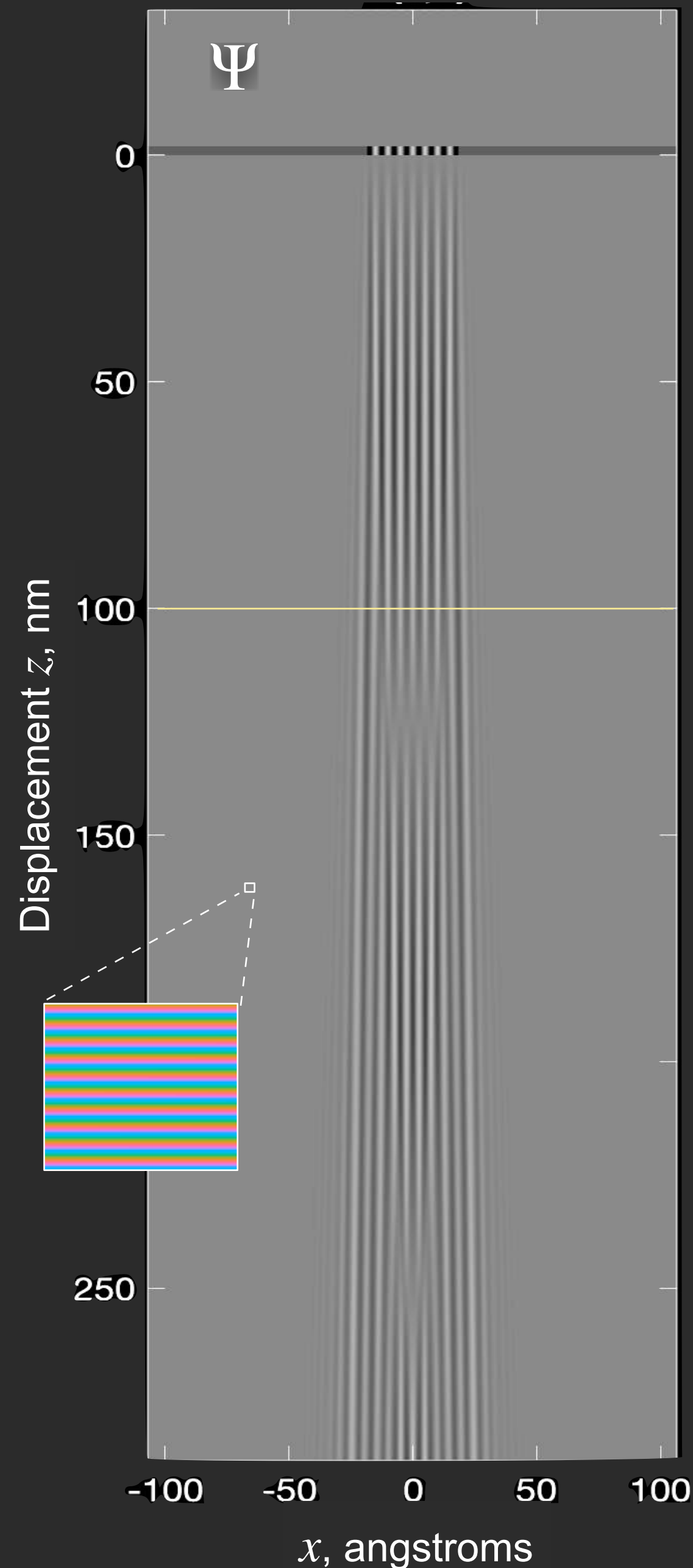


The grating $\phi(x)$



Interference between the undiffracted wave and diffracted waves produces contrast.

Waves interfere to make contrast



- The two diffracted waves Ψ_+ and Ψ_- travel at very small angles $+\theta$ and $-\theta$ to the undiffracted wave.
- To reach a distance z below the specimen, they take a path longer than Ψ_0 does. Let ζ = the path length difference.

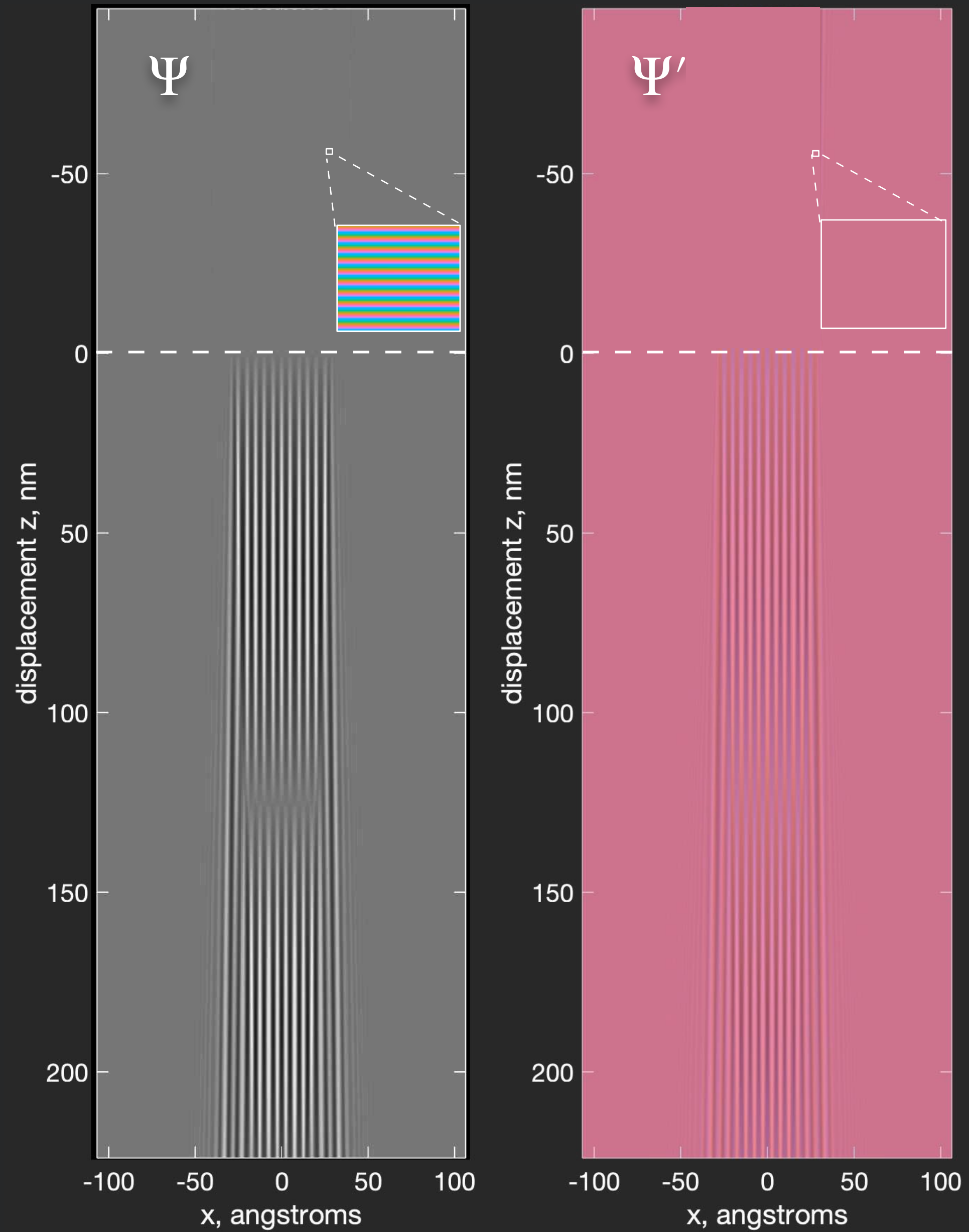
$$\zeta = \frac{z}{\cos \theta} - z \approx z\lambda^2/2d^2.$$

- In our example $\lambda = .02\text{\AA}$ and the grating $d = 5\text{\AA}$. At the level $z = 100 \text{ nm}$, $\zeta = .008\text{\AA}$, about half a wavelength.
- Define χ = the phase difference between the undiffracted and diffracted waves.

$$\begin{aligned}\chi &= 2\pi\zeta/\lambda \\ &= \pi\lambda z/d^2\end{aligned}$$

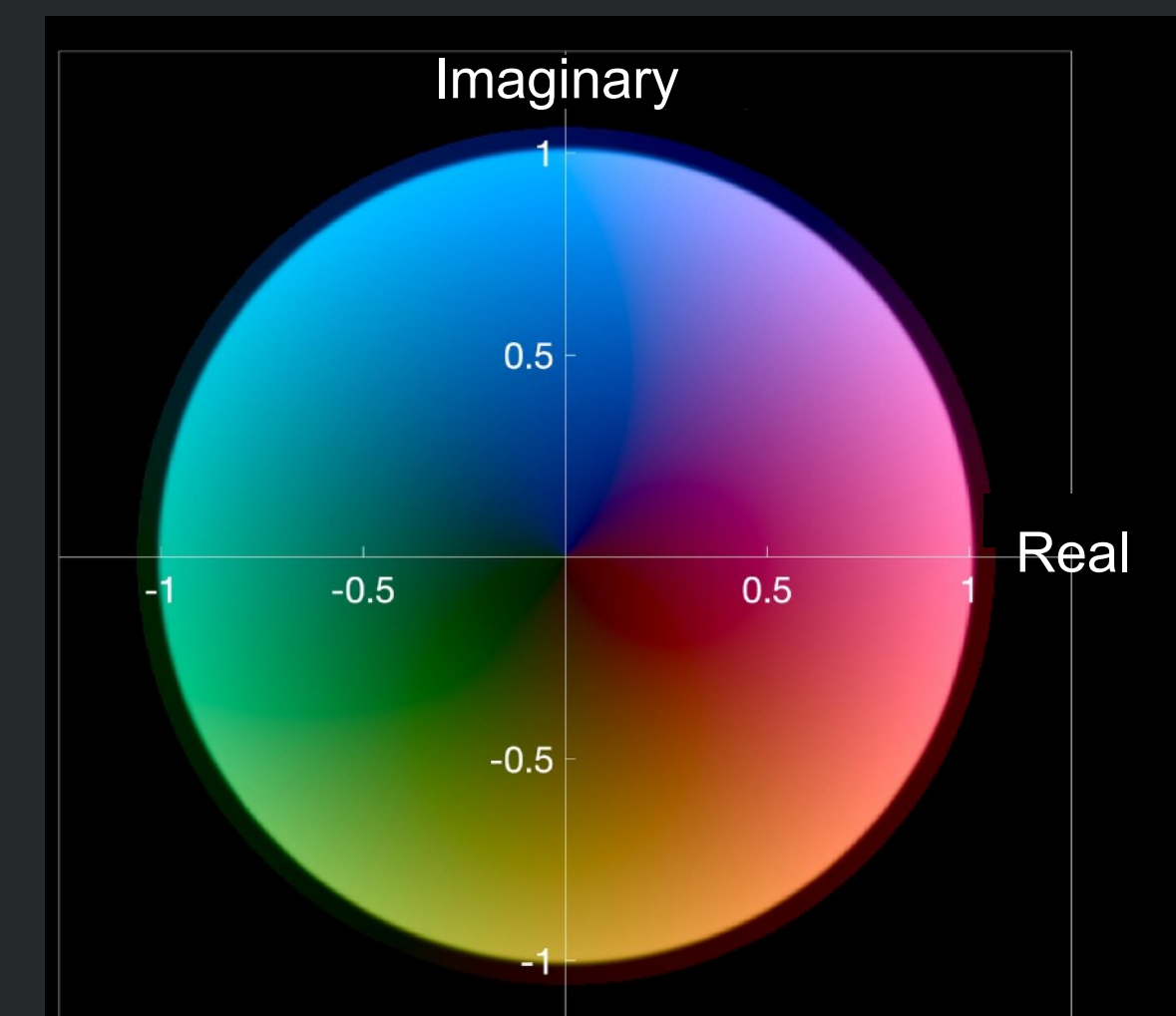
- In this example $\chi = 0.8\pi$

Where the phase of the diffracted waves is right, we have contrast.

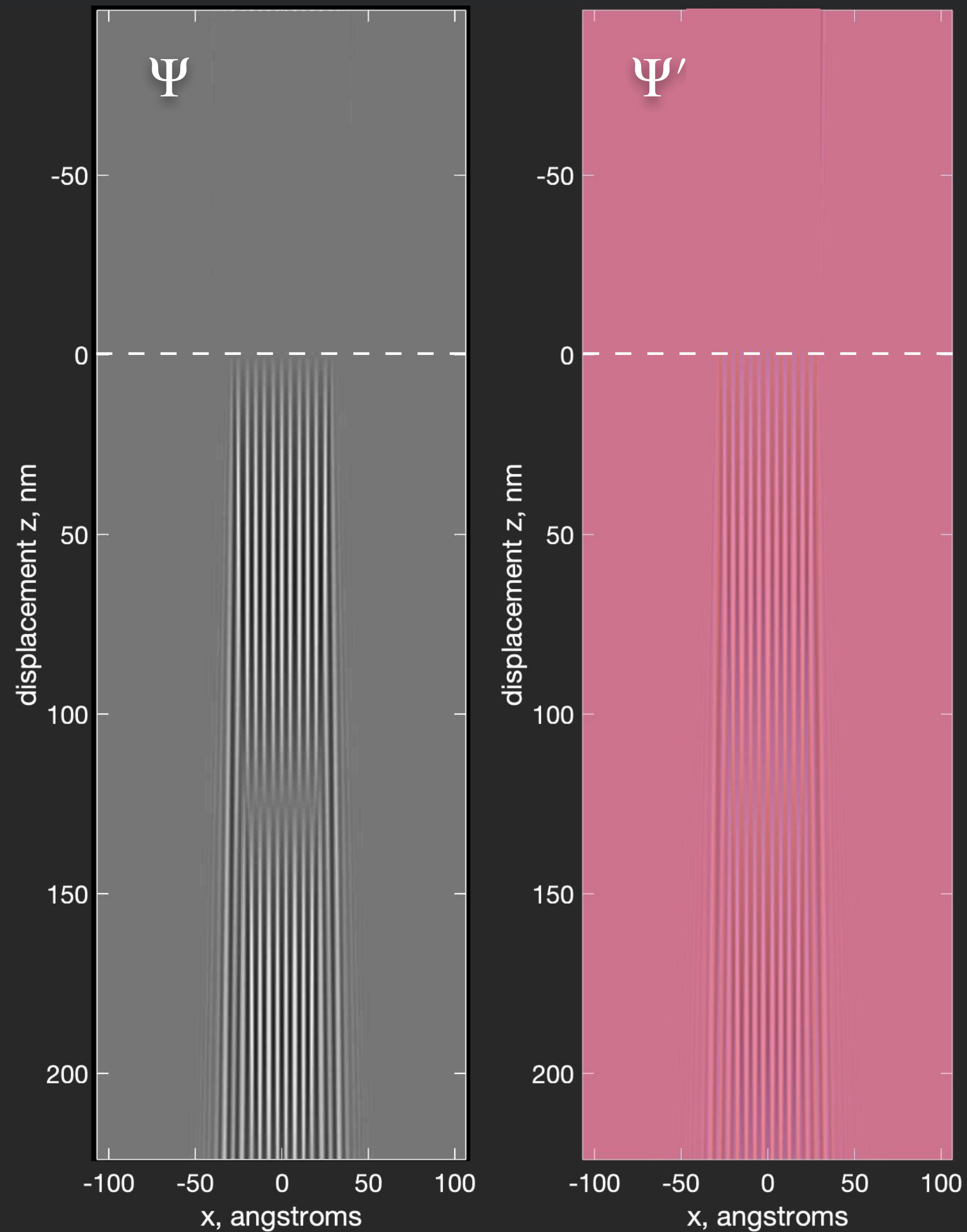


Let's unwrap the oscillations in Ψ :
We'll define $\Psi' = \Psi/\Psi_0$

Complex number color scheme



Where the phase of the diffracted waves is right, we have contrast.



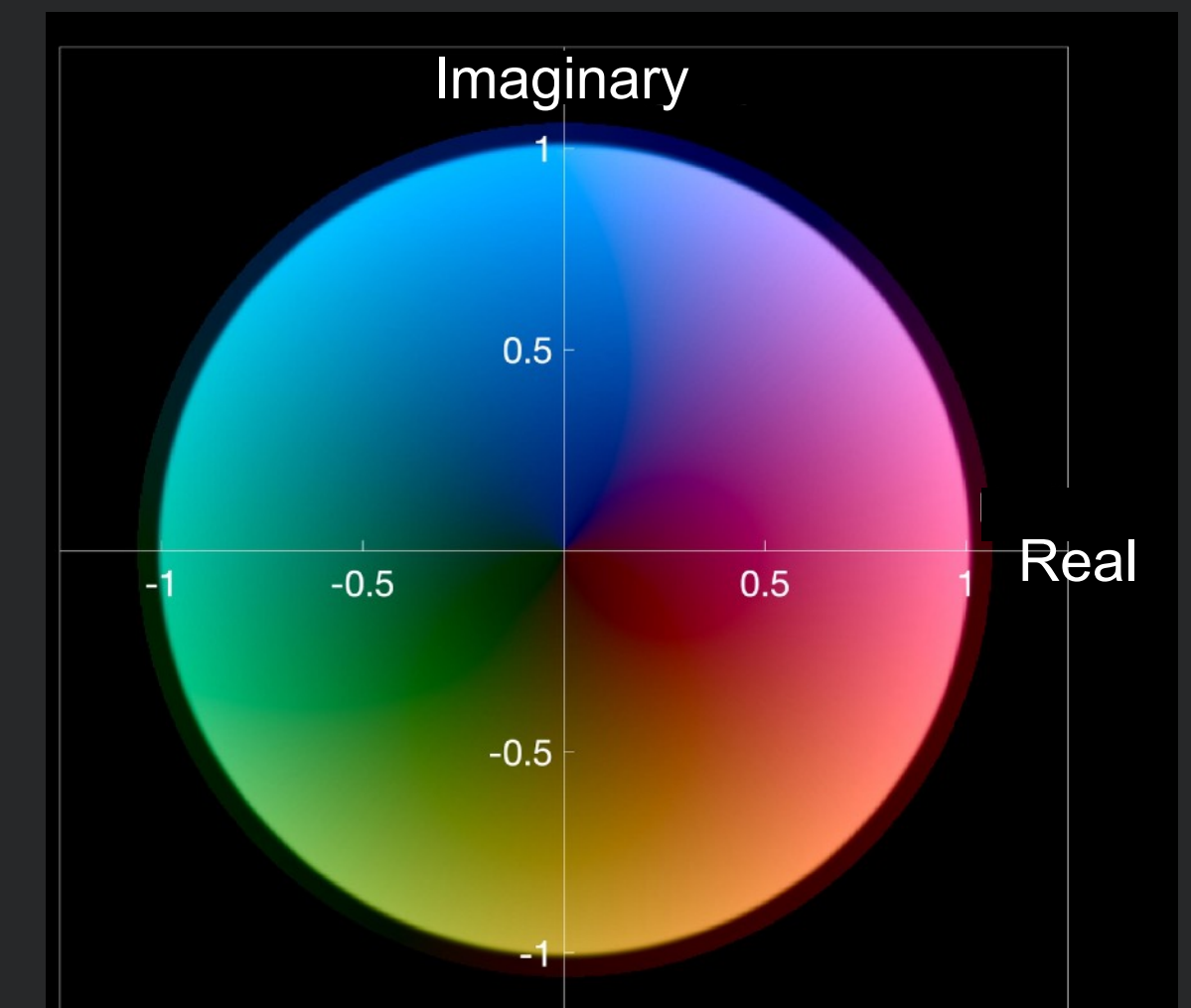
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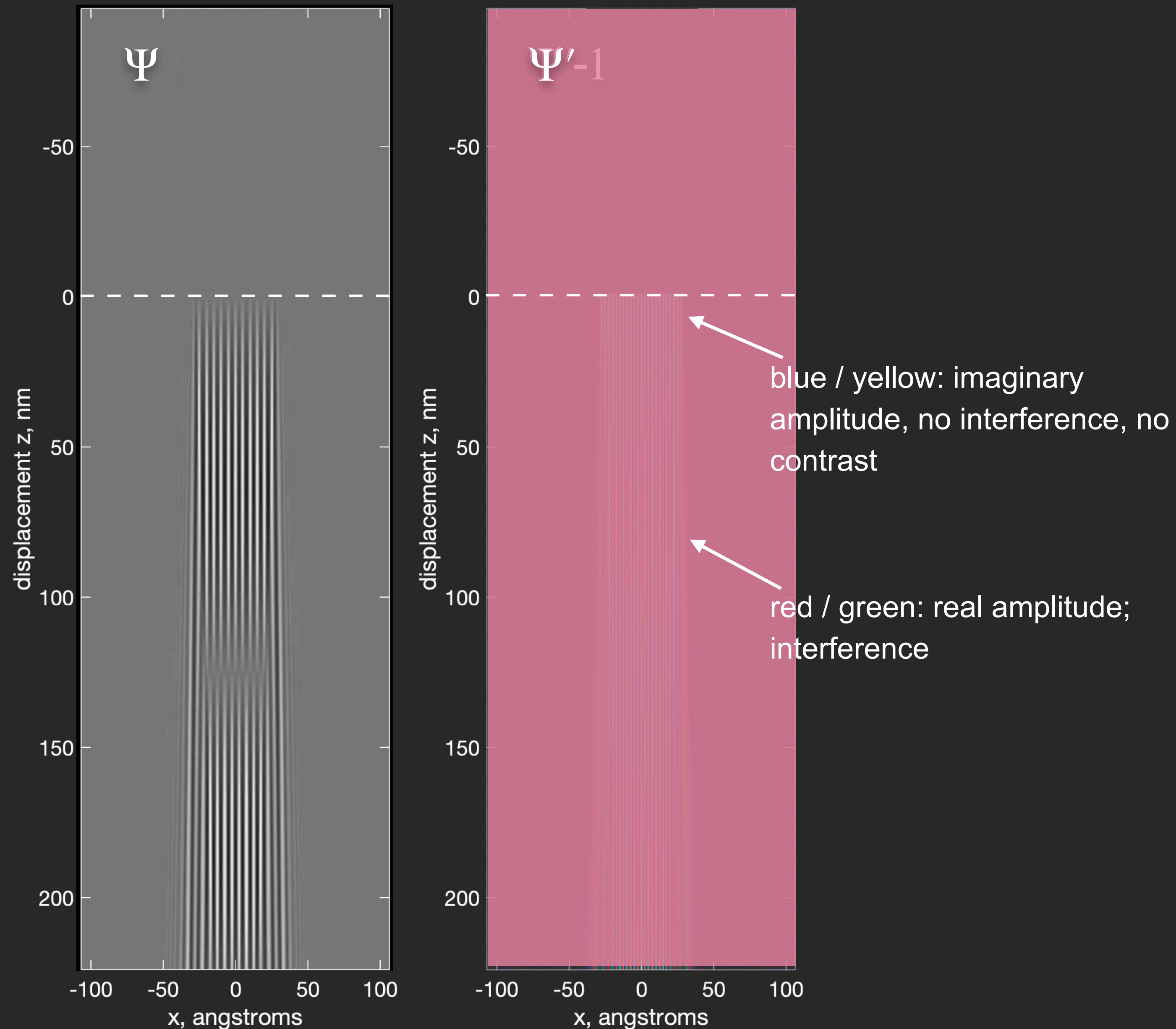
Let's remove the undiffracted wave, so we have just the diffracted waves,

$$(\Psi' - 1) = \Psi_+ + \Psi_-$$

Complex number color scheme



When the phase of the diffracted waves is right, we have contrast.



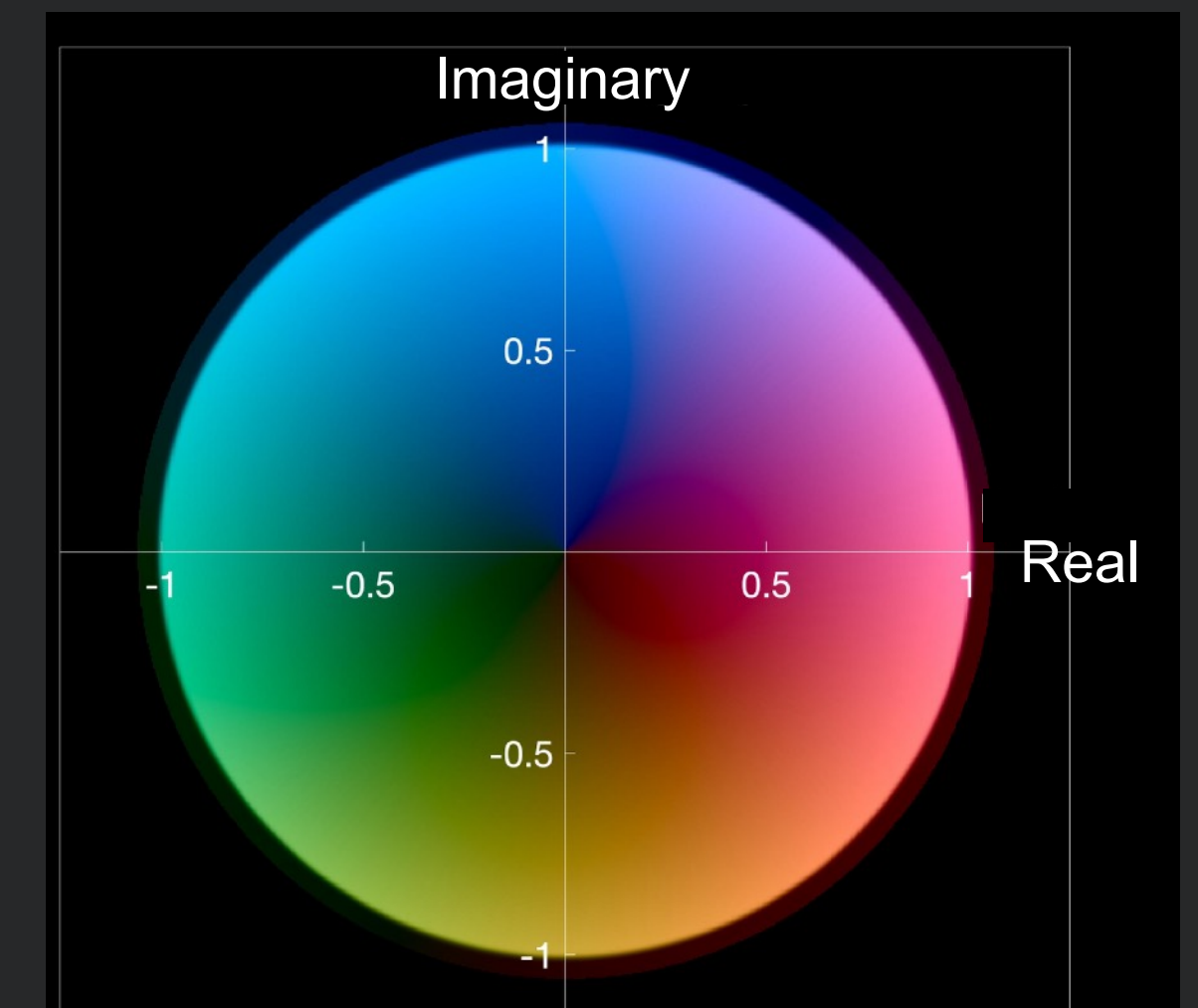
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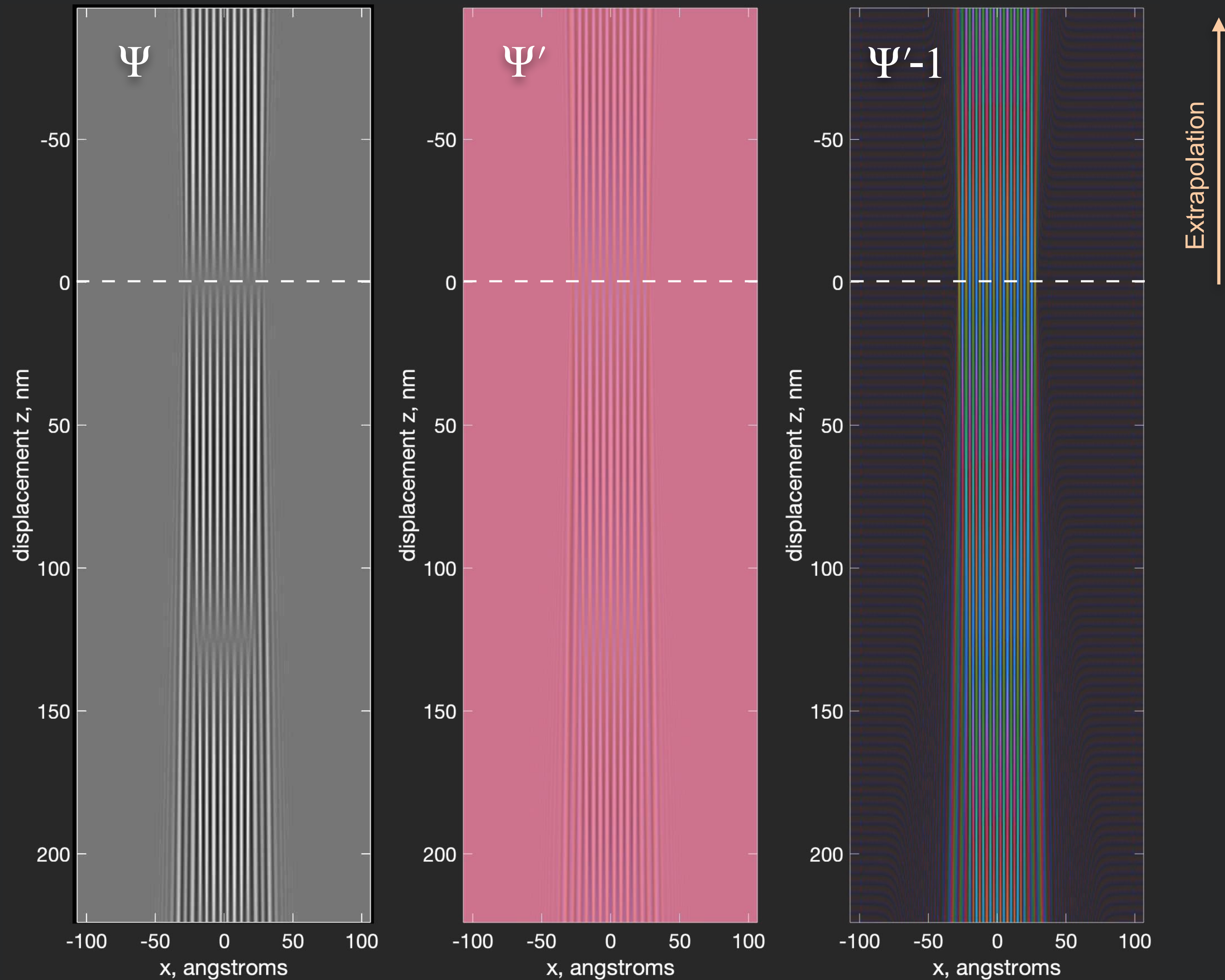
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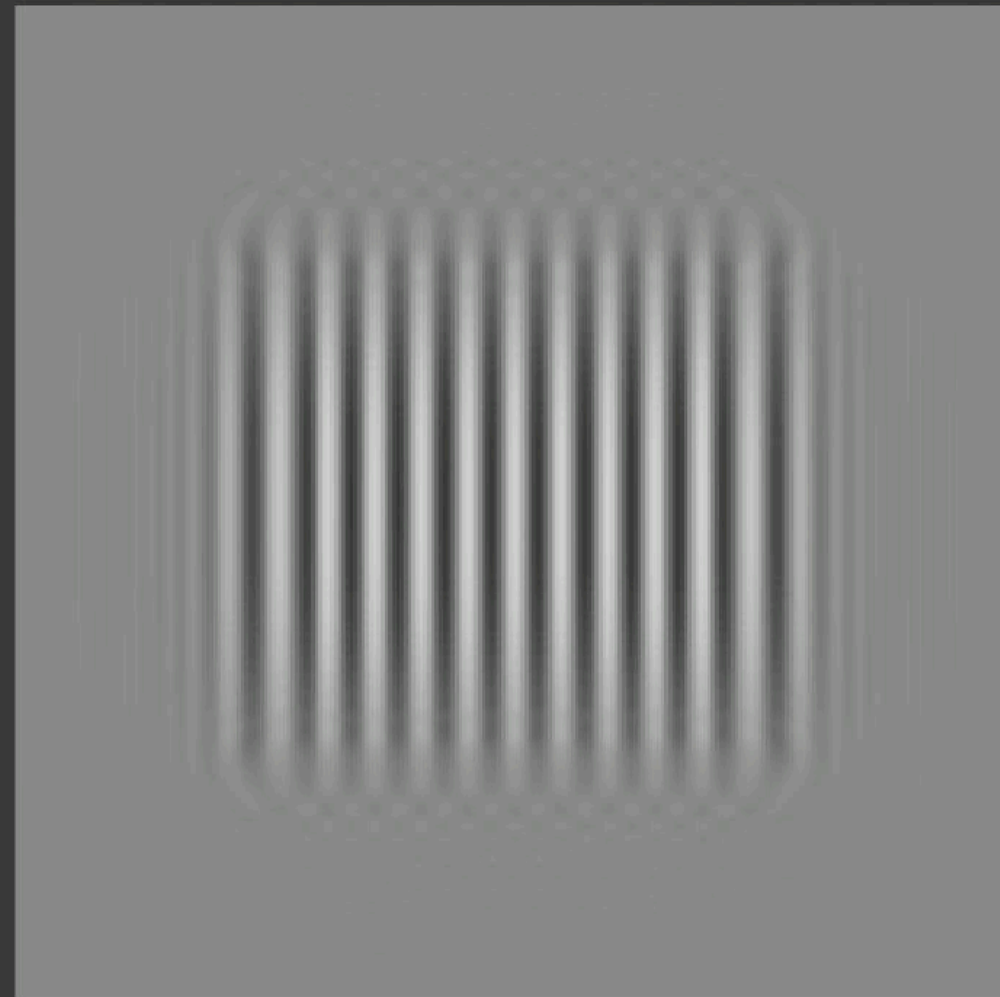
What happens when the objective lens is focused *above* the specimen?



What wavefunction **above** the specimen would give rise to what we see below it?

We can back-propagate Ψ :
this is what the objective lens “sees”

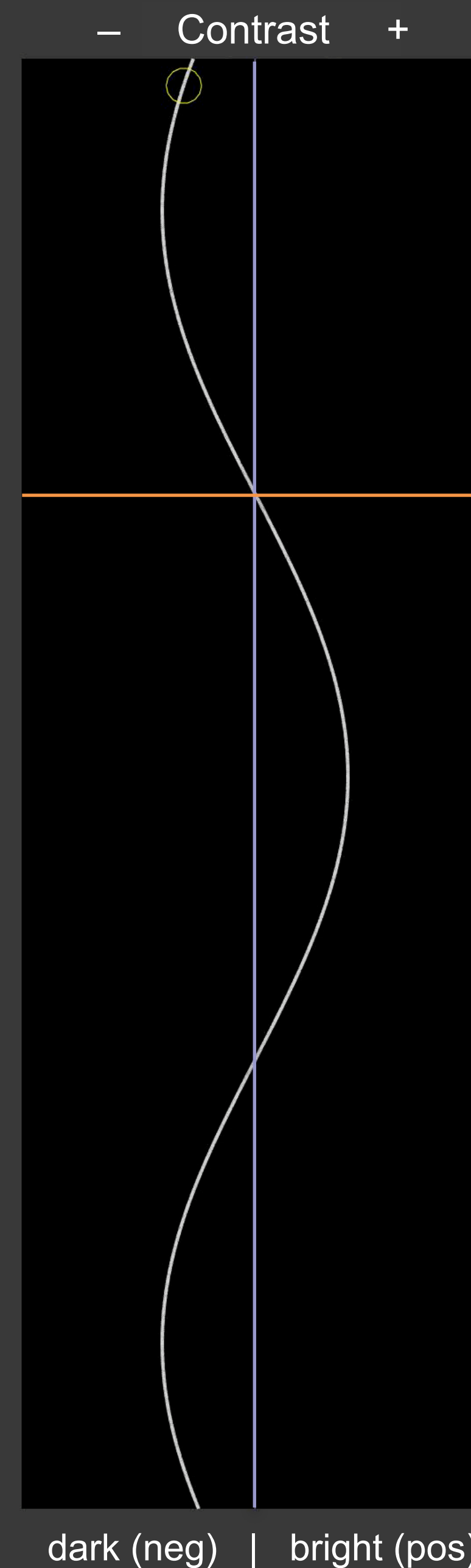
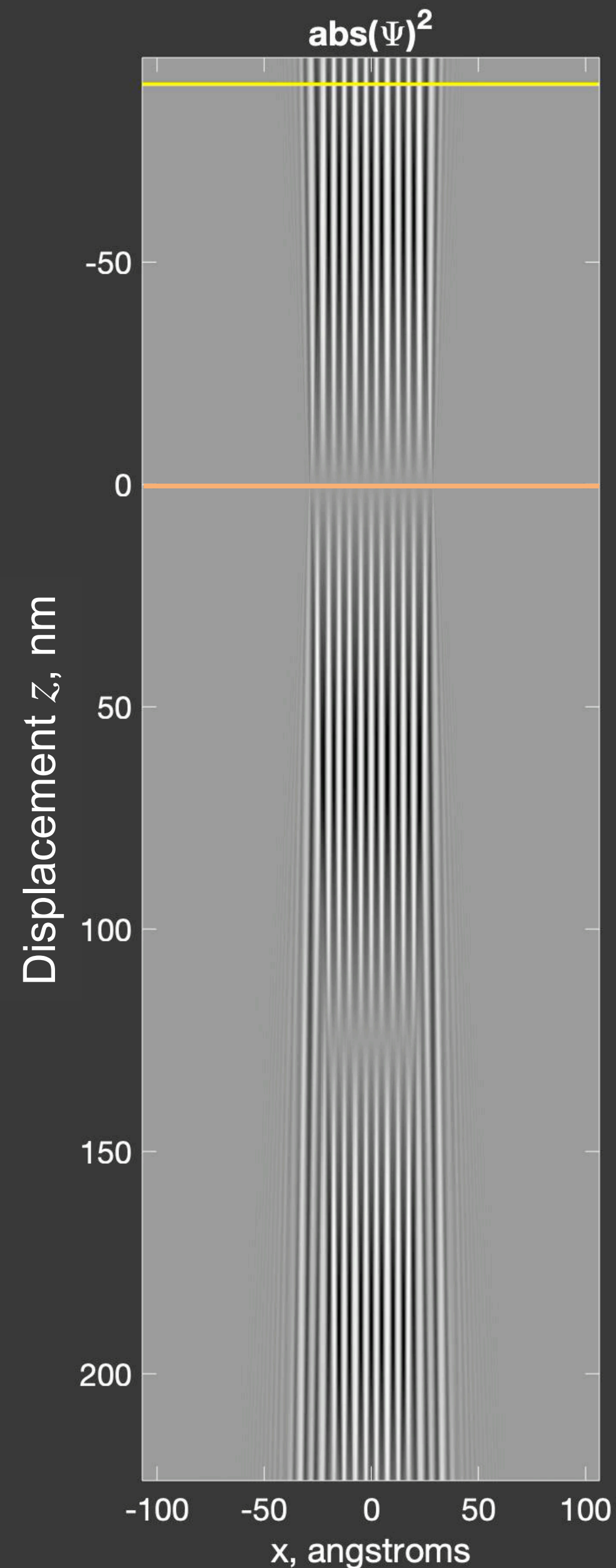
What happens when the objective lens is focused *above* the specimen?



Intensity at z



The grating $\phi(x)$

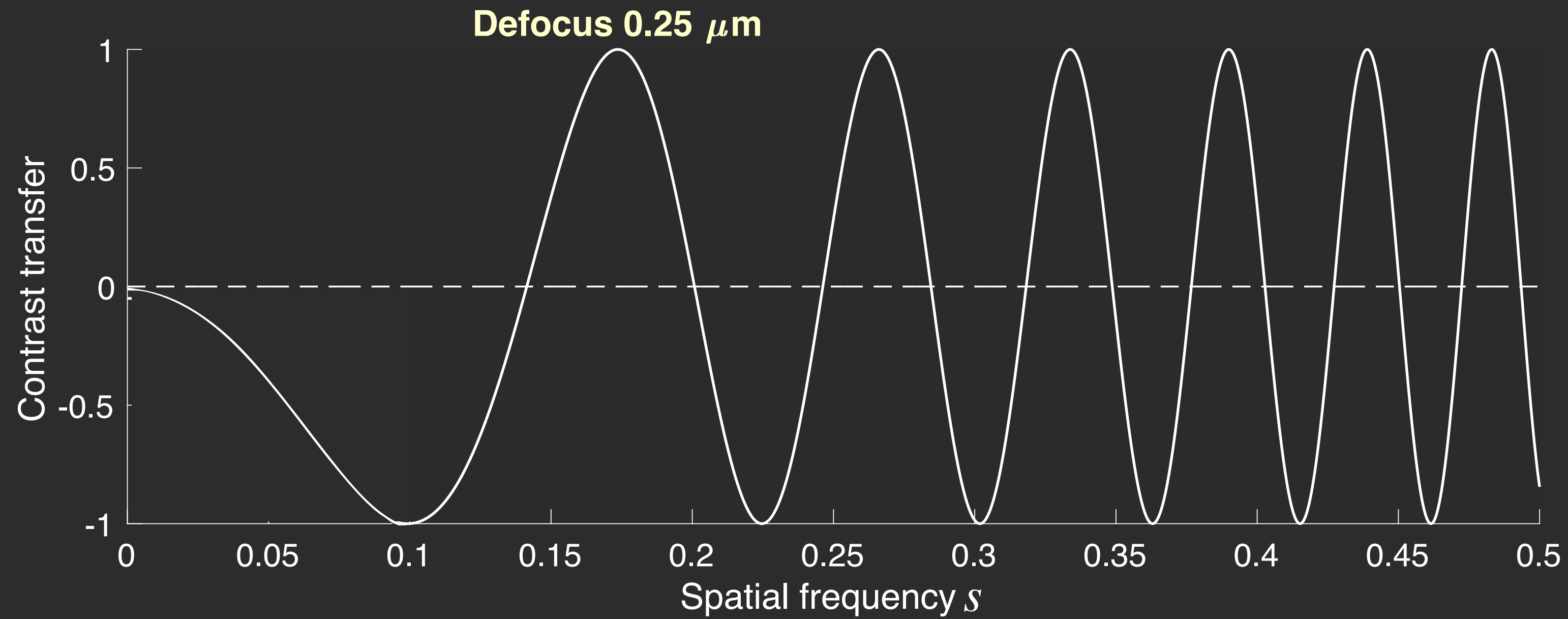


Terminology

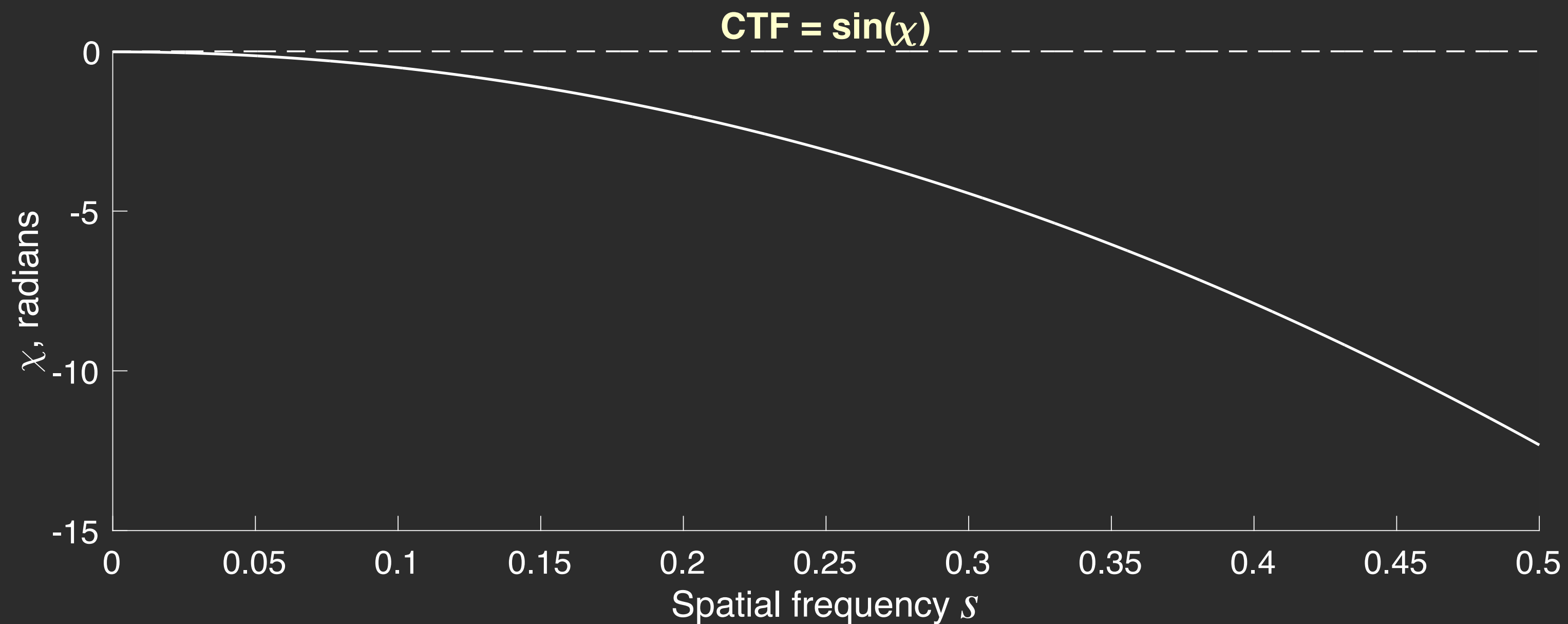
- “Underfocus” is focusing the objective lens above the specimen.
- By convention, defocus values δ are positive for underfocus:
 $\delta = -z$
- Spatial frequency is $s = 1/d$
- The phase shift χ is proportional to δ .
- The contrast transfer function is given by

$$\begin{aligned} \text{CTF} &= \sin(\chi) \\ &= \sin(-\pi\lambda\delta s^2) \end{aligned}$$

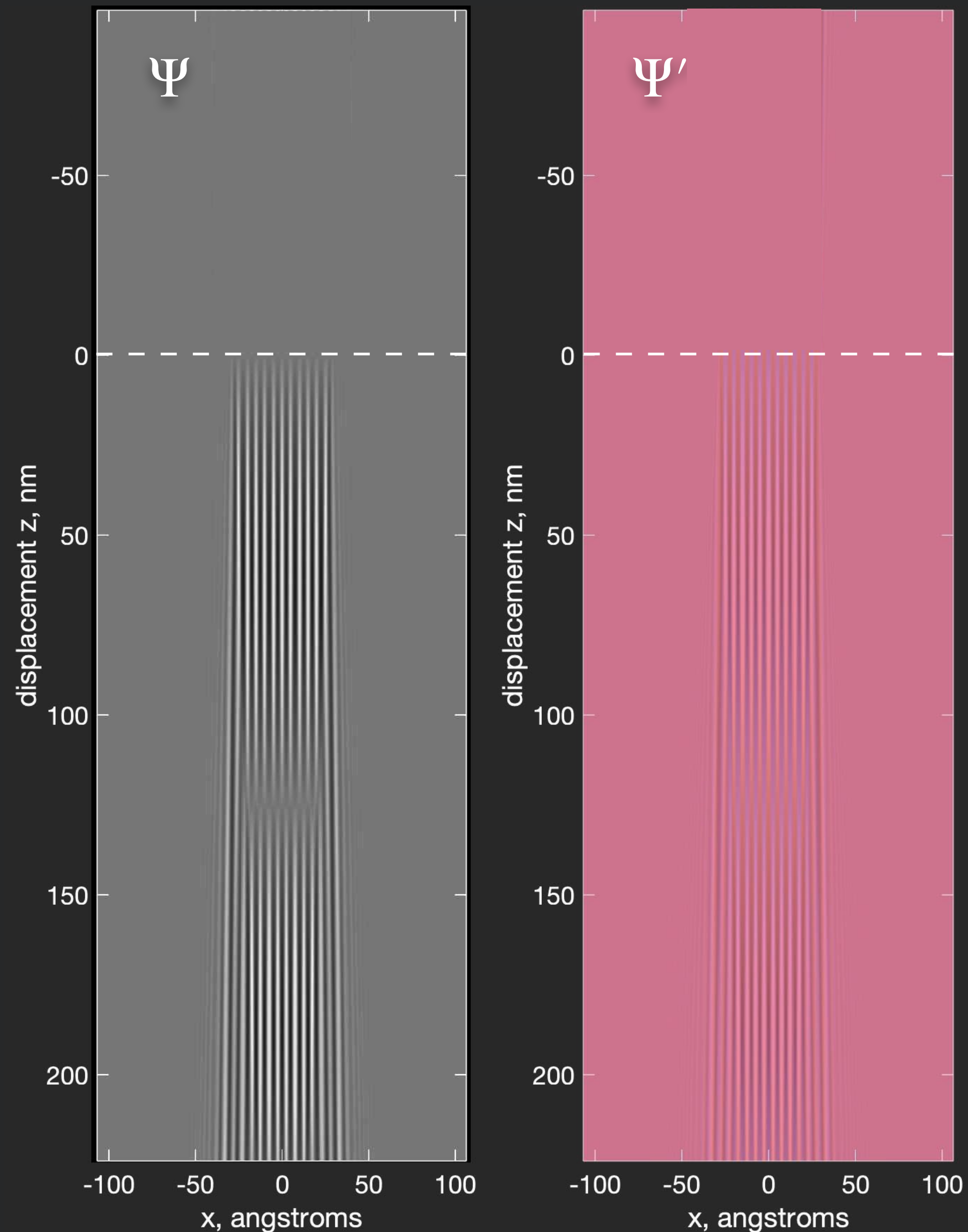
The basic contrast-transfer function as a function of s



$$\text{CTF} = \sin(-\pi\lambda\delta s^2)$$



Formal derivation of the defocus-contrast CTF



We define

$$\Psi' = \Psi / \Psi_0$$

$$\Psi' = 1 + ie^{-ik\zeta} \cdot \epsilon \cos(2\pi x/d)$$

and can be written as

$$\Psi' = 1 + ie^{-i\chi} \epsilon \phi(x).$$

Grating object:

$$\epsilon \phi(x) = \epsilon \cos(2\pi x/d)$$

Electron propagation:

$$k = 2\pi/\lambda$$

Diffracted wave path difference:

$$\zeta \approx z\lambda^2/2d^2$$

Wave aberration function:

$$\chi = k\zeta \approx \pi\lambda z/d^2$$

Formal derivation of the CTF for a grating of spacing d

$$\Psi' = 1 + ie^{-i\chi} \epsilon \phi(x).$$

The measured intensity is

$$\begin{aligned} |\Psi|^2 &= |\Psi'|^2 = (\text{real part})^2 + (\text{imag part})^2 \\ &= [1 + \sin(\chi) \epsilon \phi(x)]^2 + [\cos(-\chi) \epsilon \phi(x)]^2 \\ &= [1 + 2 \sin(\chi) \epsilon \phi(x) + \mathcal{O}(\epsilon^2)] + [\mathcal{O}(\epsilon^2)]. \end{aligned}$$

Grating object:

$$\epsilon \phi(x) = \epsilon \cos(2\pi x/d)$$

Wave aberration function:

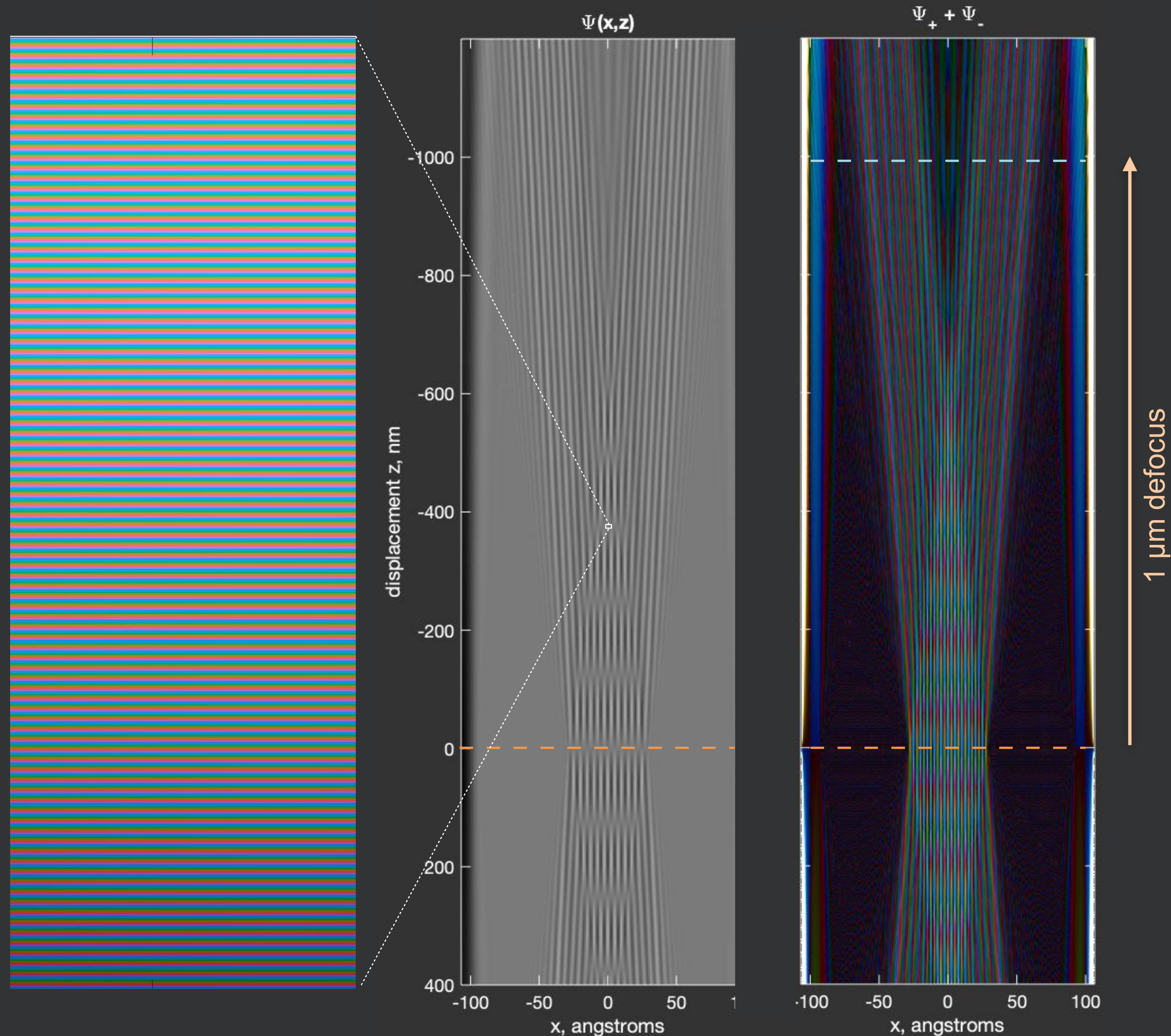
$$\chi \approx \pi \lambda z / d^2$$

In practice

- We ignore the constant background intensity.
- Everyone ignores the factor of 2 also.
- So we say the transfer from phase shift to intensity change is

$$\text{CTF} = \frac{\Delta \text{Intensity}}{\Delta \text{Electron phase}} = \sin(\chi)$$

A little defocus is actually a long distance

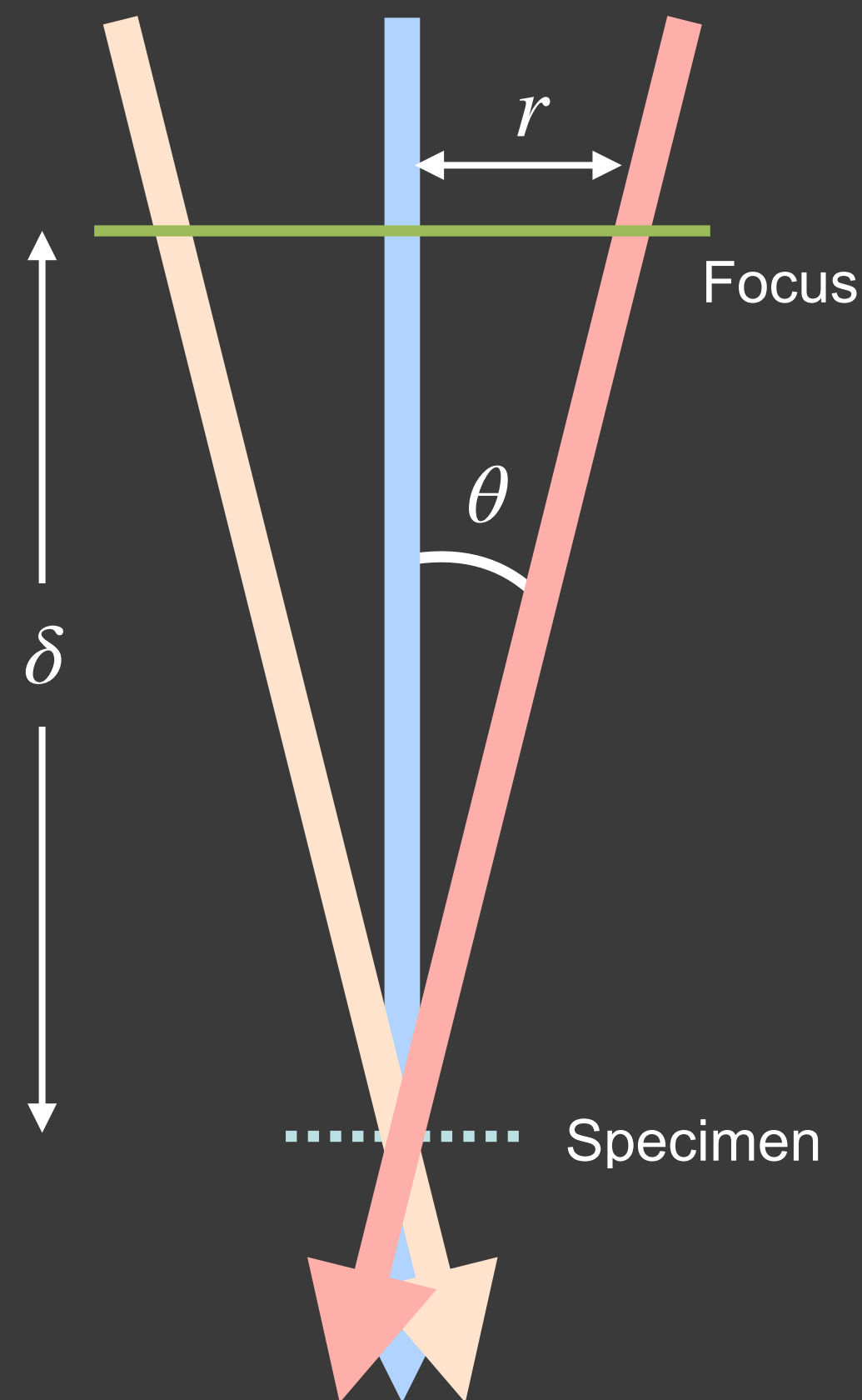


1 μm —a moderate defocus for cryo-EM imaging—is 500,000 wavelengths!

This has ramifications regarding

- beam coherence
- specimen charging
- delocalization

With large defocus, how bad is the image delocalization?



The dispersion radius is given by

$$r = \delta \tan \theta$$
$$= \delta \lambda s \text{ (small angle approx*)}$$

For example at 3 μm defocus and 3 $\text{\AA}$ resolution

$$\delta = 3 \times 10^4 \text{\AA}$$

$$\lambda = .02 \text{\AA}$$

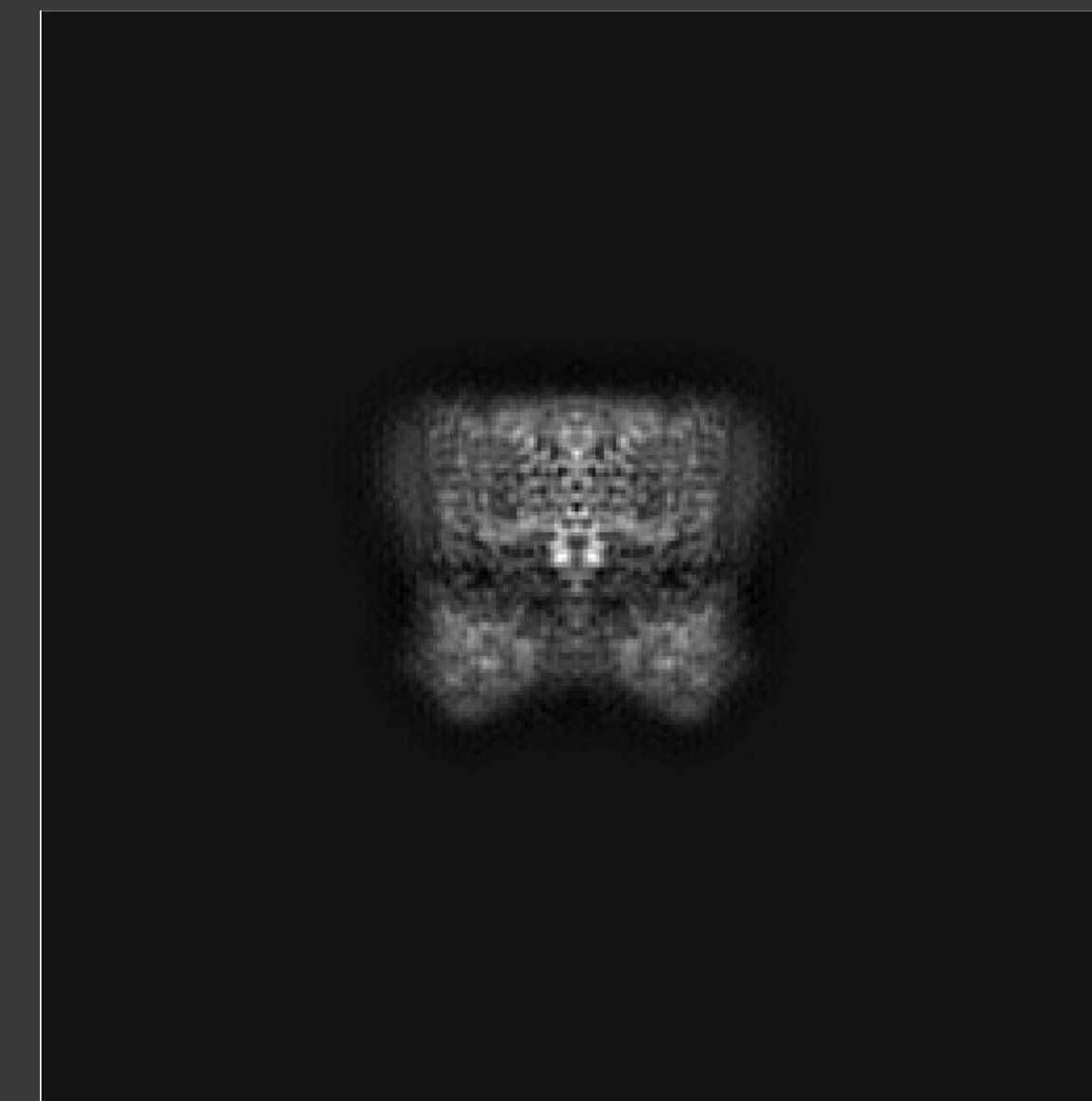
$$s = 0.33 \text{\AA}^{-1}$$

then

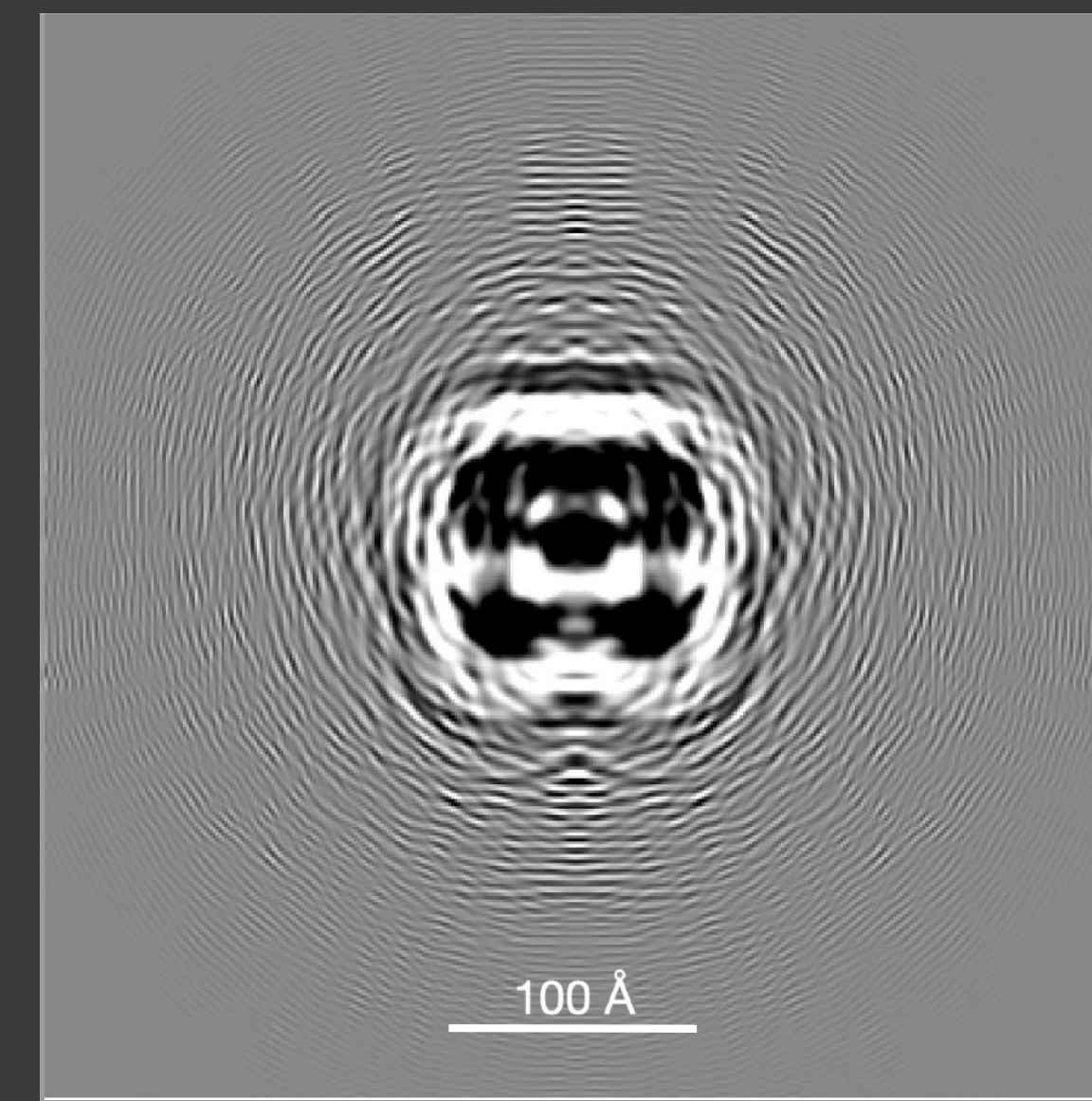
$$r = 200 \text{\AA}$$

In this case one would want 200 $\text{\AA}$ of space in the box around each particle image.

*Note: beyond about 3 $\text{\AA}$, spherical aberration needs to be taken into account too.



Object

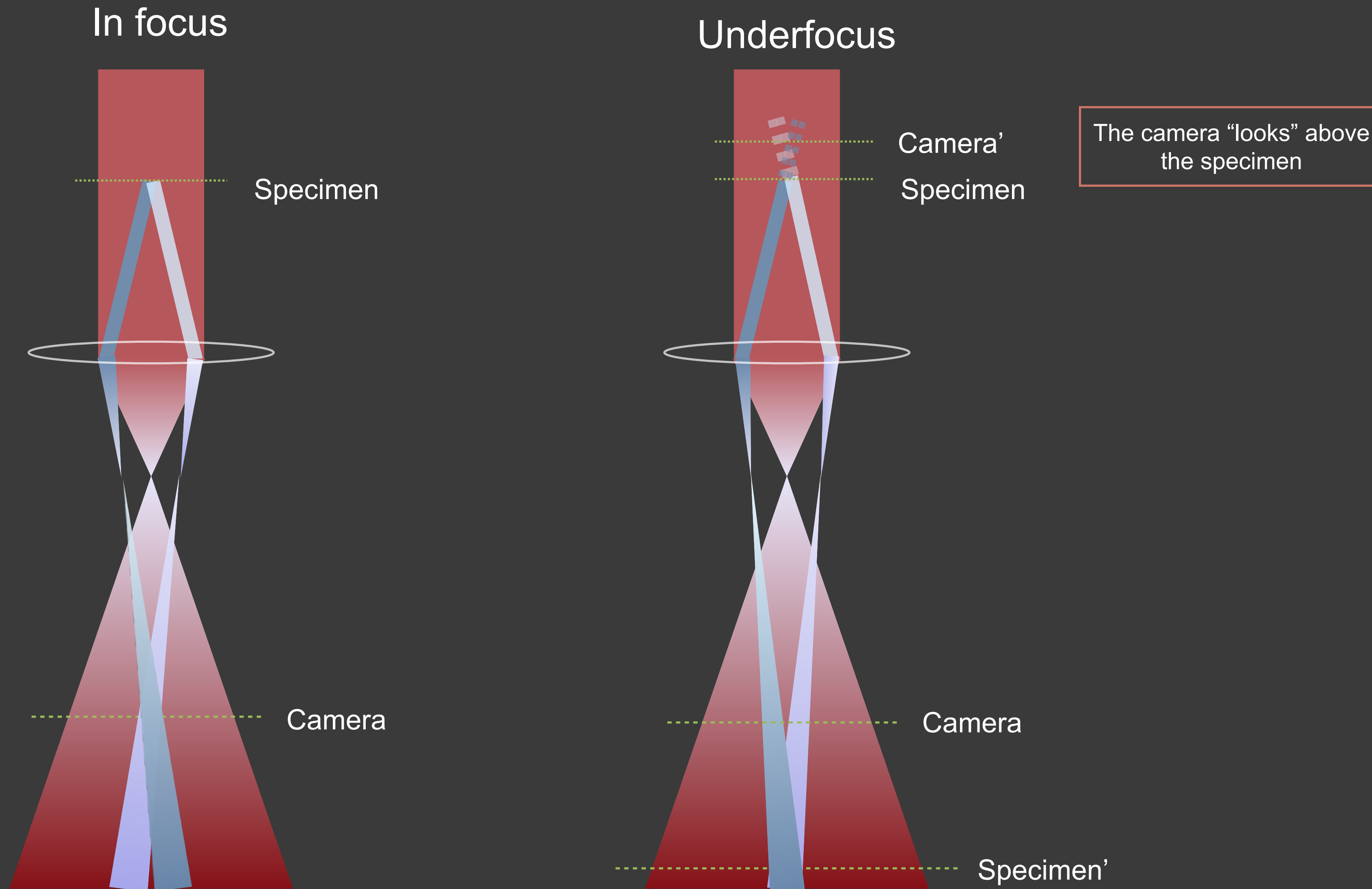


3 μm
defocus

Phase contrast and the contrast transfer function

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An objective lens reproduces interference patterns at the camera



With spherical aberration a lens bends high-angle rays more strongly

Spherical aberration changes
the defocus by

$$\delta' = -C_s \lambda^2 s^2 / 2.$$

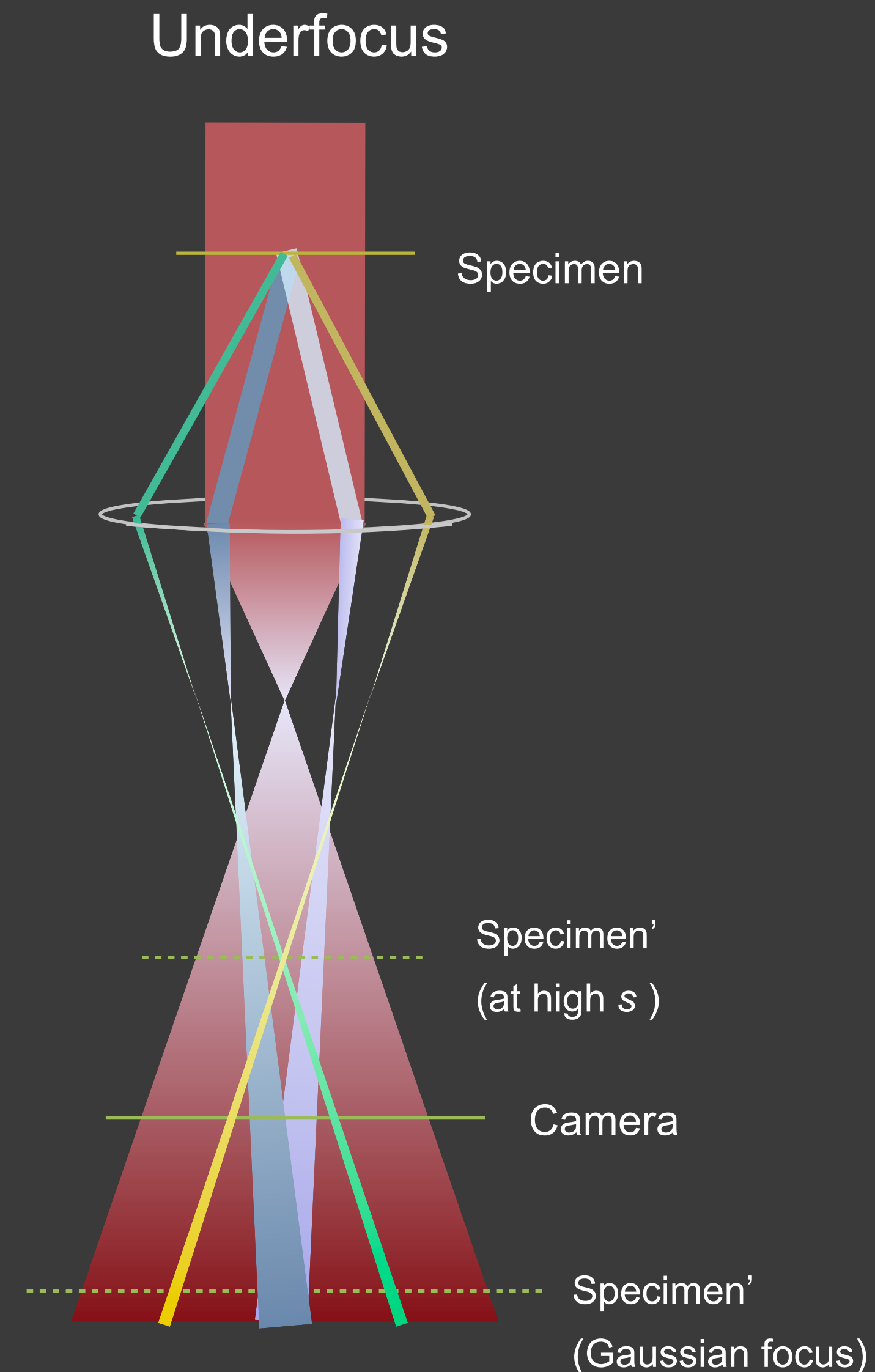
The contrast transfer function now includes δ' ,

$$\text{CTF} = \sin(-\pi\lambda (\delta + \delta') s^2)$$

or, expanded,

$$\text{CTF} = \sin(-\pi\lambda\delta s^2 + \frac{\pi}{2}C_s\lambda^3s^4)$$

The coefficient C_s is typically ~2mm. Spherical aberration typically becomes important for $s \gtrsim 0.25 \text{\AA}^{-1}$, or about 4 $\text{\AA}$ resolution.



Very high-angle scattering yields amplitude contrast

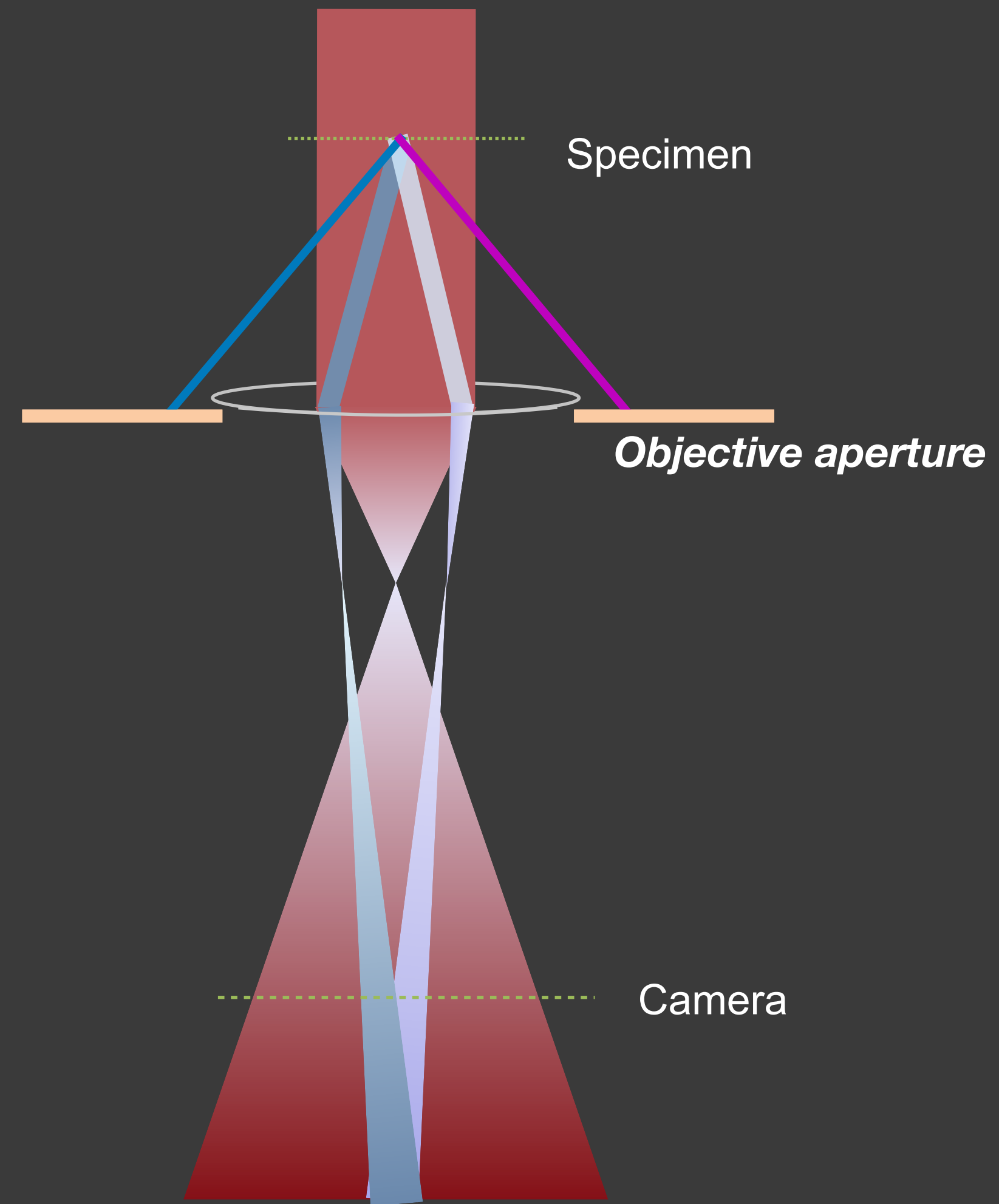
Electrons that pass very close to an atomic nucleus are scattered at high angles, and are caught by the objective aperture.

- The loss of these electrons results in a small amount of negative amplitude contrast.
- For proteins α is typically around 0.05.
- The amplitude contrast term allows the CTF to have a small negative value even at zero spatial frequency.

Combining all these terms, the contrast transfer function is given by

$$\text{CTF} = \sin(-\pi\lambda\delta s^2 + \frac{\pi}{2}C_s\lambda^3s^4 - \alpha)$$

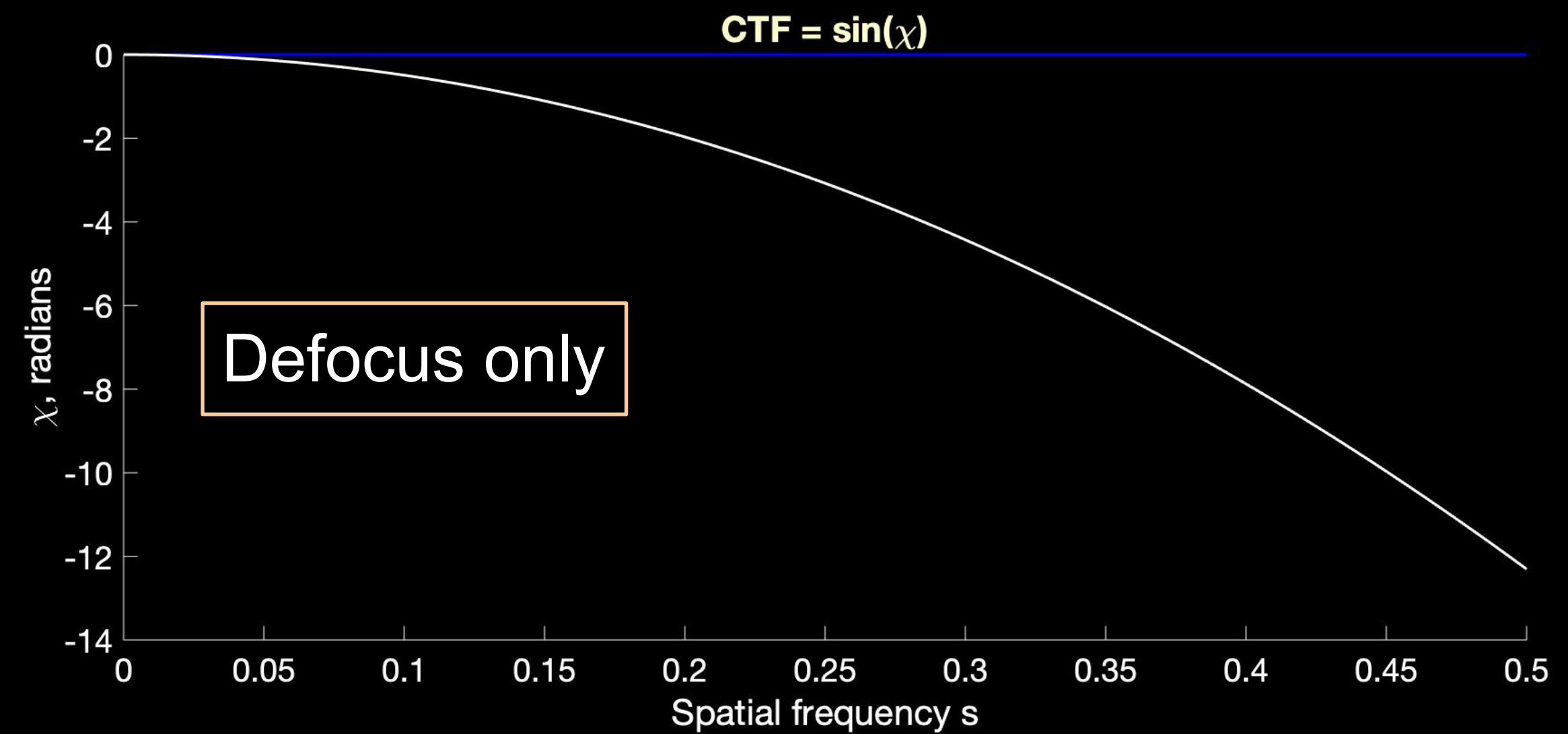
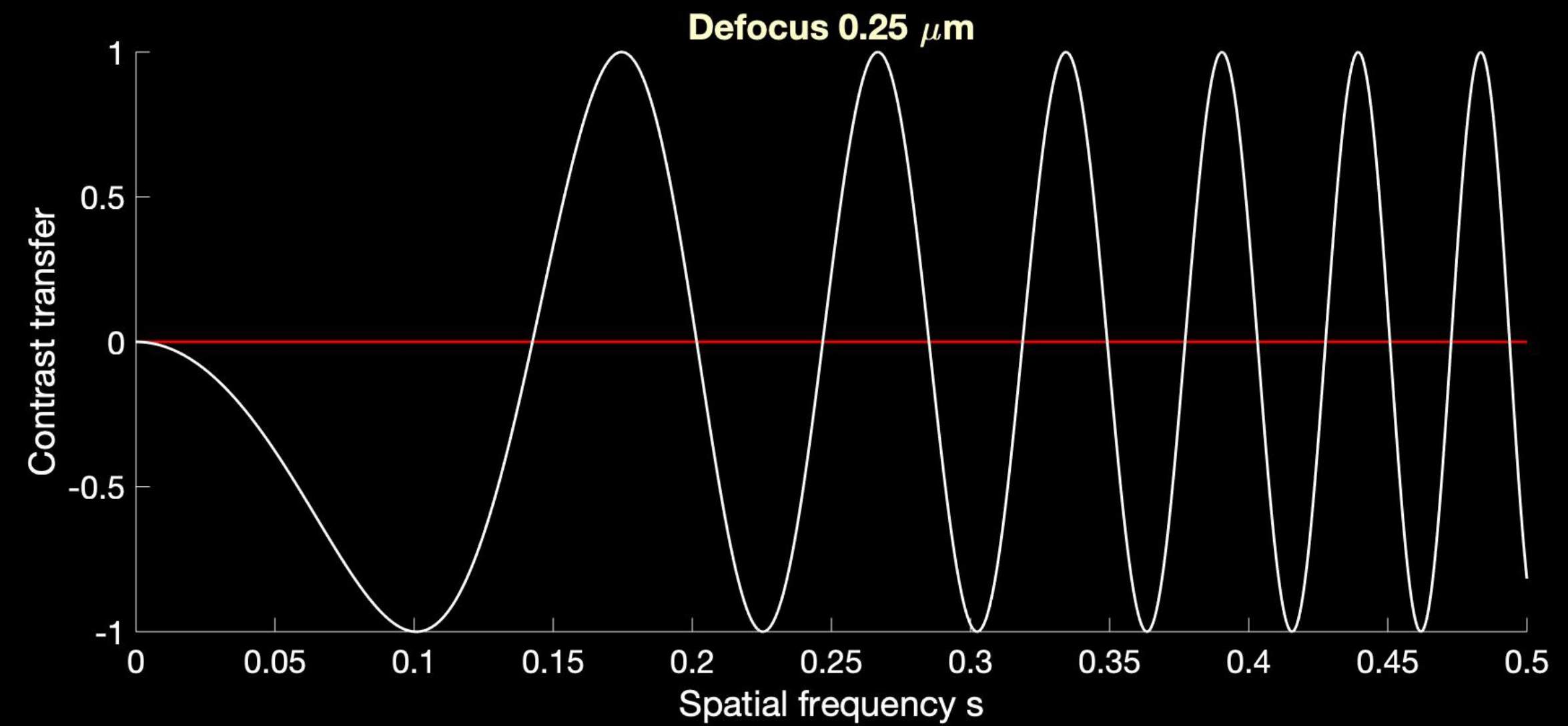
defocus *sphere abb.* *amplitude*



The simple defocus contrast is what we've seen before

$$\text{CTF} = \sin(-\pi\lambda\delta s^2 + \frac{\pi}{2}C_s\lambda^3s^4 - \alpha)$$

defocus sphere abb. amplitude



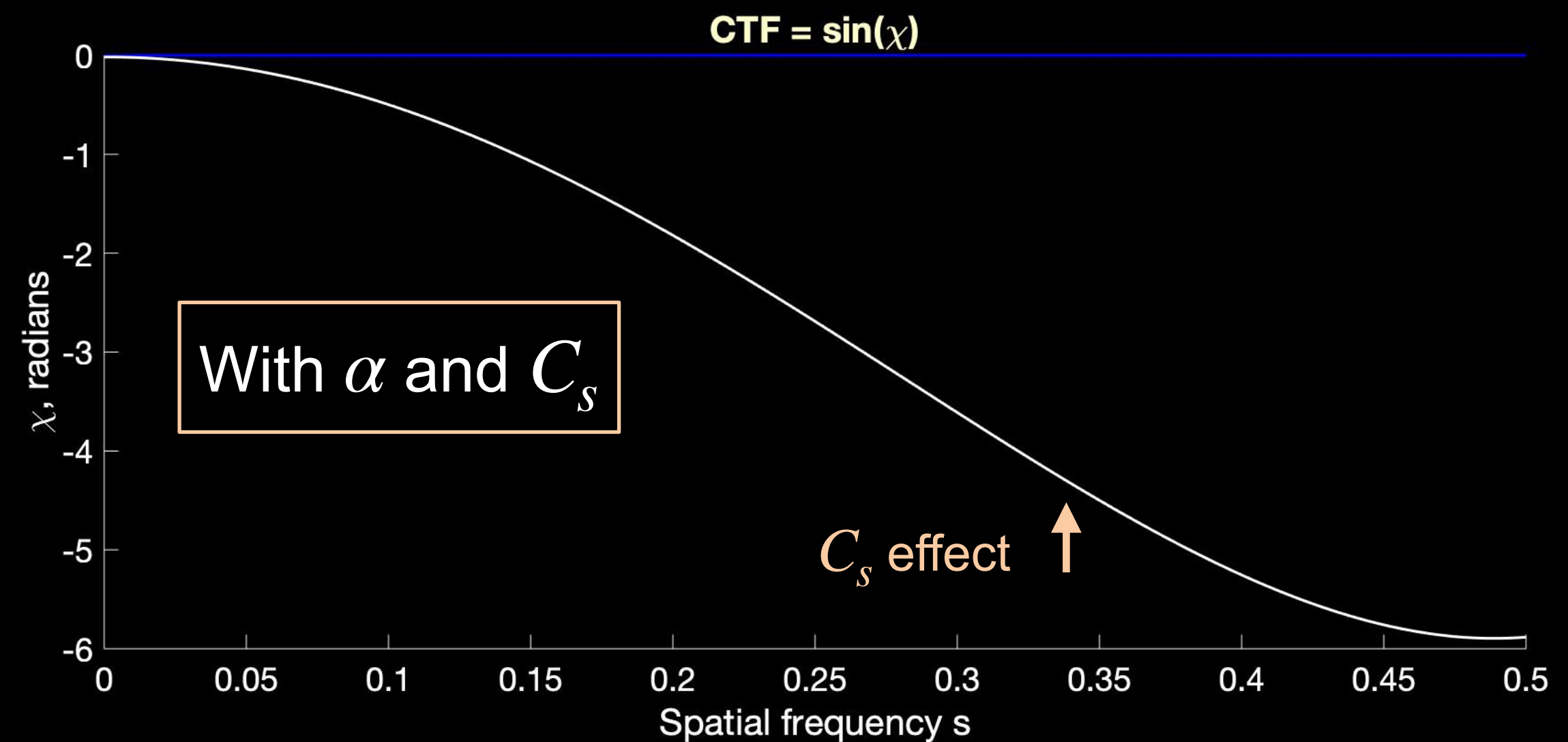
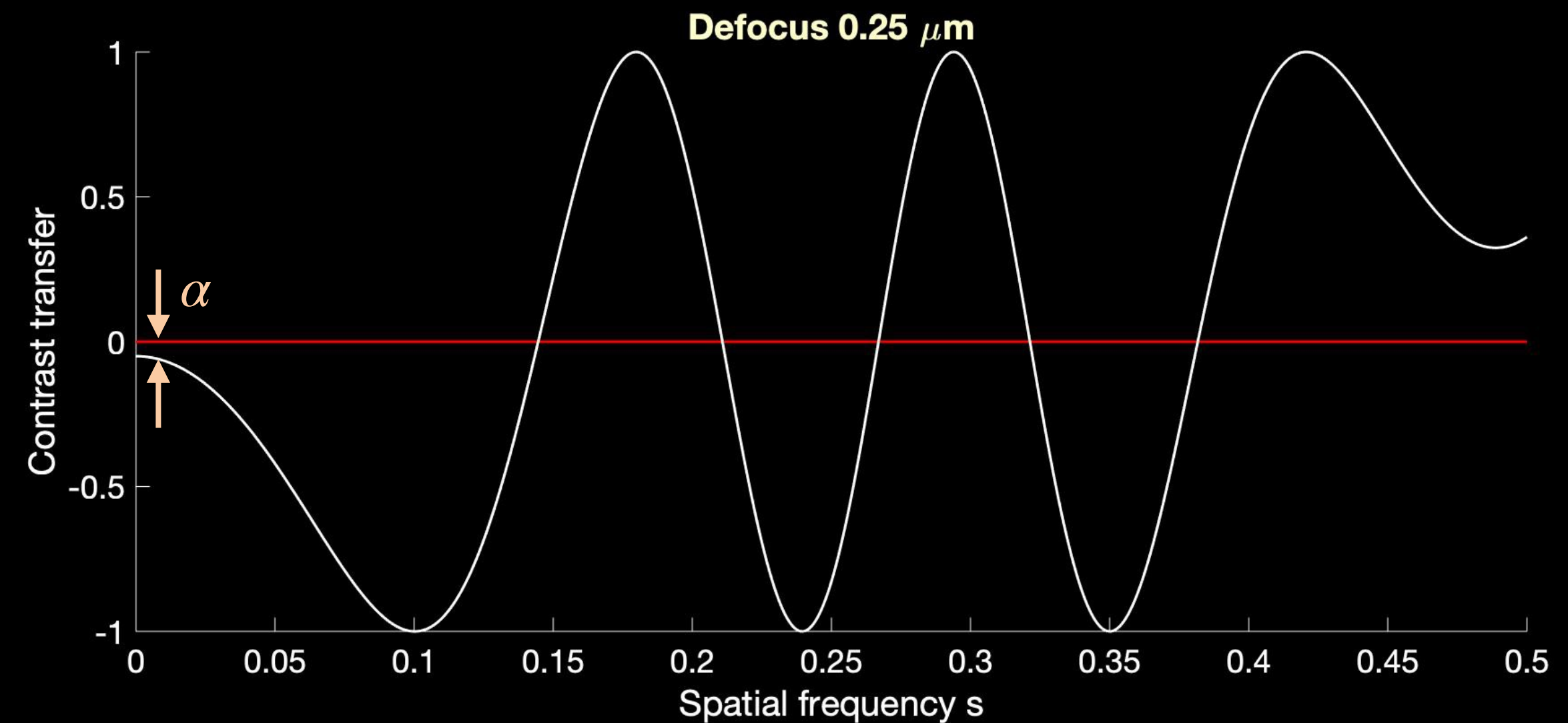
Now adding in spherical aberration and amplitude contrast

Here you can see why everyone uses underfocus: the amplitude contrast and defocus contrast are additive in this case.

Also, C_s has the effect of reversing some of the oscillations in the CTF.

Combining all these terms, the contrast transfer function is given by

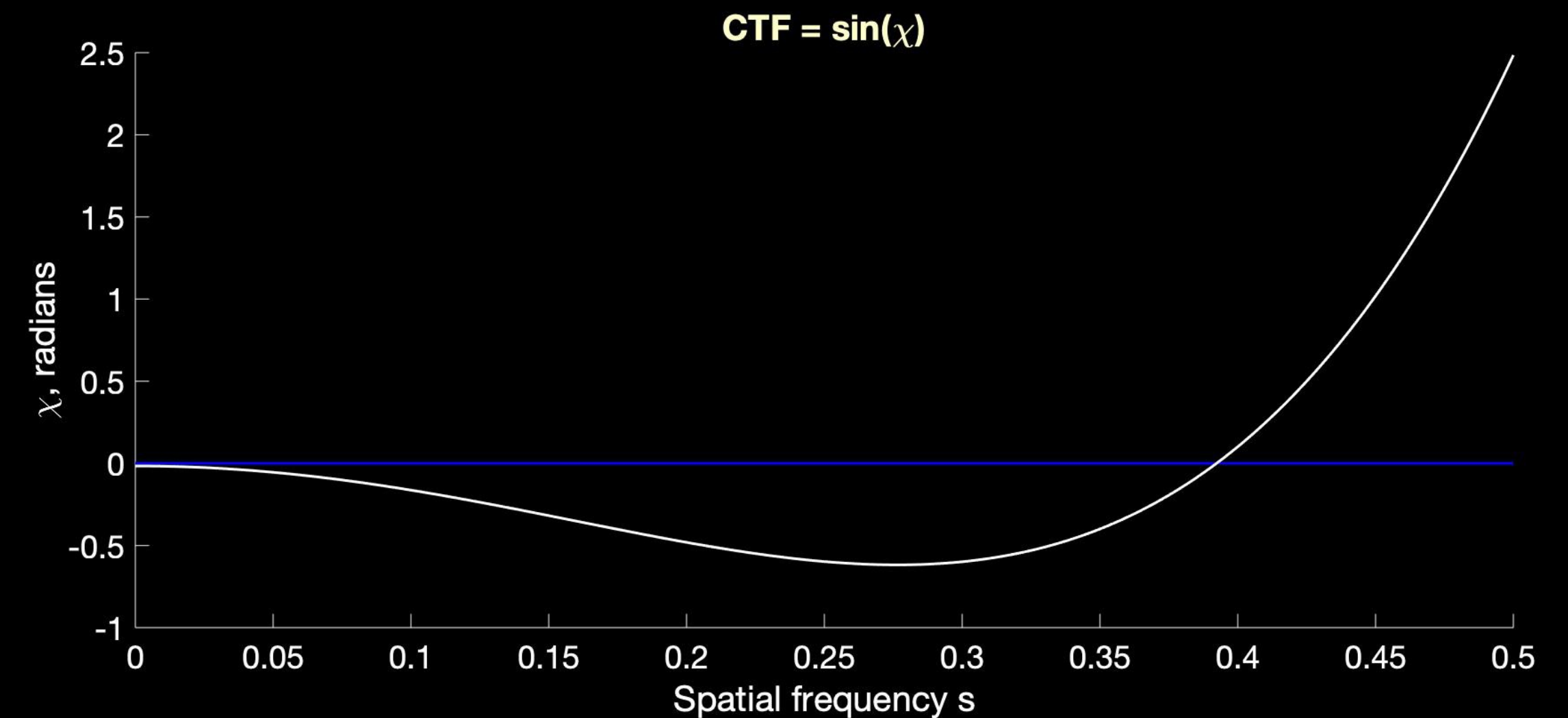
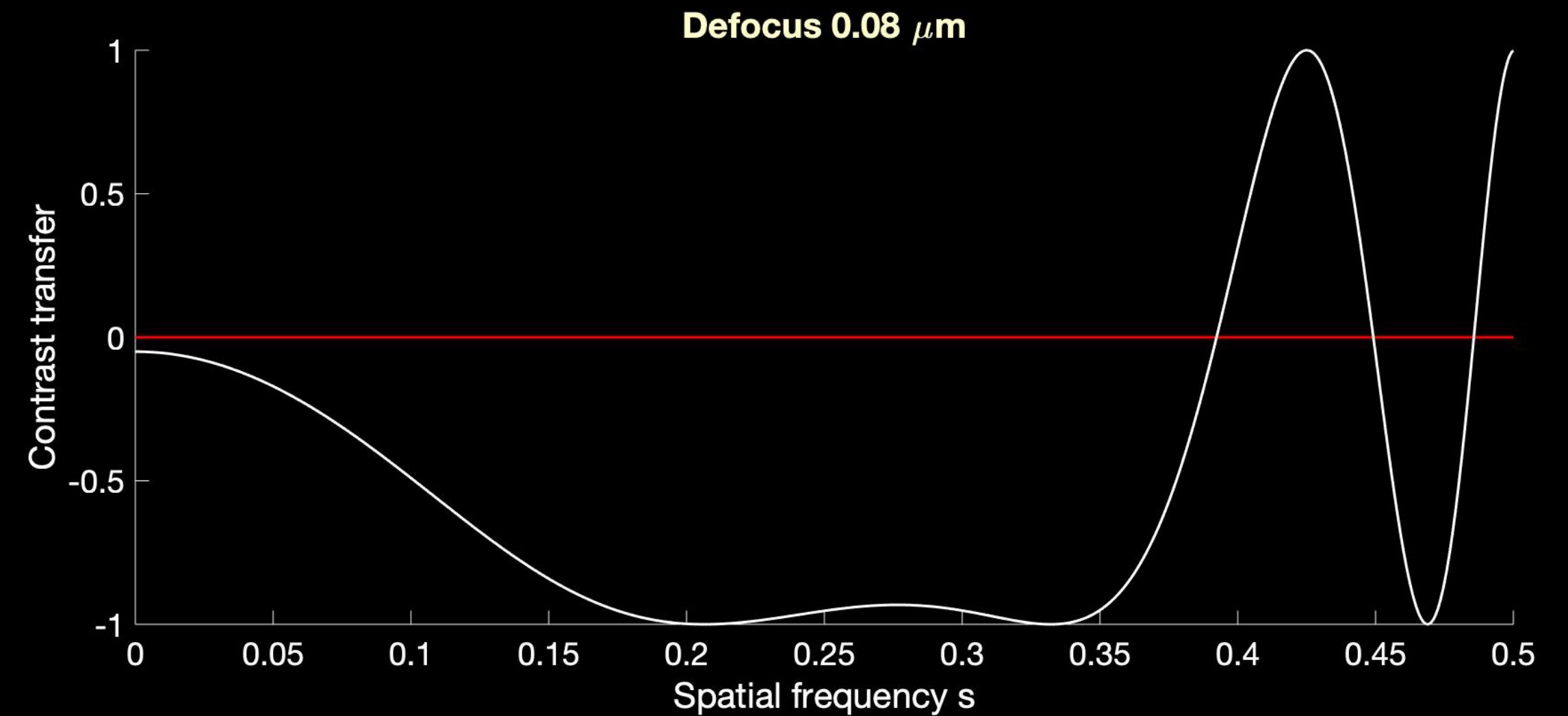
$$\text{CTF} = \sin(\underbrace{-\pi\lambda\delta s^2}_{\text{defocus}} + \underbrace{\frac{\pi}{2}C_s\lambda^3 s^4}_{\text{sphere abb.}} - \underbrace{\alpha}_{\text{amplitude}})$$



Spherical aberration can be our friend

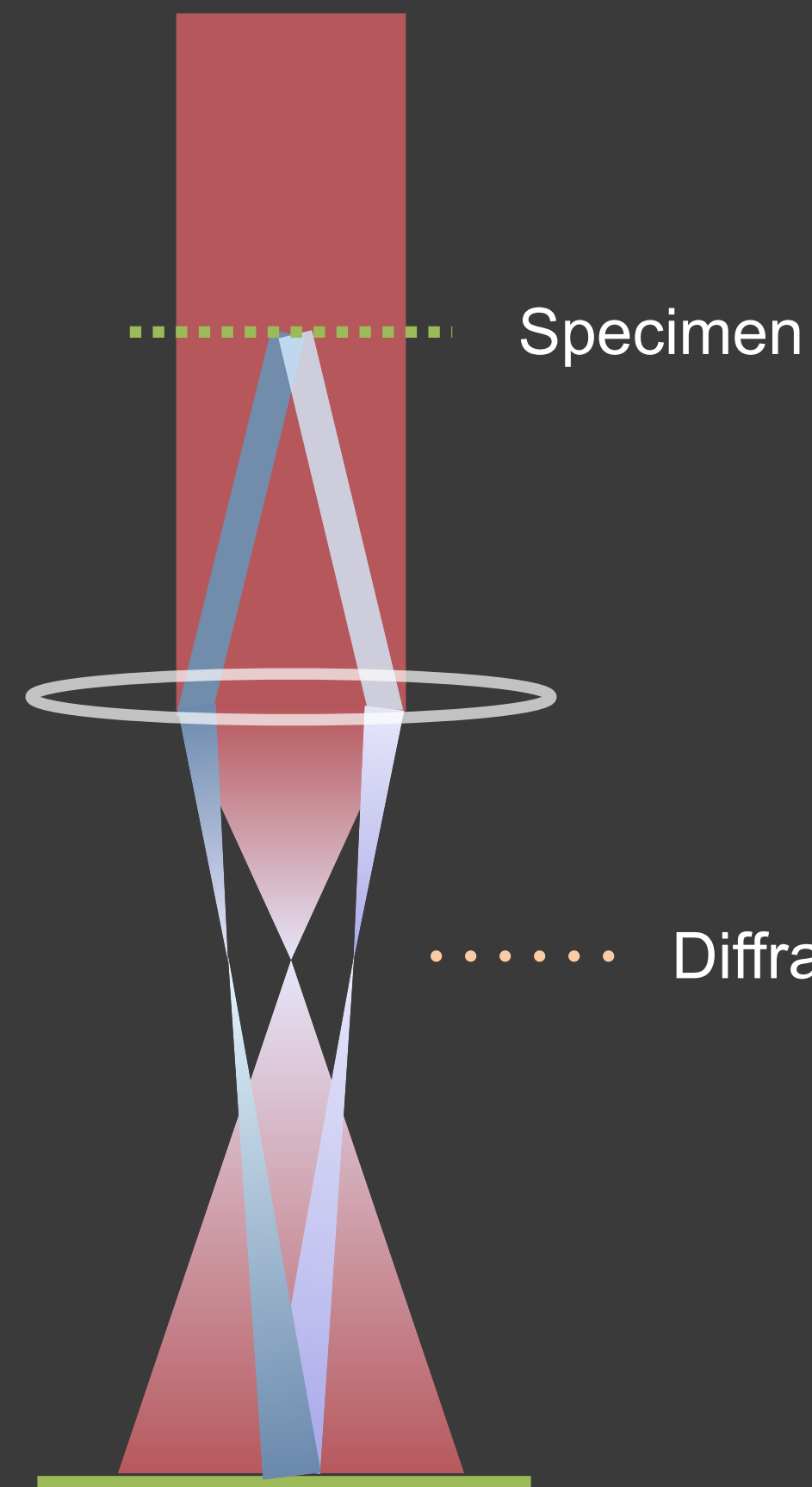
If we're not using image processing to remove CTF effects, Scherzer defocus is a good solution: just enough defocus to give signal over a broad range of spatial frequencies.

It's popular in materials science but not much for cryoEM: the signal transfer at low frequencies is poor.

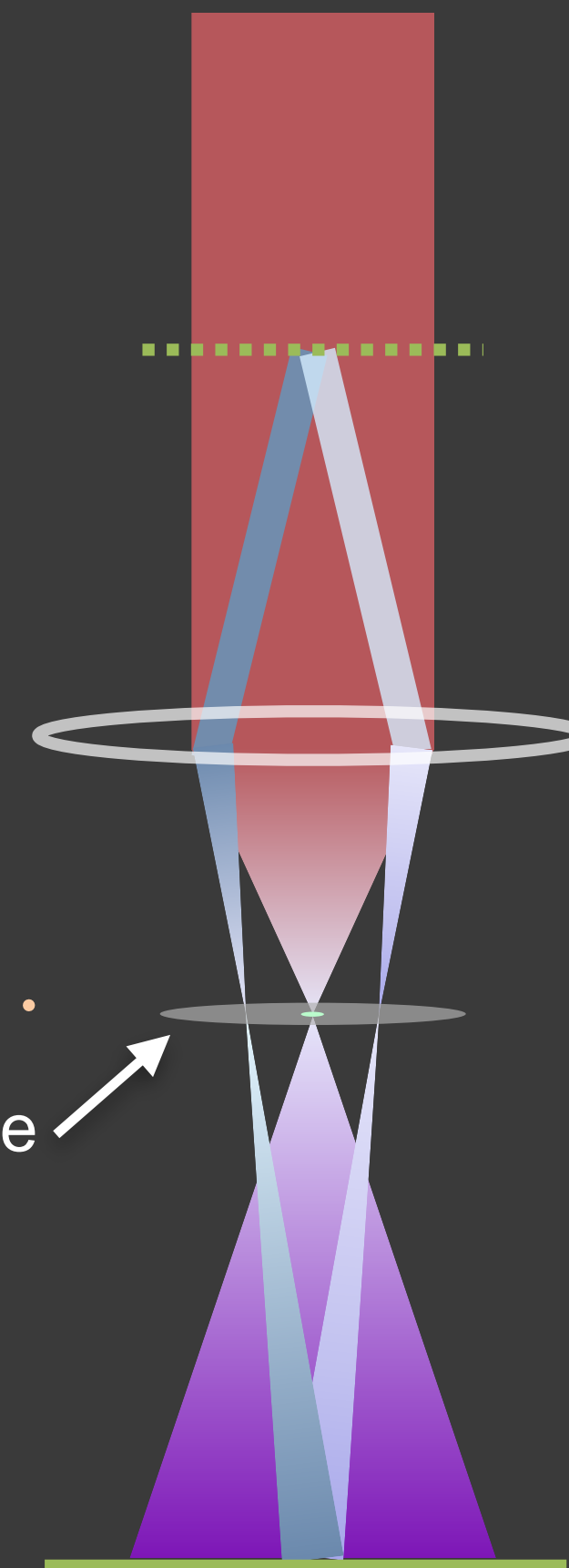


A phase plate modifies the interference of electron waves at the camera

In focus



Phase plate



The phase plate shifts the phase of the undiffracted beam Ψ_0 by some angle ϕ .

Then $\text{CTF} = \sin(\chi - \phi)$.

If $\phi = 90^\circ$ then

$$\text{CTF} = -\cos(\chi)$$

The phase plate allows in-focus imaging, given precise focusing.

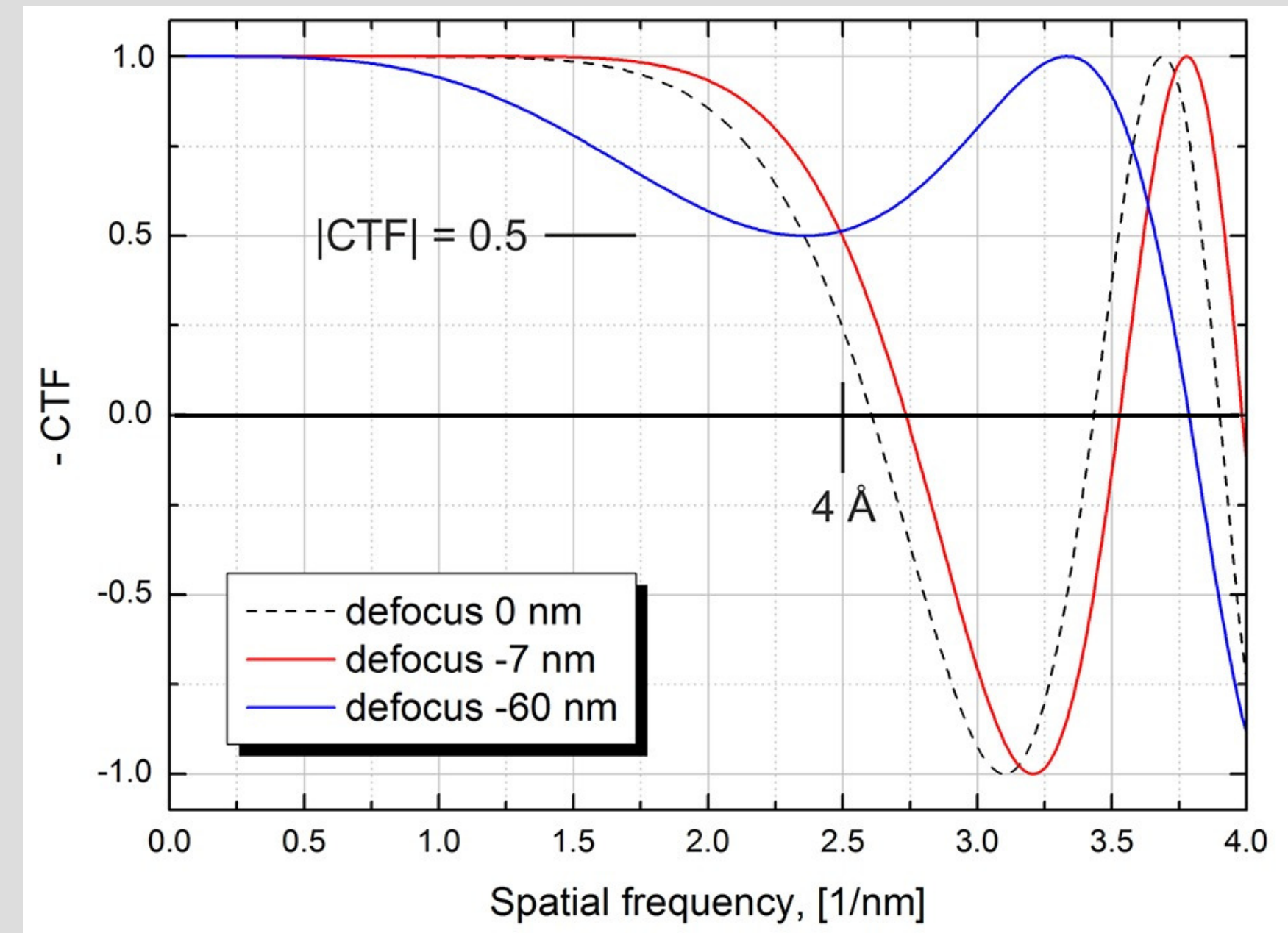
Cryo-EM single particle analysis with the Volta phase plate

Radostin Danev*, Wolfgang Baumeister

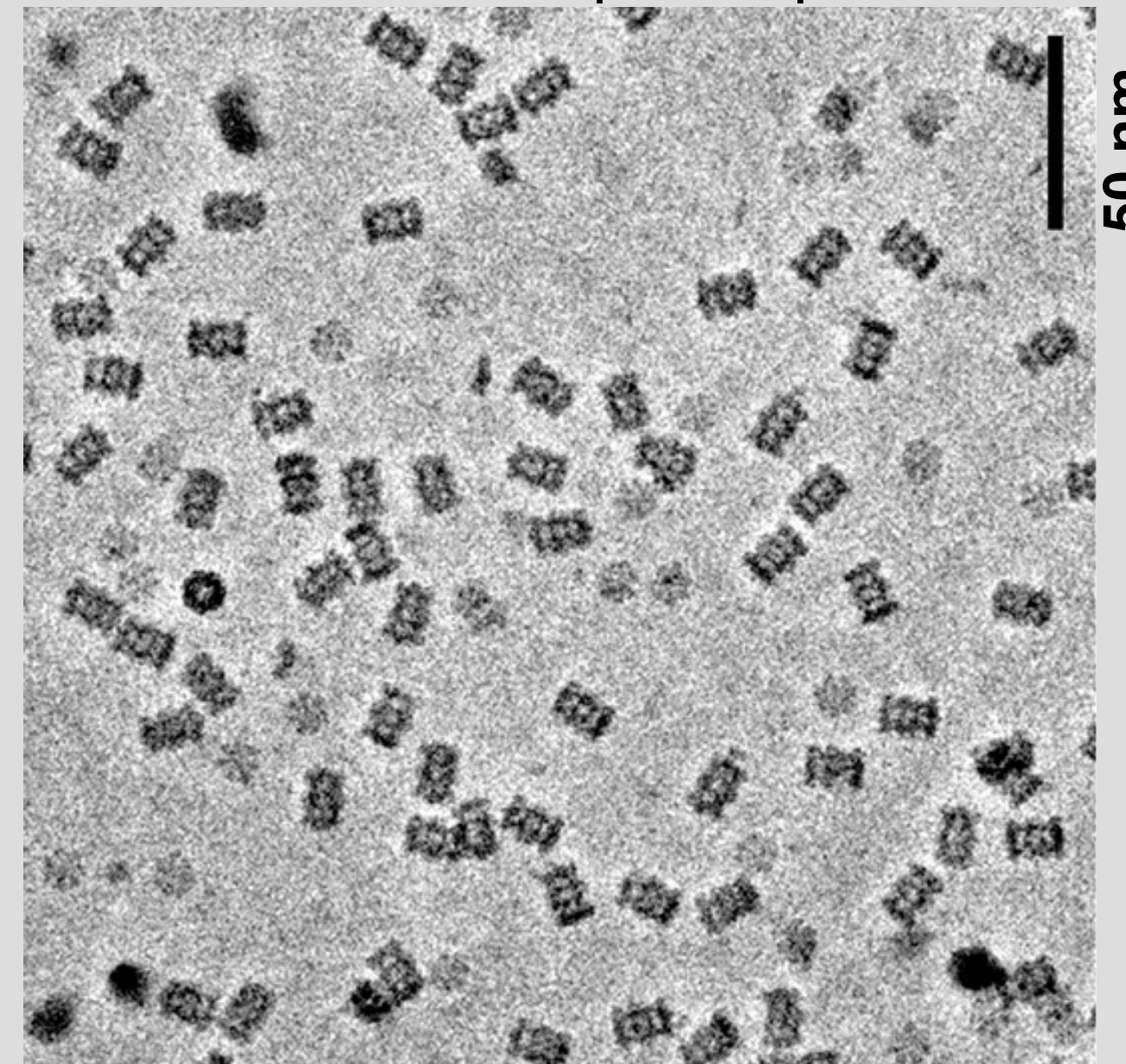
Department of Molecular Structural Biology, Max Planck Institute of Biochemistry, Martinsried, Germany

eLife 2016

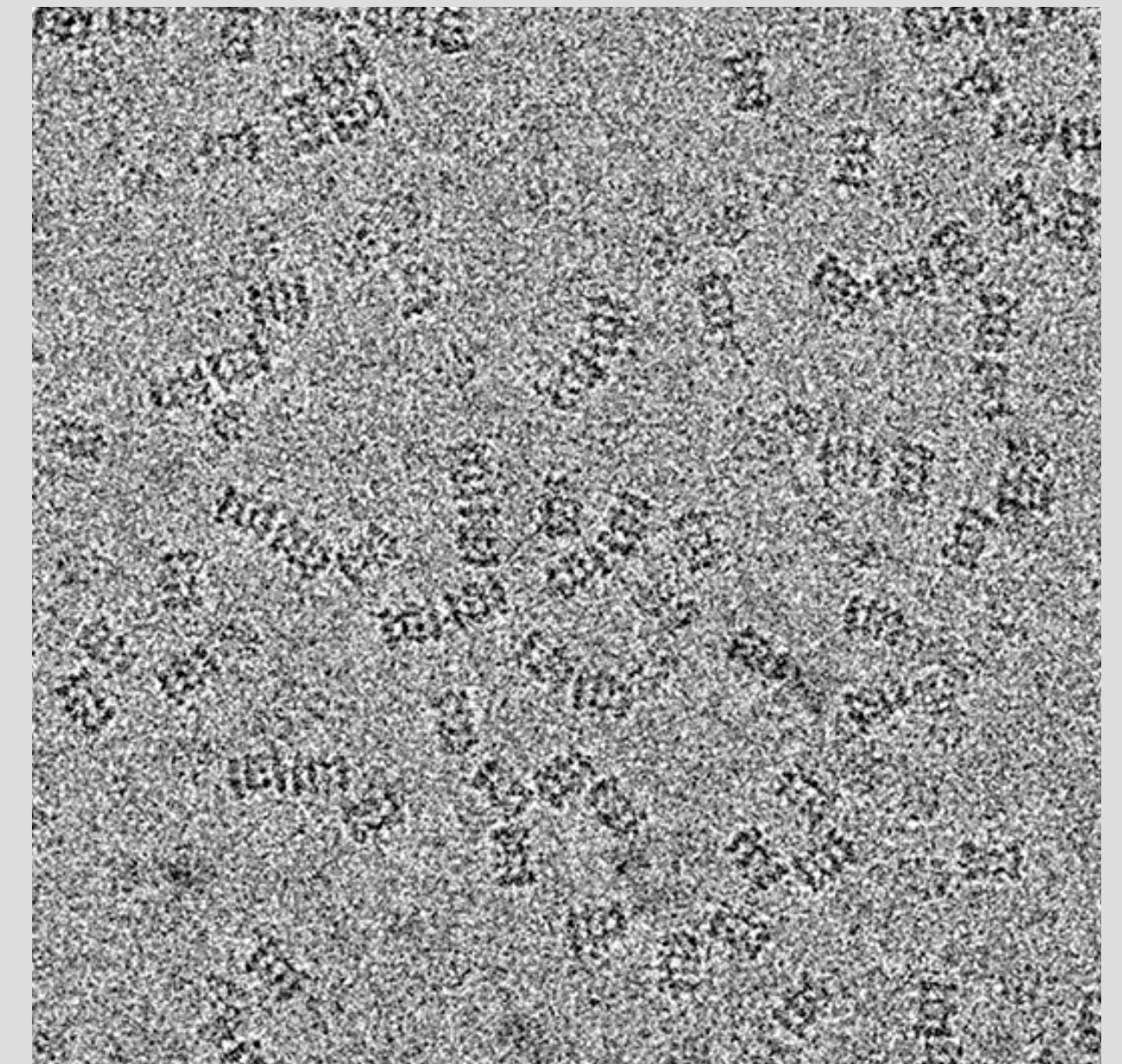
- The better low-frequency contrast makes particles much more visible.
- The defocus value must be precise within 60 nm in order to get 4 Å resolution.



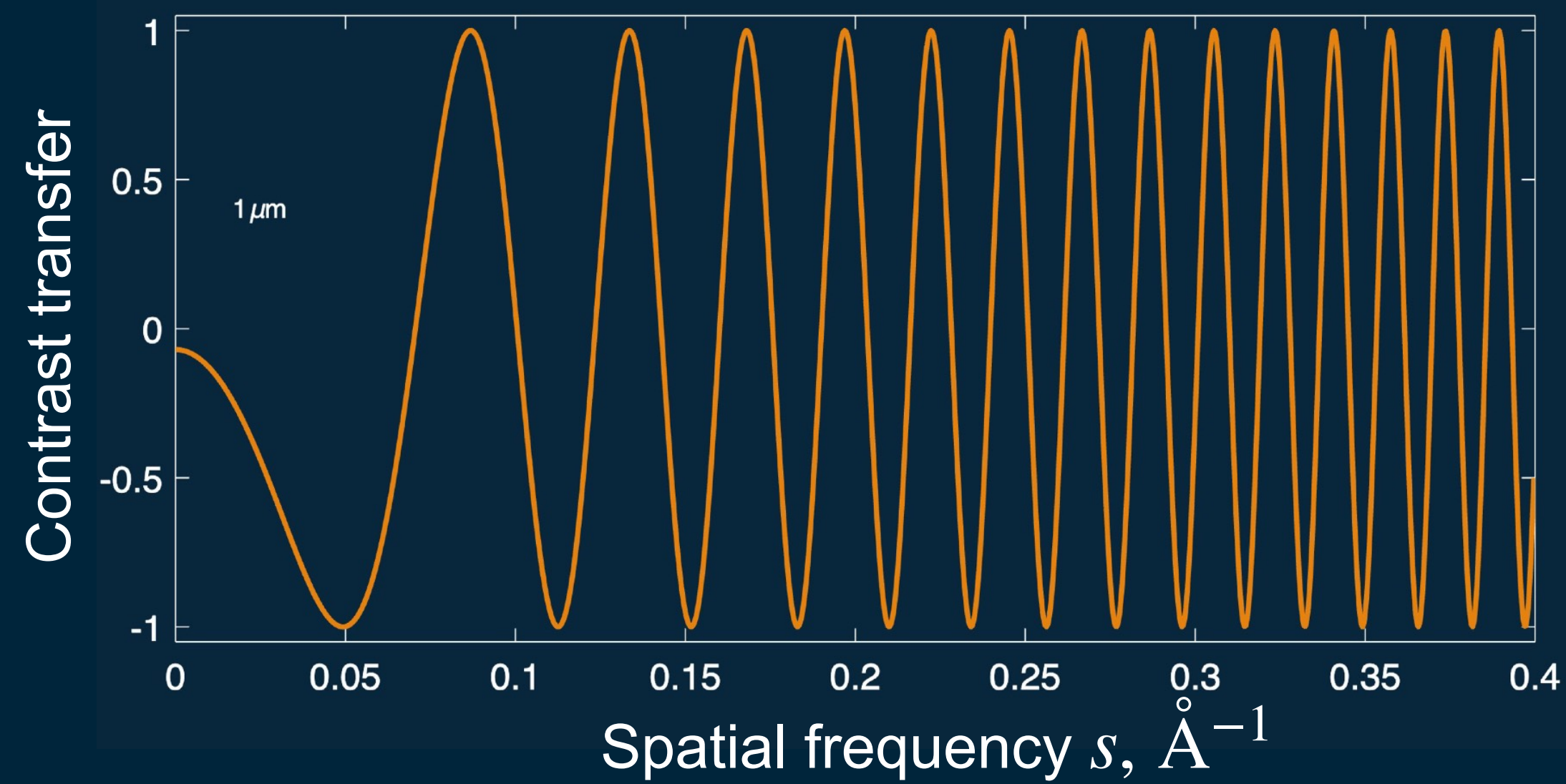
In-focus phase plate



Defocus contrast

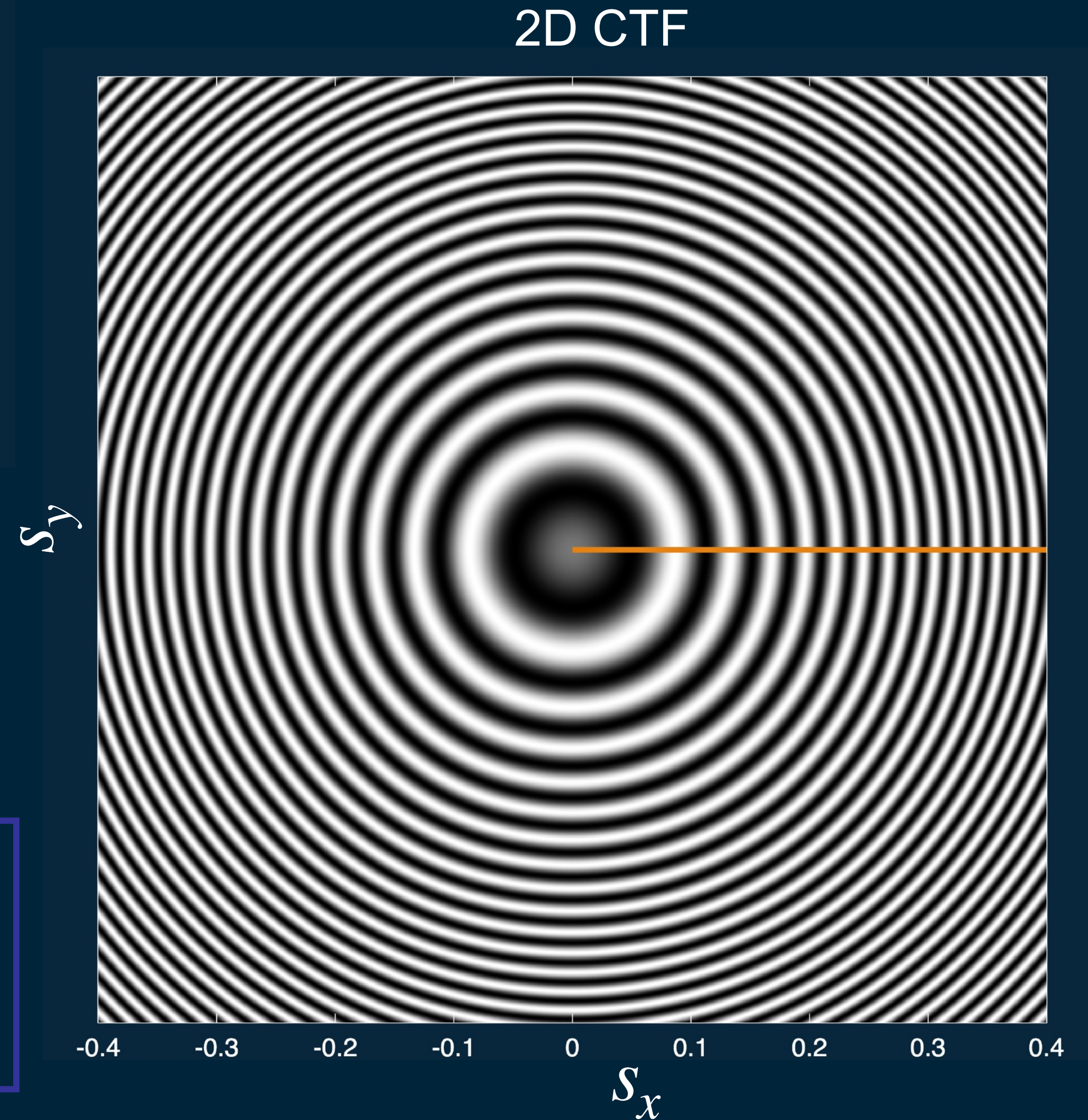


The CTF actually is a 2D function

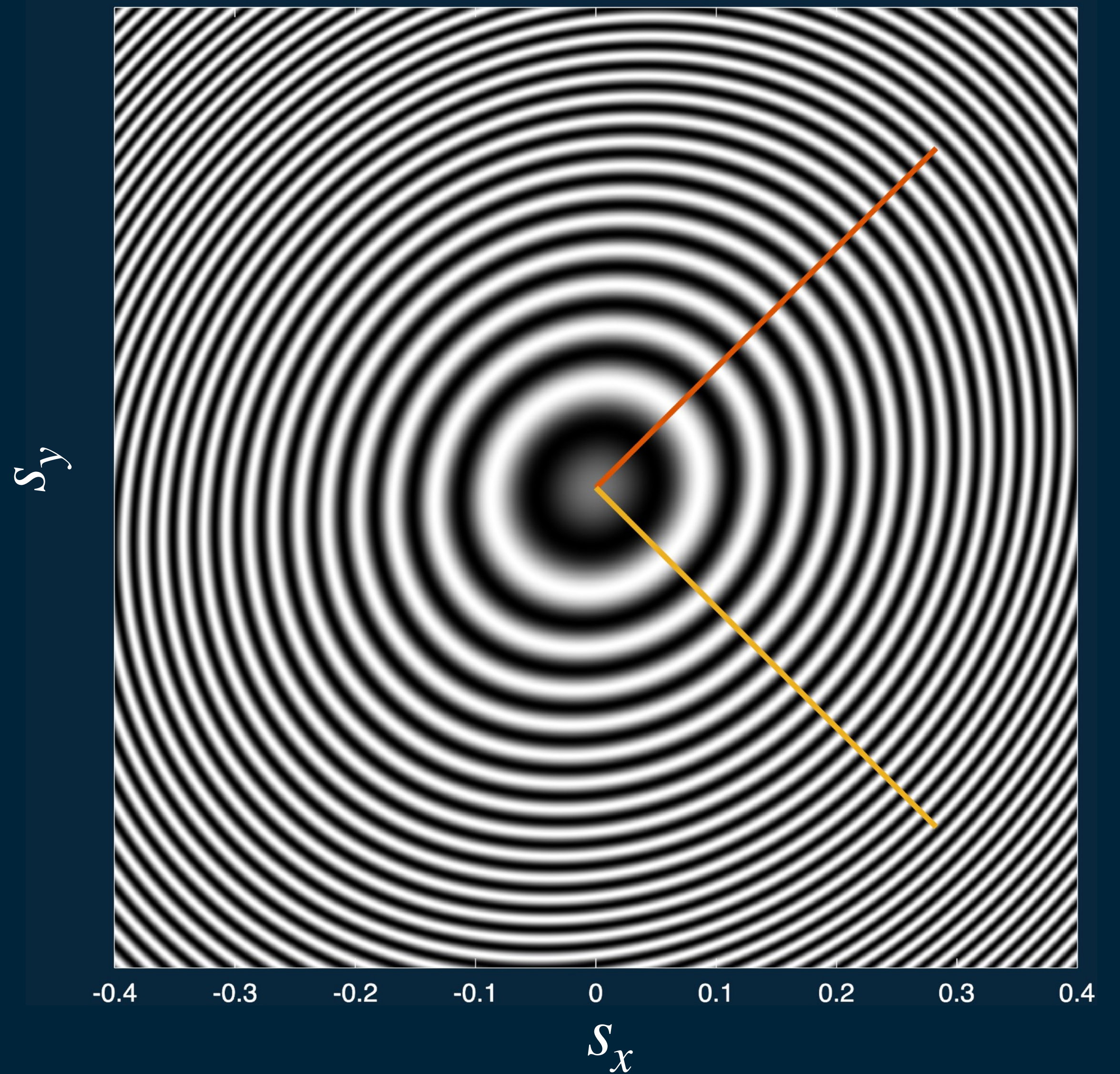
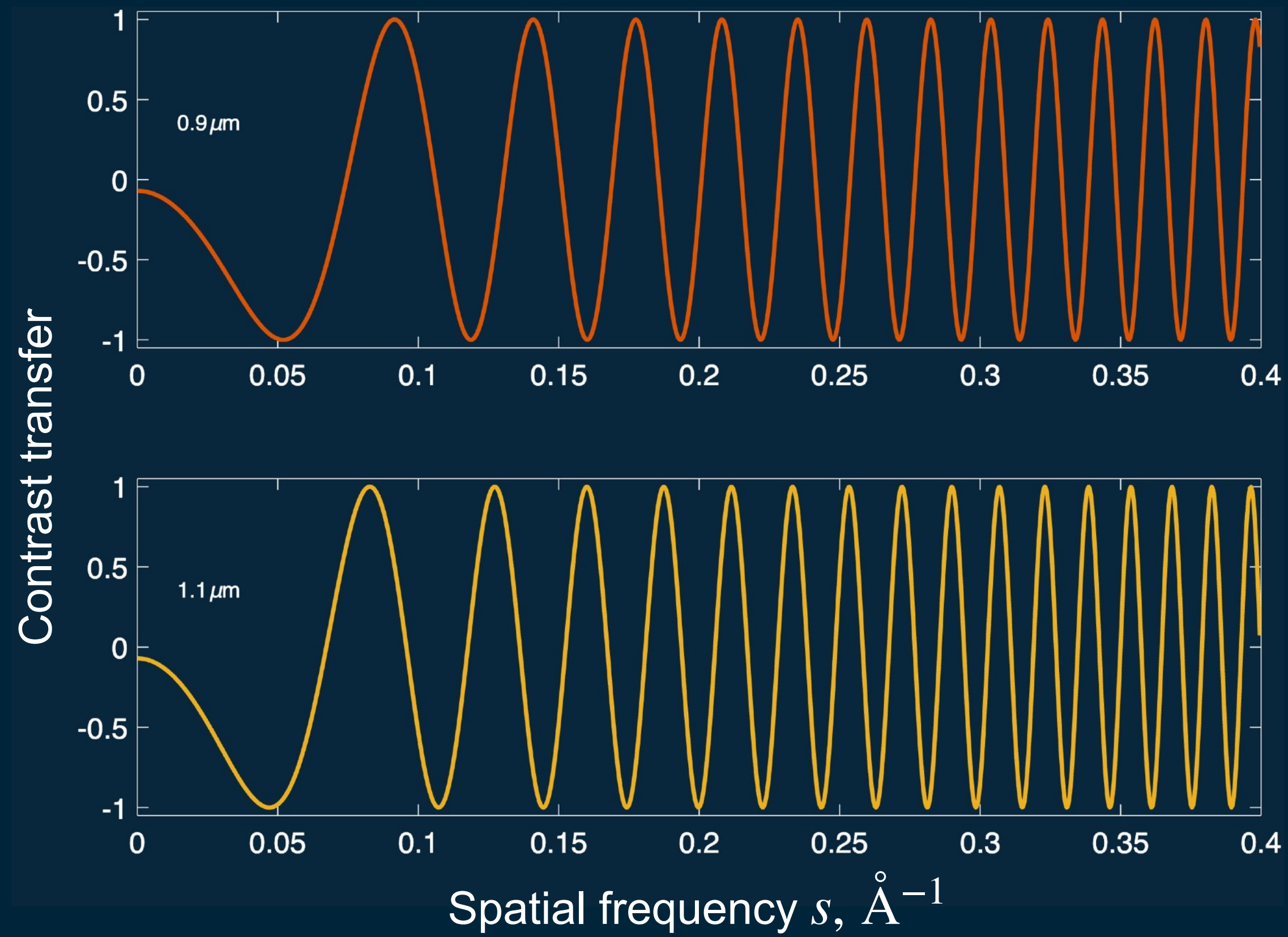


$$\text{CTF} = \sin\left(\underbrace{-\pi\lambda\delta s^2}_{\text{defocus}} + \underbrace{\frac{\pi}{2}C_s\lambda^3 s^4}_{\text{sphere abb.}} - \underbrace{\alpha}_{\text{amplitude}}\right)$$

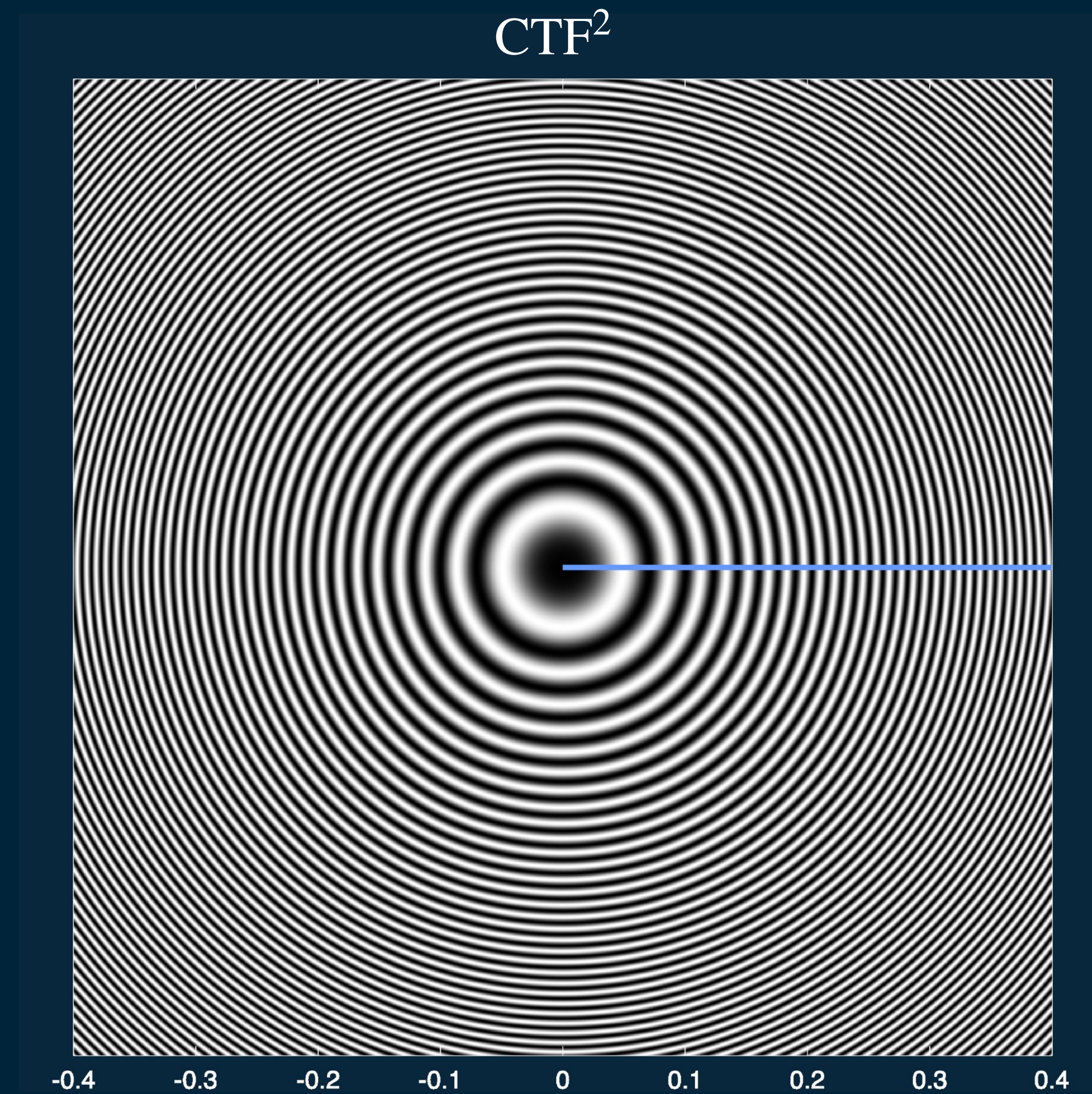
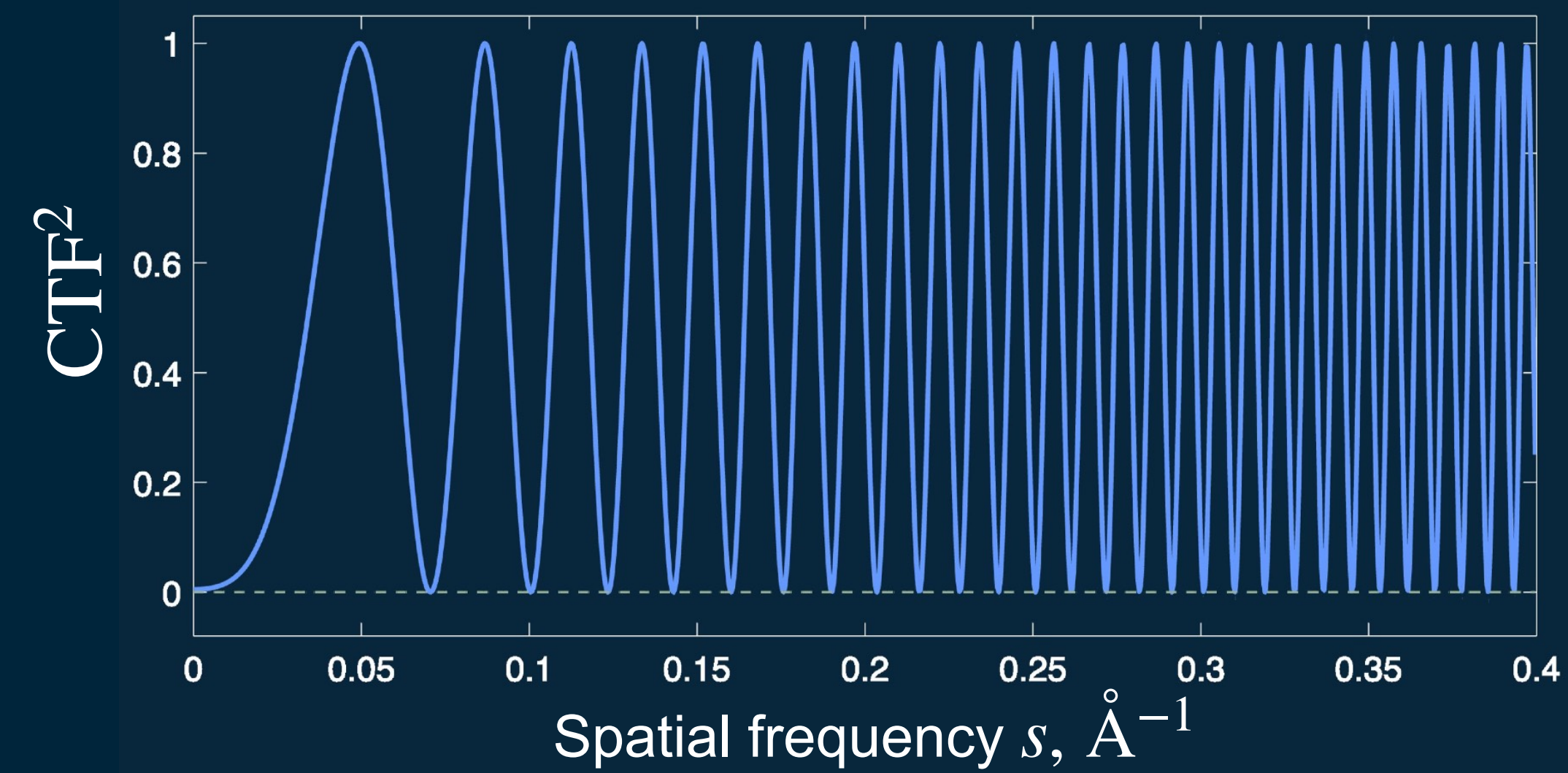
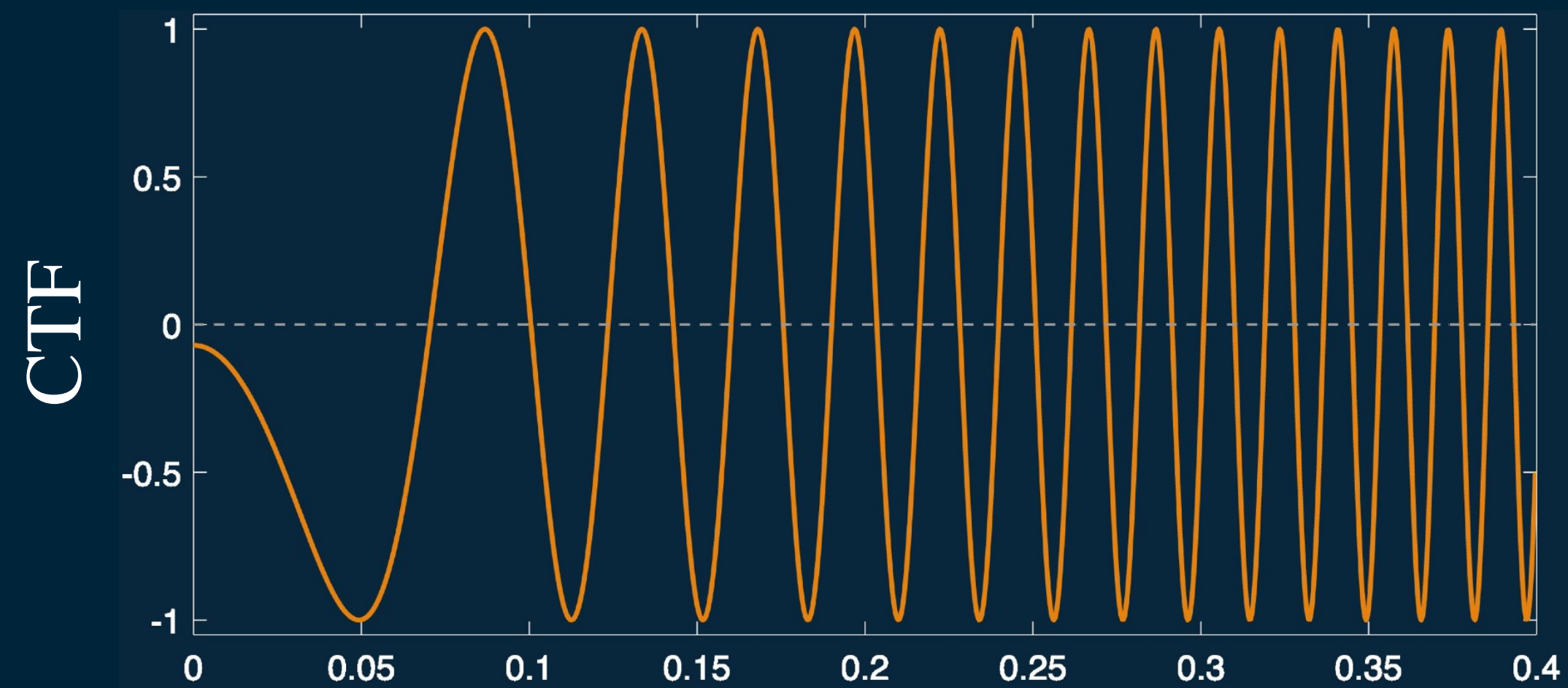
$$\text{CTF} = \sin\left(-\pi\lambda\delta(s_x^2 + s_y^2) + \frac{\pi}{2}C_s\lambda^3(s_x^2 + s_y^2)^2 - \alpha\right)$$



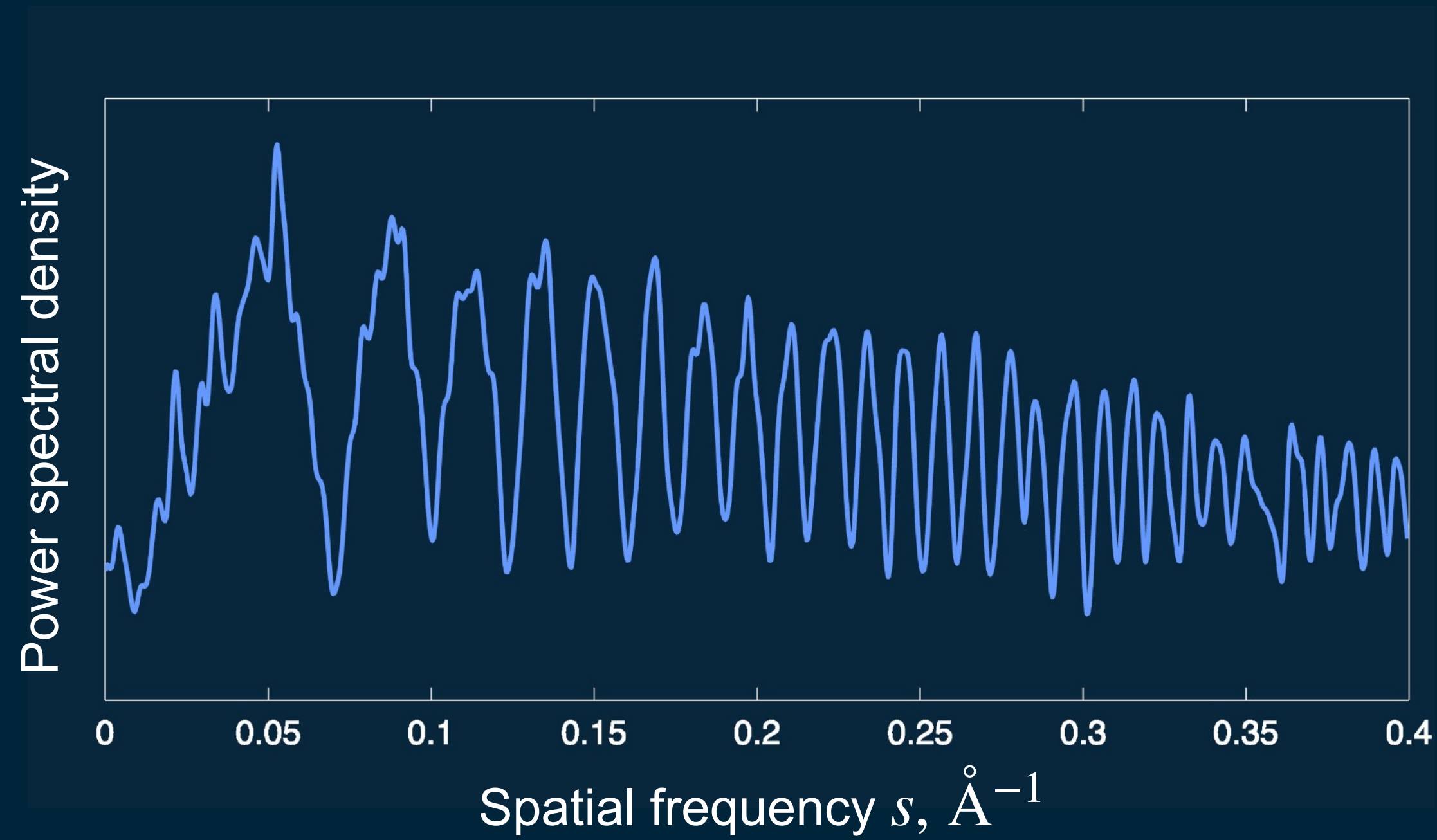
Astigmatism yields a varying defocus depending on the angle



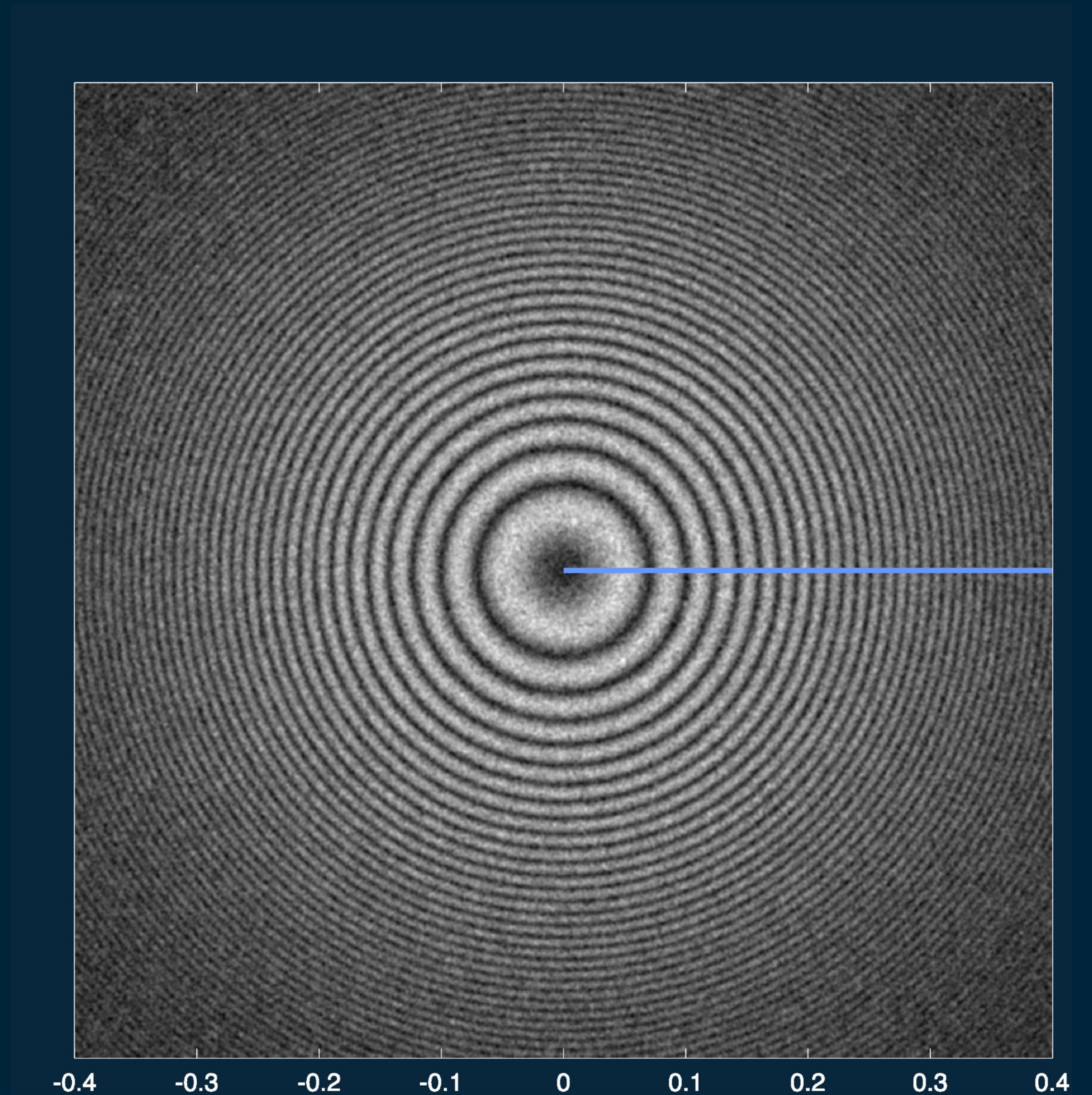
Black rings in CTF^2 show the zeros in the CTF



The power spectrum shows the same dark “Thon rings”

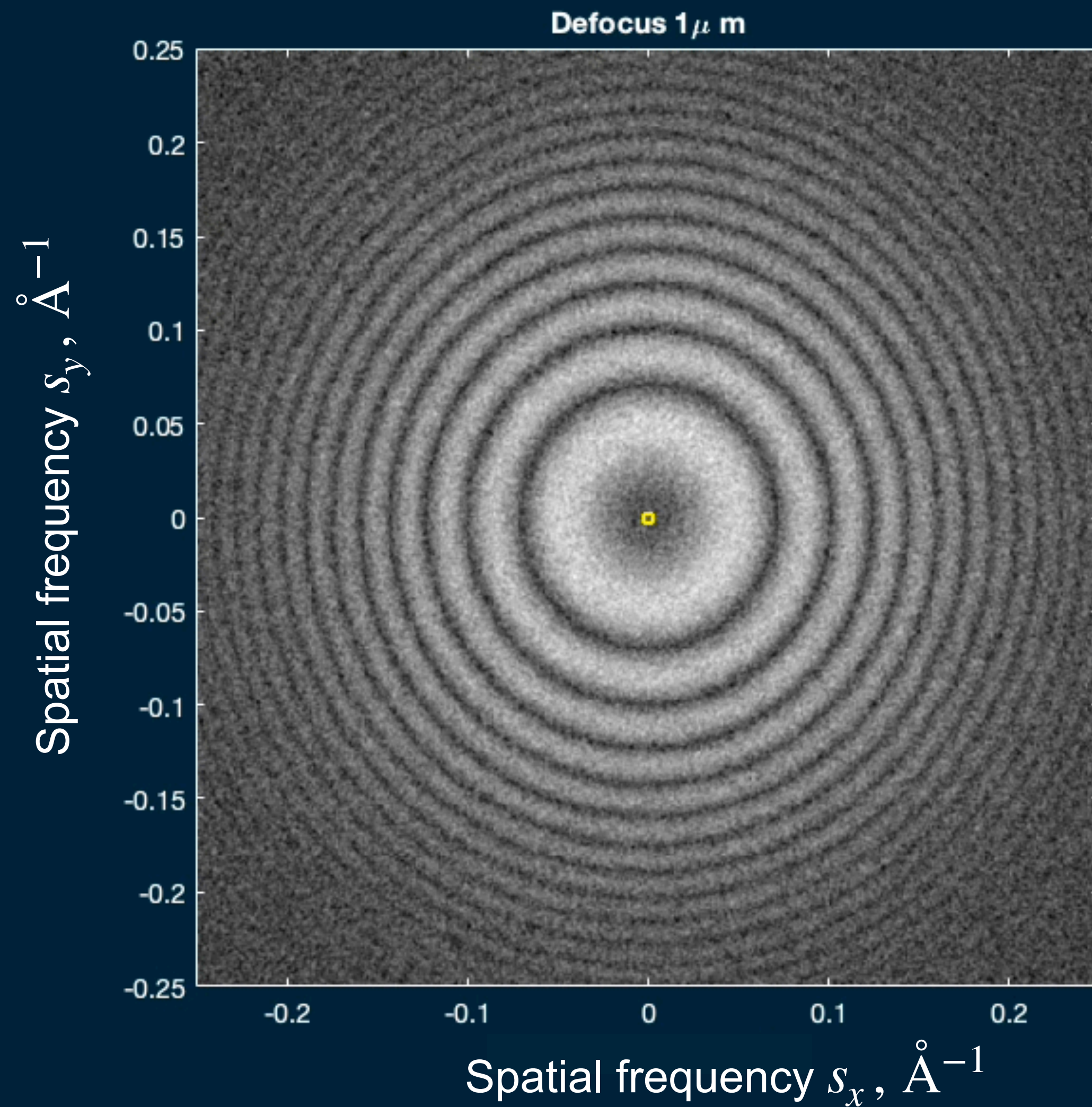


The defocus and other CTF parameters can be estimated by curve fitting.

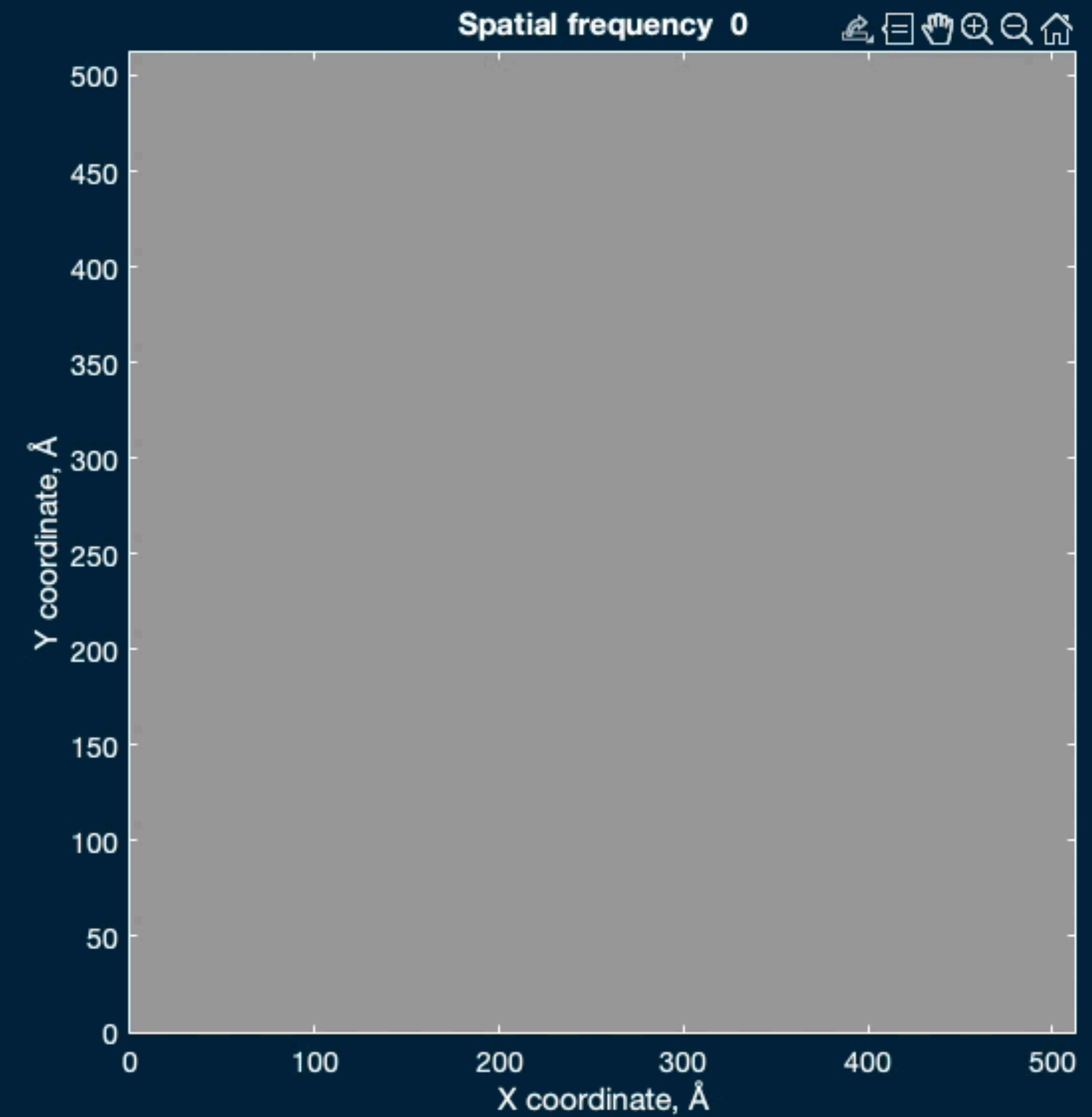


The power spectrum shows the magnitude of an image's FT

Power spectrum



Grating at the spatial frequency $s = (s_x, s_y)$



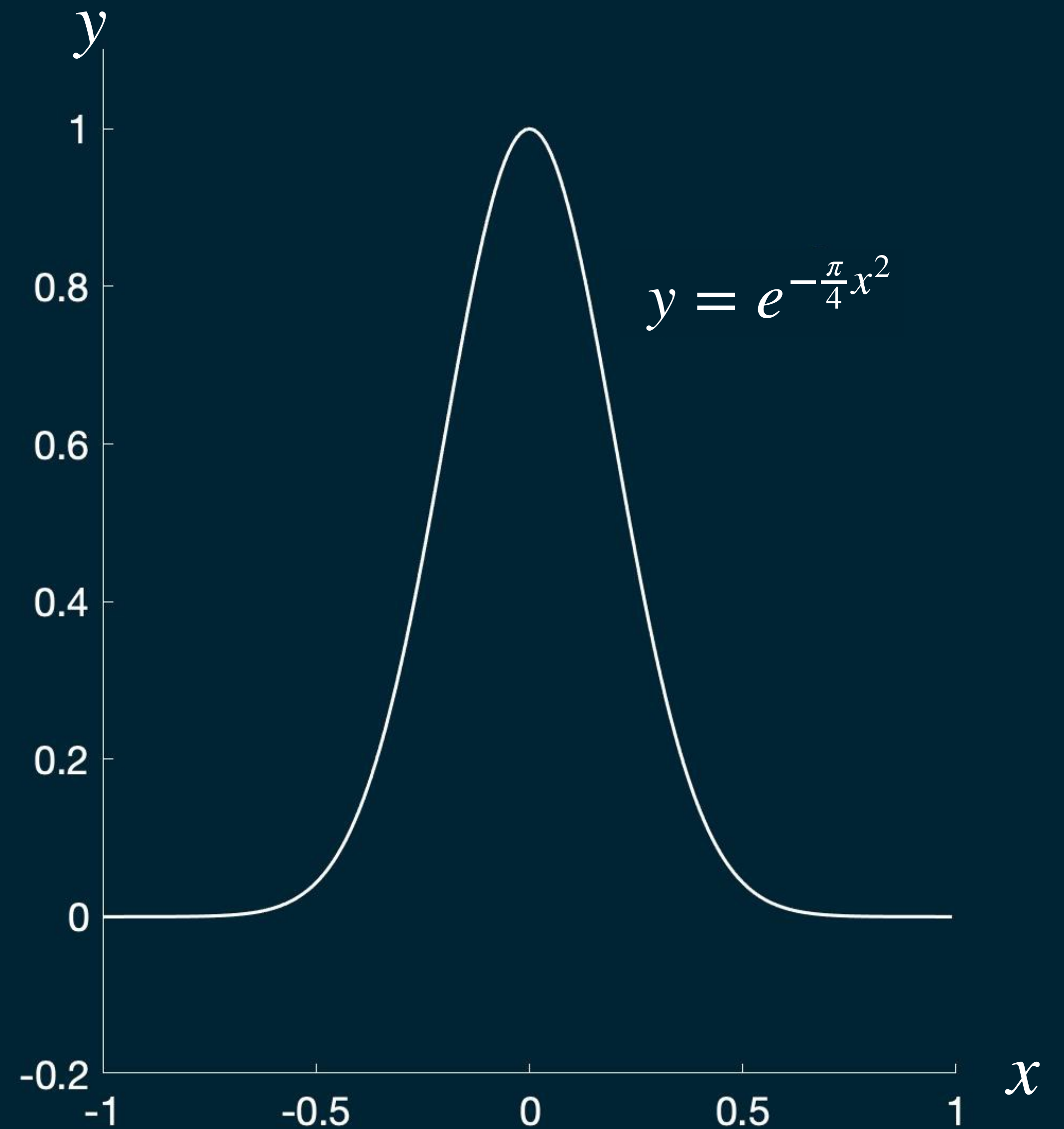
Defocus contrast: a summary

1. Electrons have really short wavelengths, and they travel through the column one by one.
2. The grating object produces diffracted waves with shifting phase
3. When the phase of the diffracted waves is right, we have contrast.
4. A lens reproduces the wavefronts at the image plane.
5. Spherical aberration and amplitude contrast introduce new terms in the CTF.
6. A phase plate alters the wavefronts after they've passed through the lens.

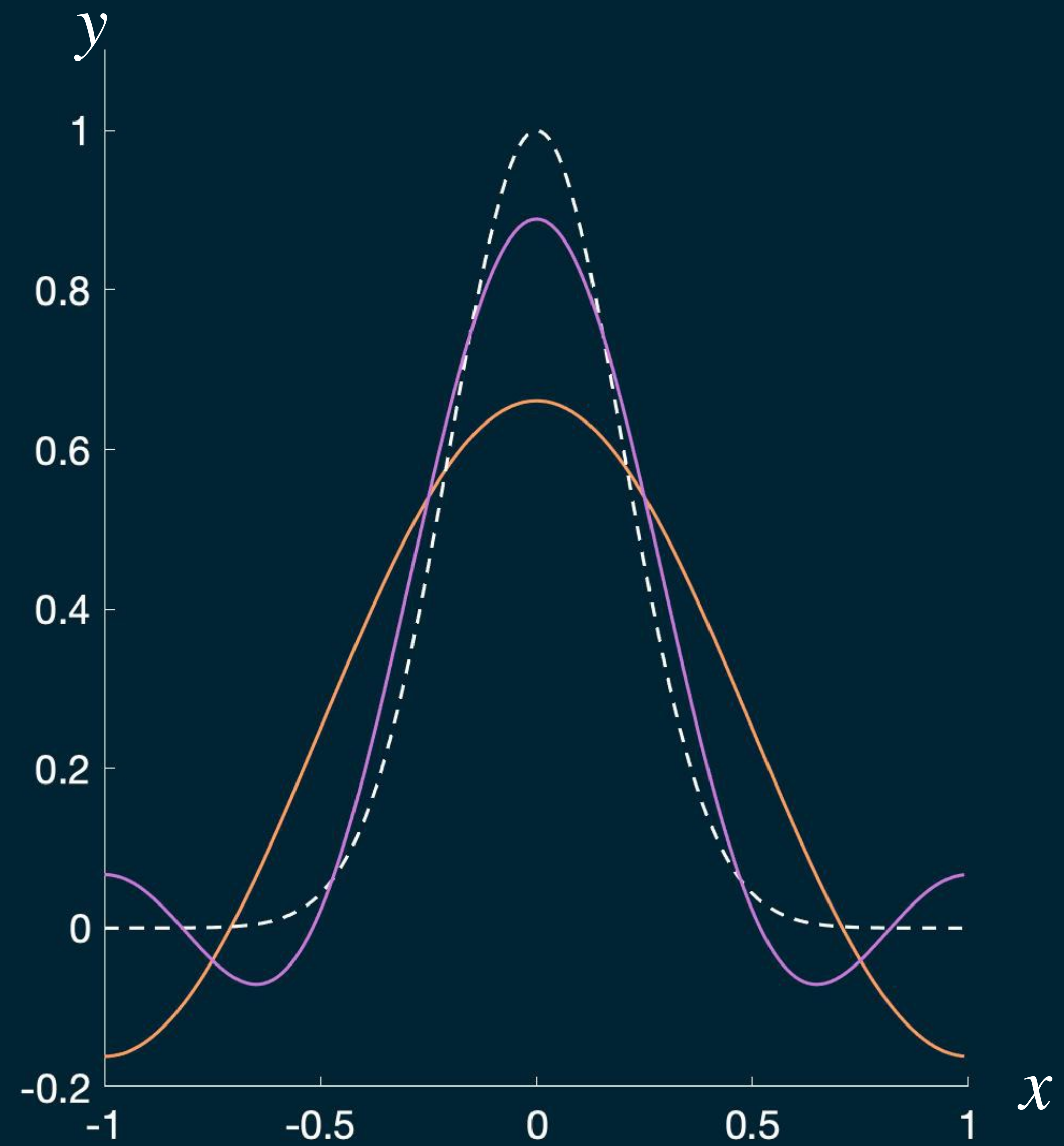
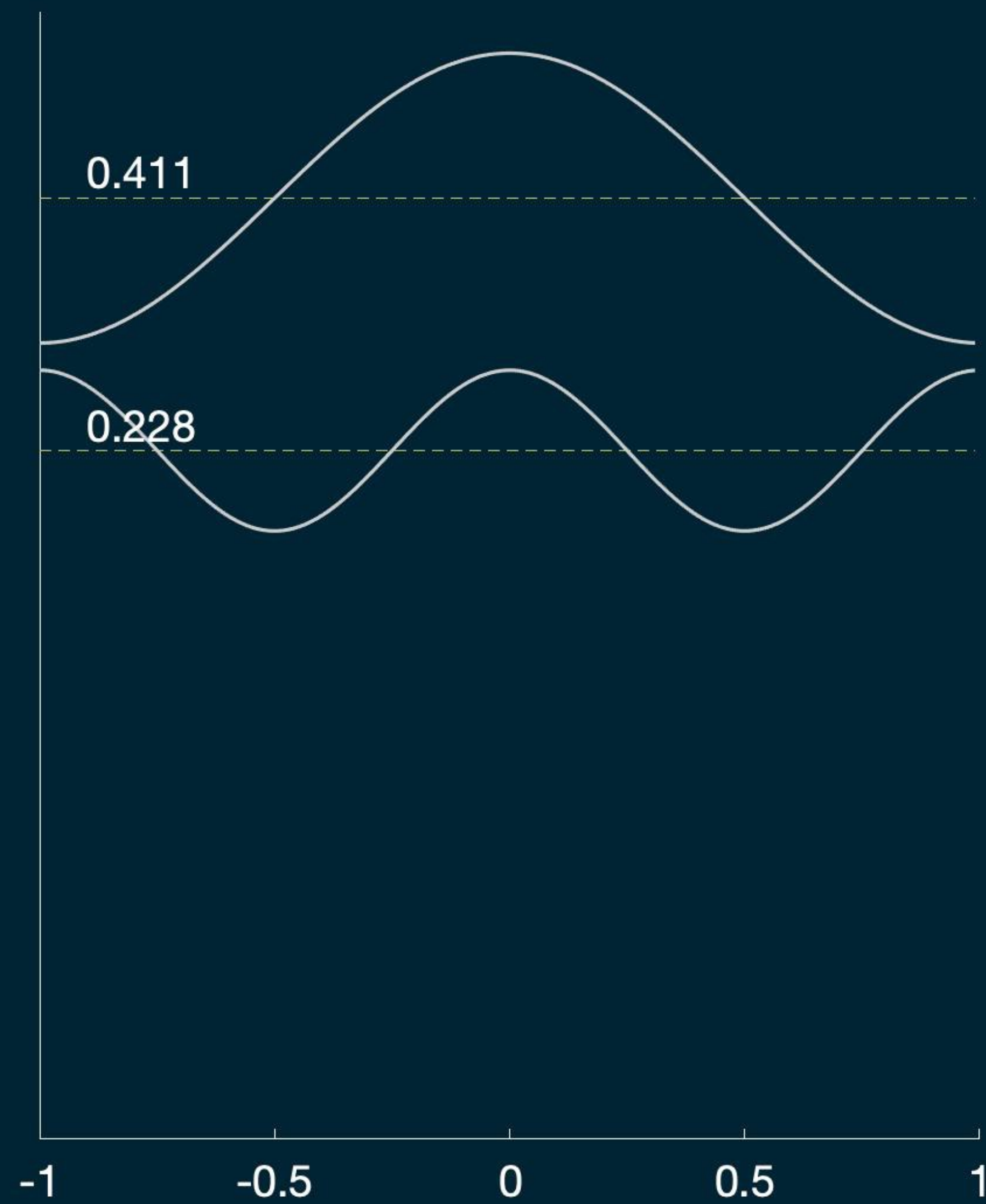
II. Fourier transforms and their properties

1. Fourier transform in 1D
2. Fourier transform in 2D
3. The Fourier slice theorem and reconstruction

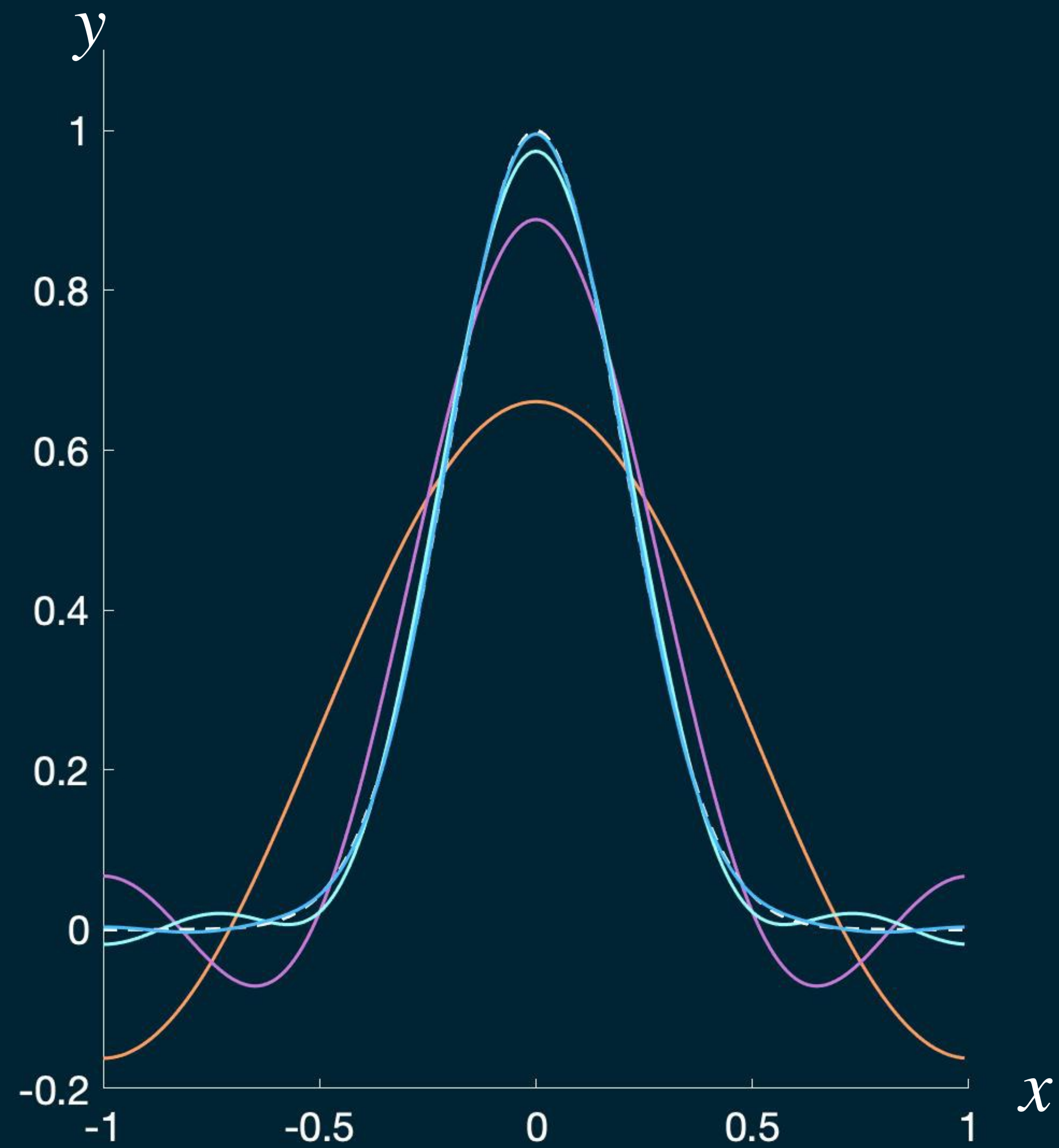
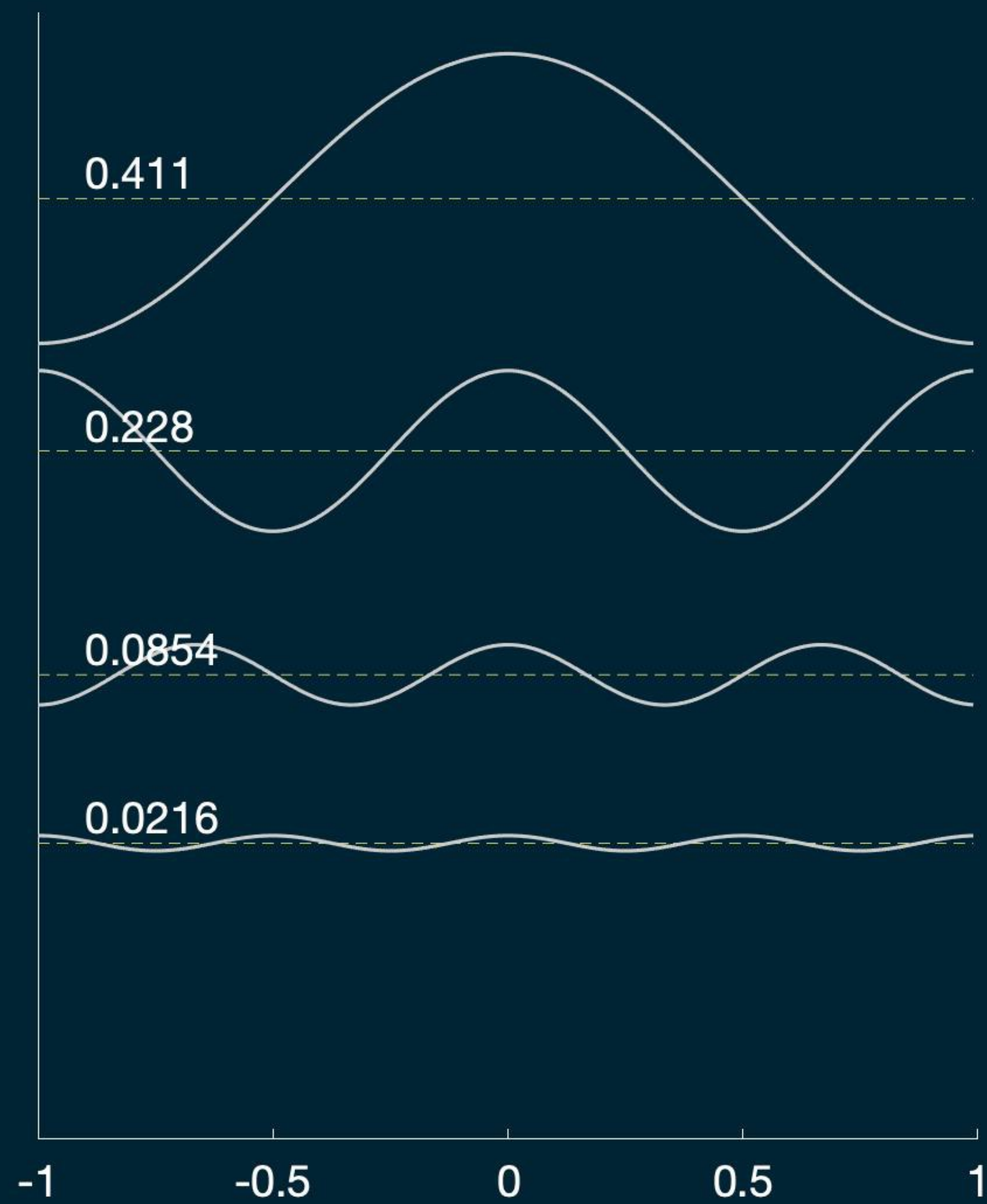
Reconstruction of a Gaussian function from cosine waves



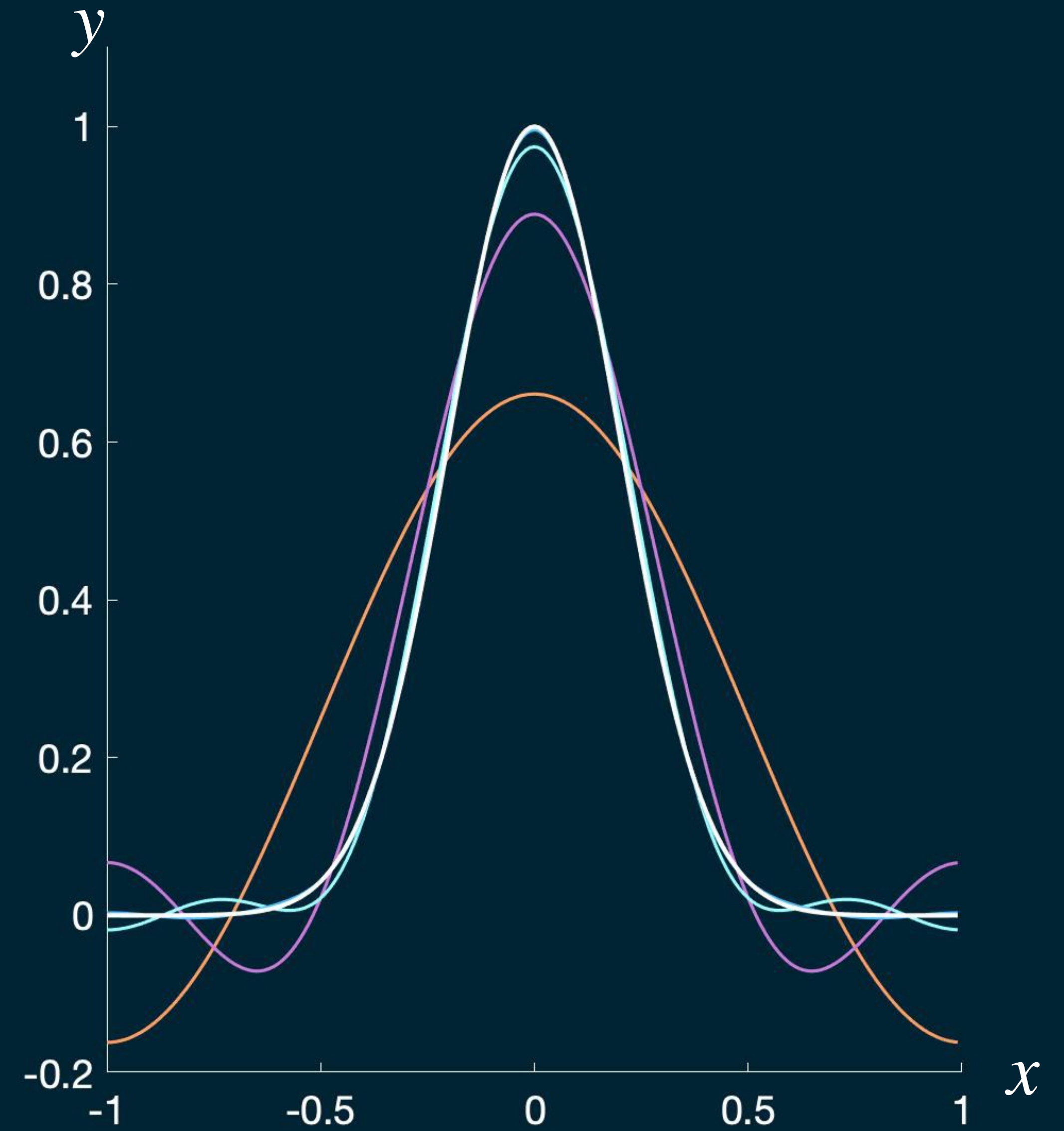
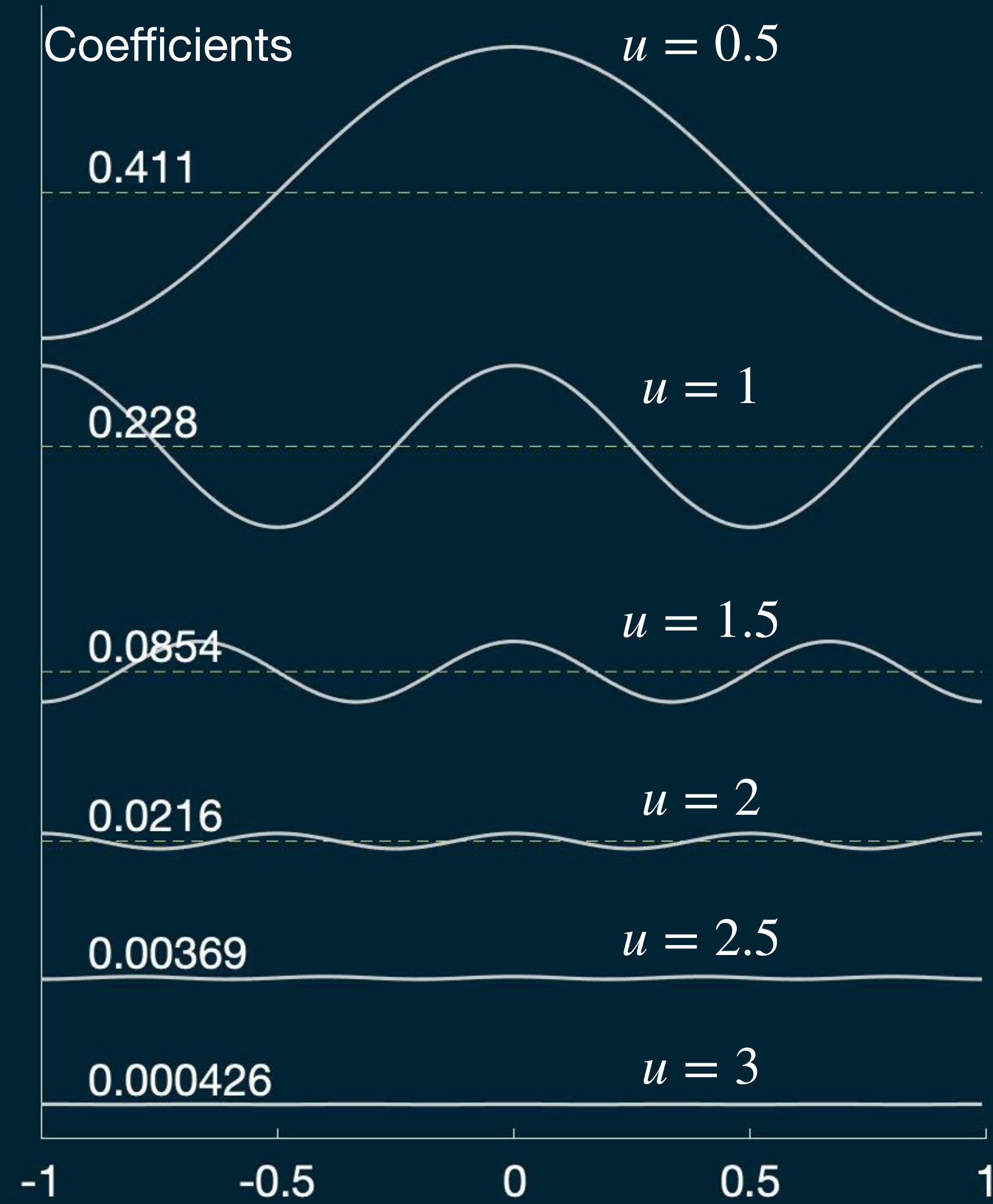
2 terms



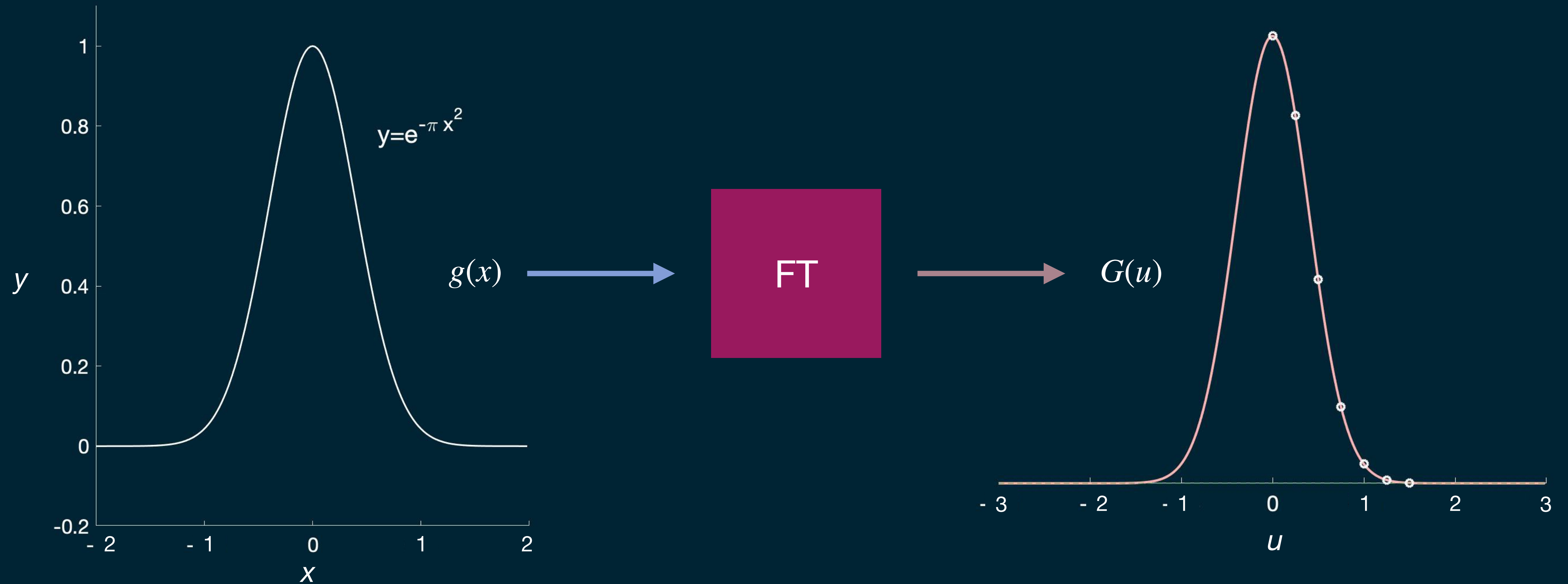
4 terms



u is the frequency variable



The Fourier Transform gives us the coefficients



A transform pair

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

Fourier transform

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

Inverse Fourier transform

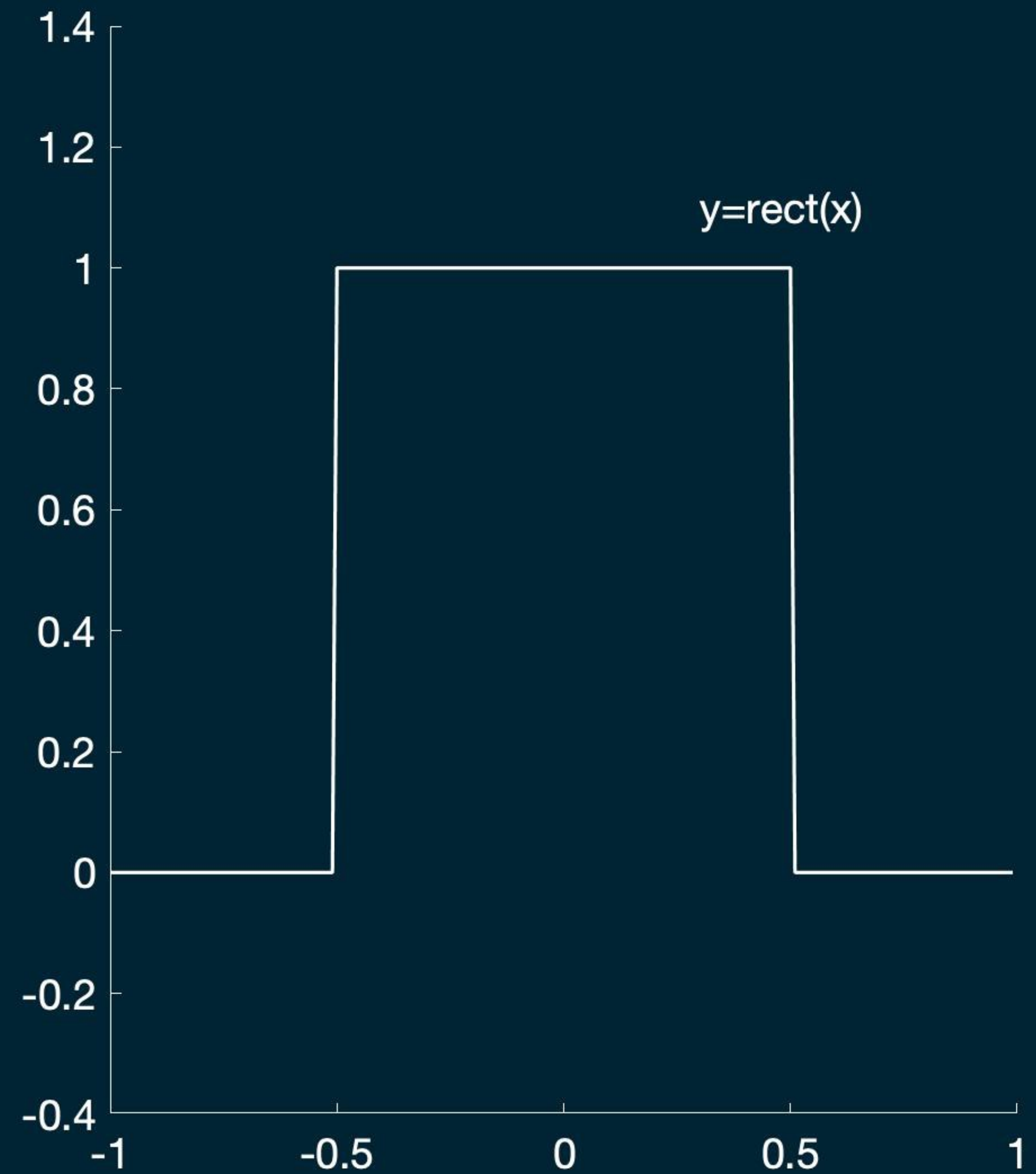
$$g(x) = \int G(u) e^{+i2\pi ux} du$$

Example:

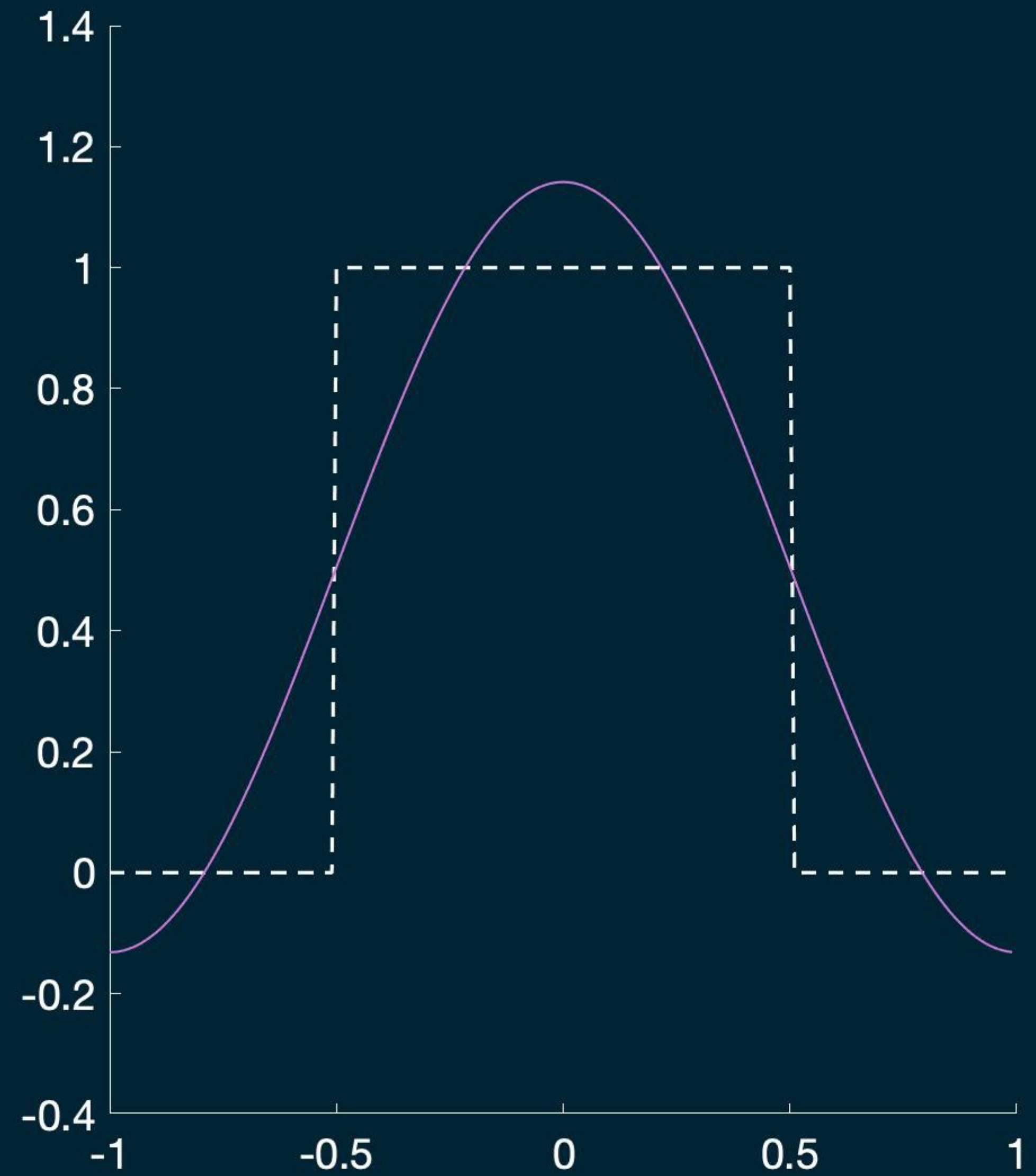
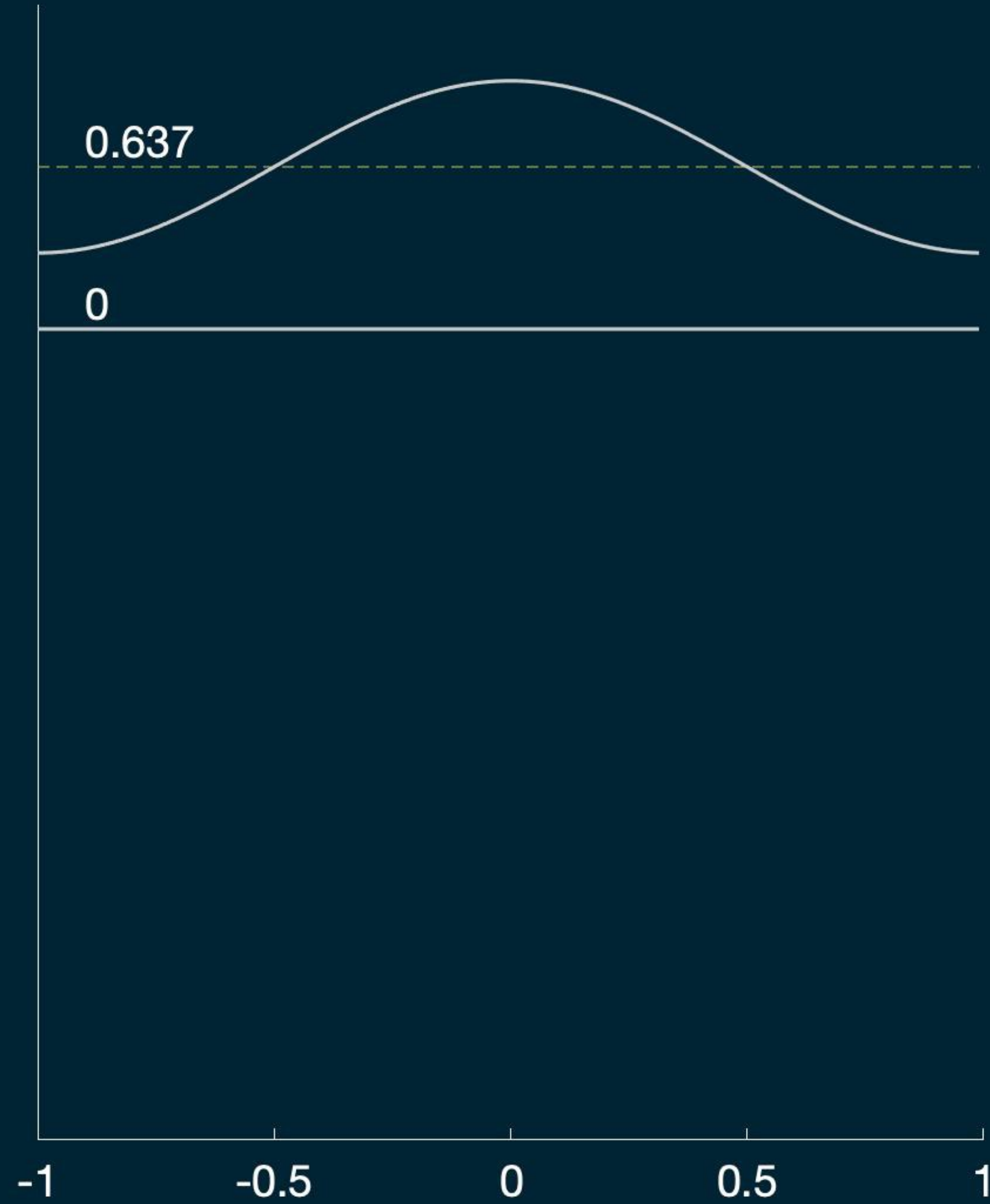
$$g(x) = e^{-\pi x^2}$$

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

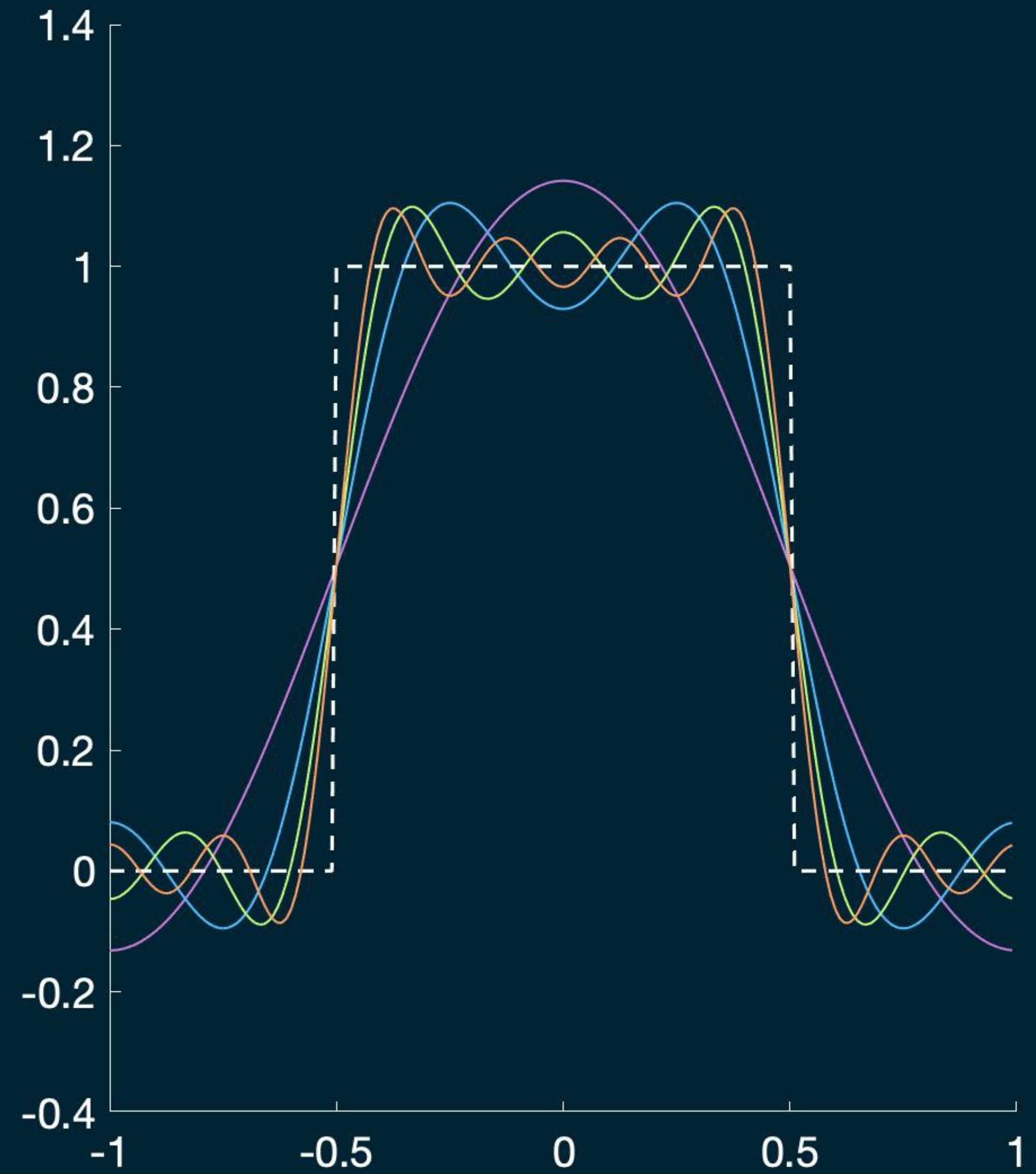
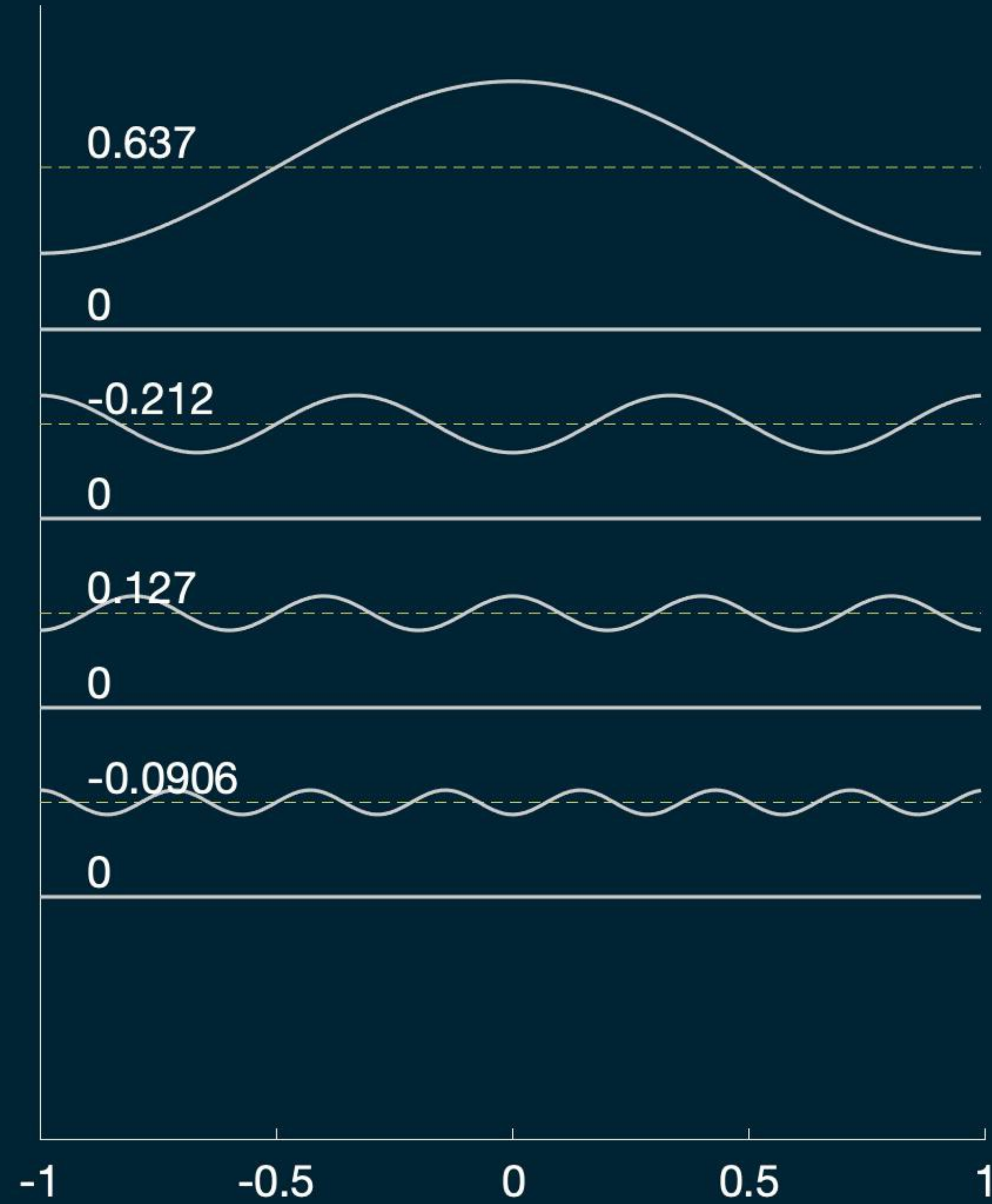
Fourier reconstruction of a rectangular function



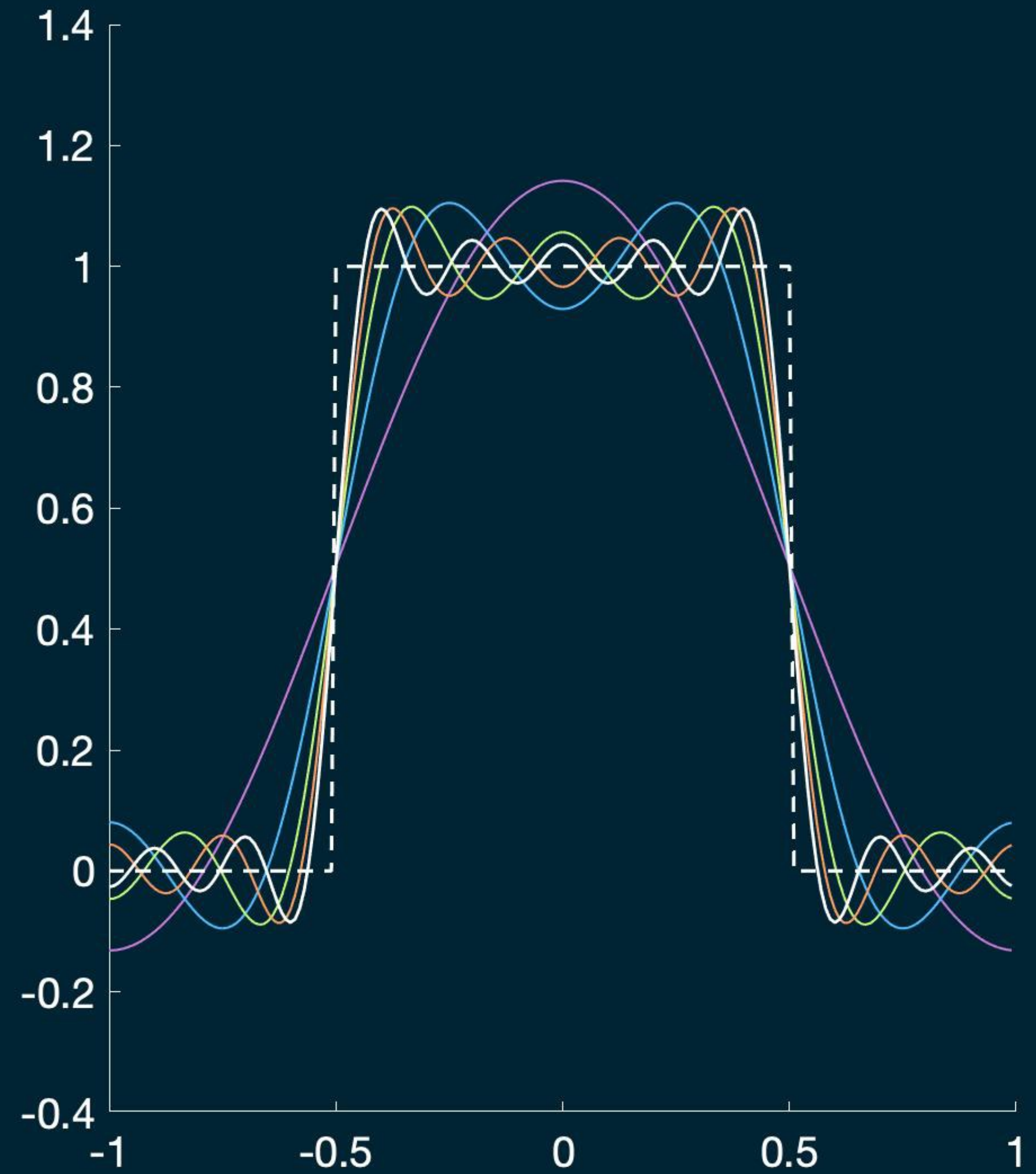
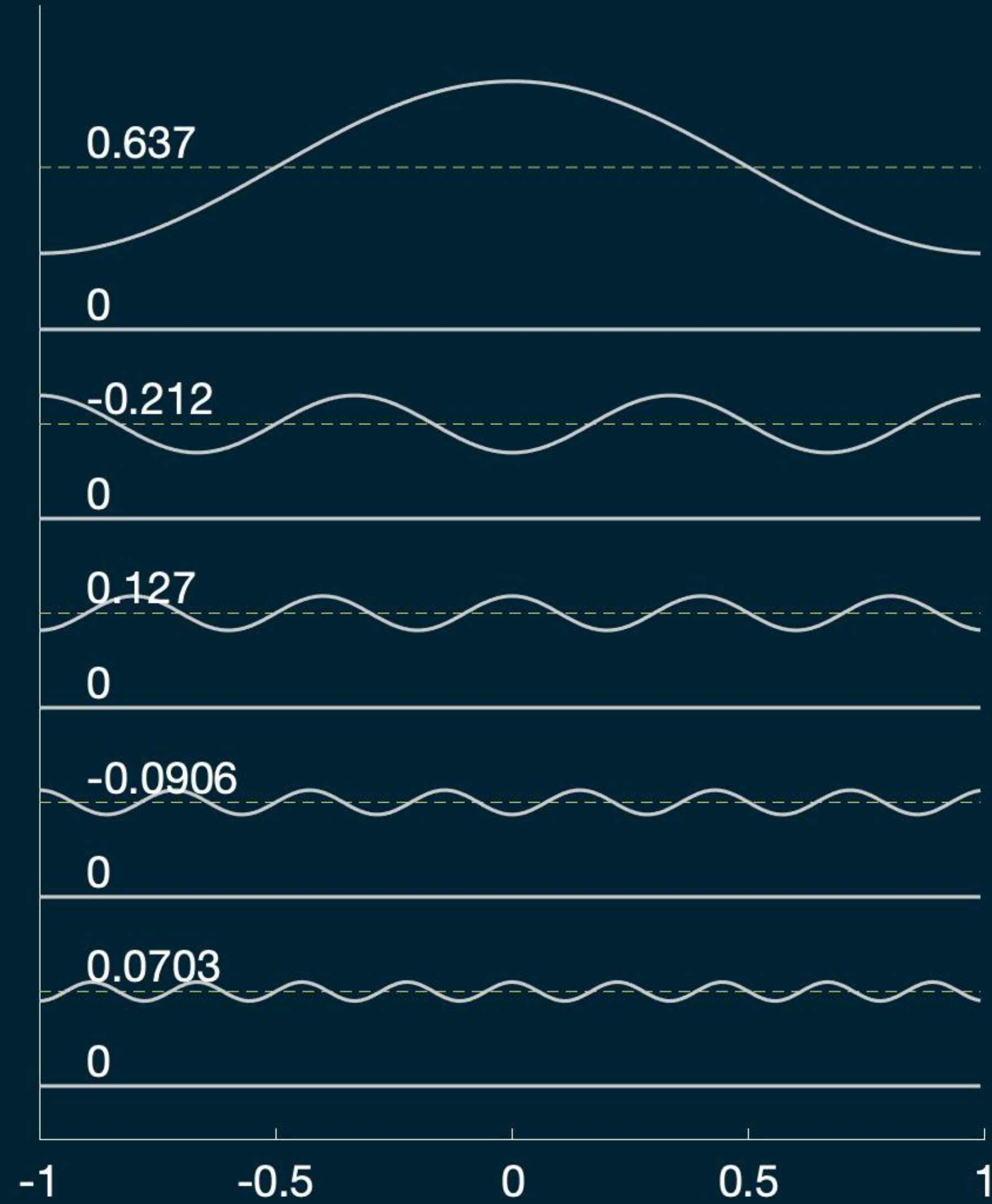
2 terms



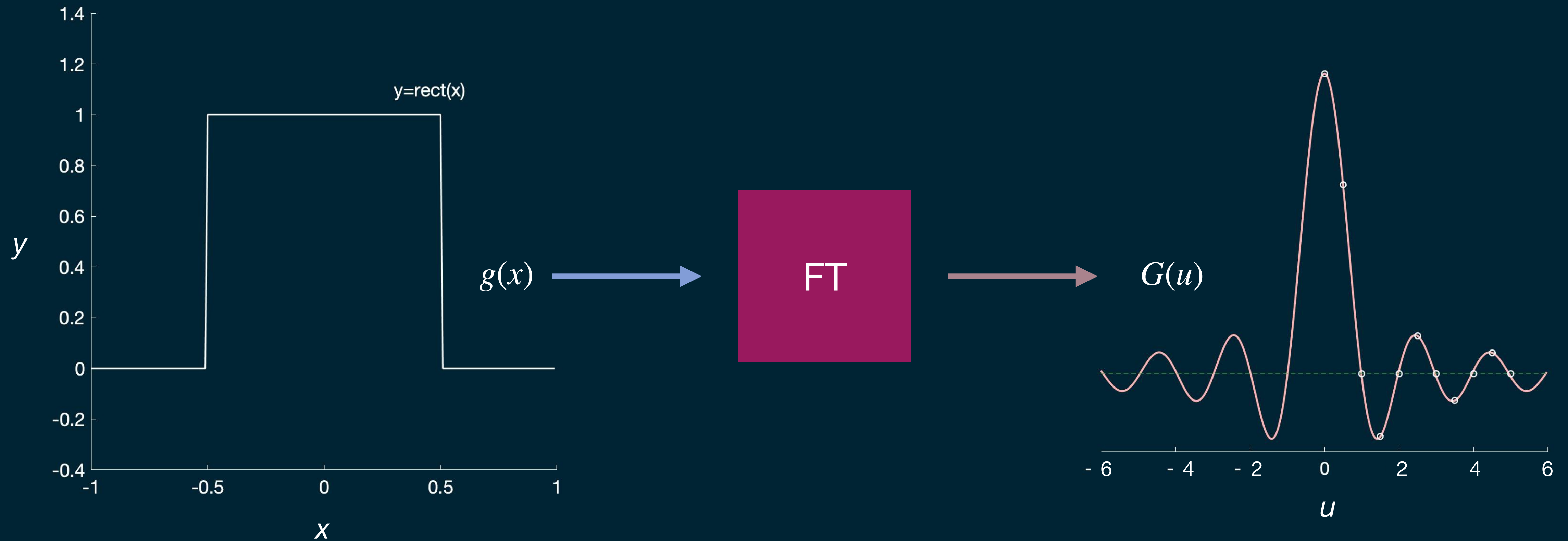
8 terms



Nowhere near convergence at 10 terms



The Fourier Transform of $\text{rect}(x)$ is $\text{sinc}(u)$

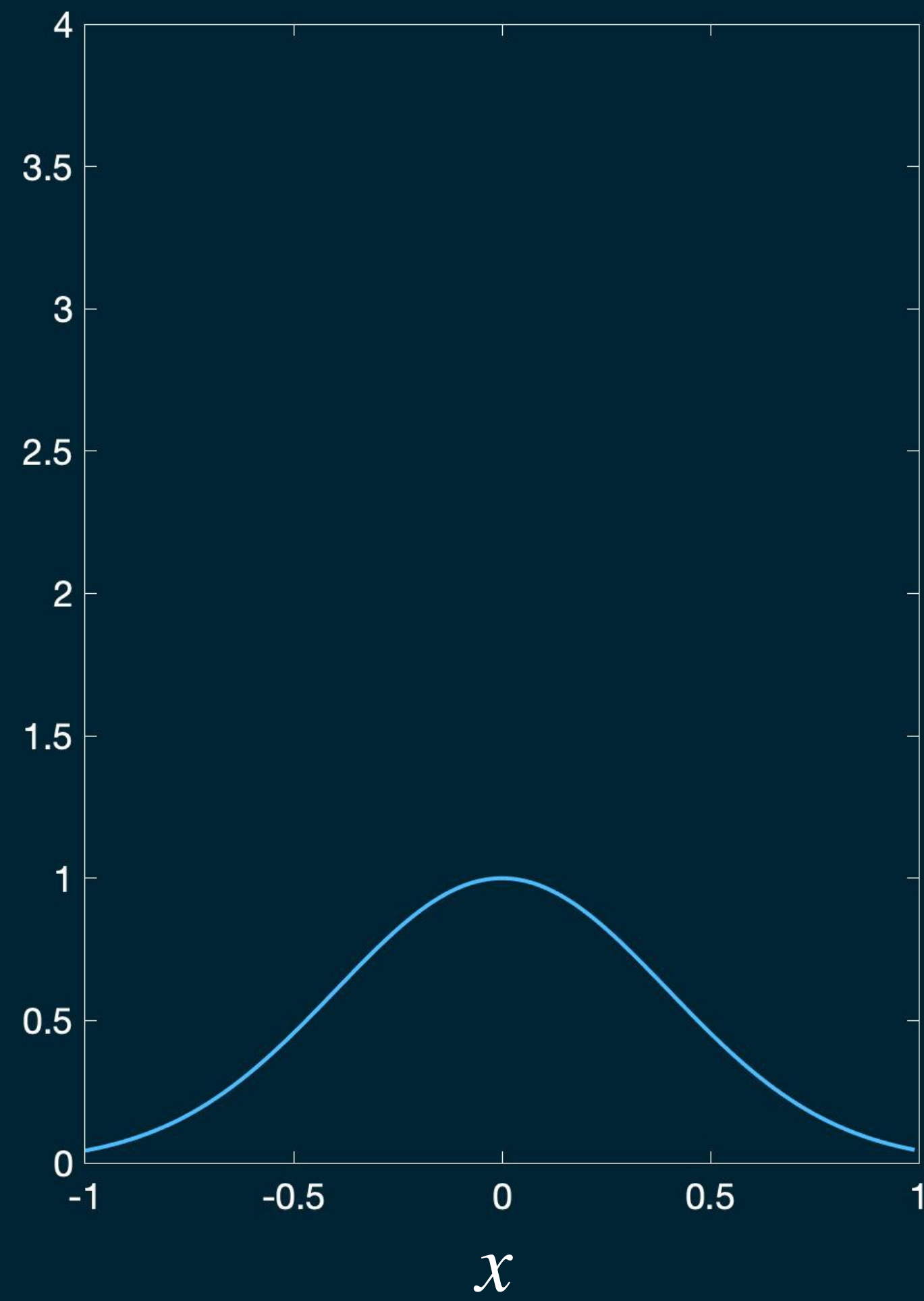


$$\text{rect}(x) \rightarrow \frac{\sin(\pi u)}{\pi u}$$

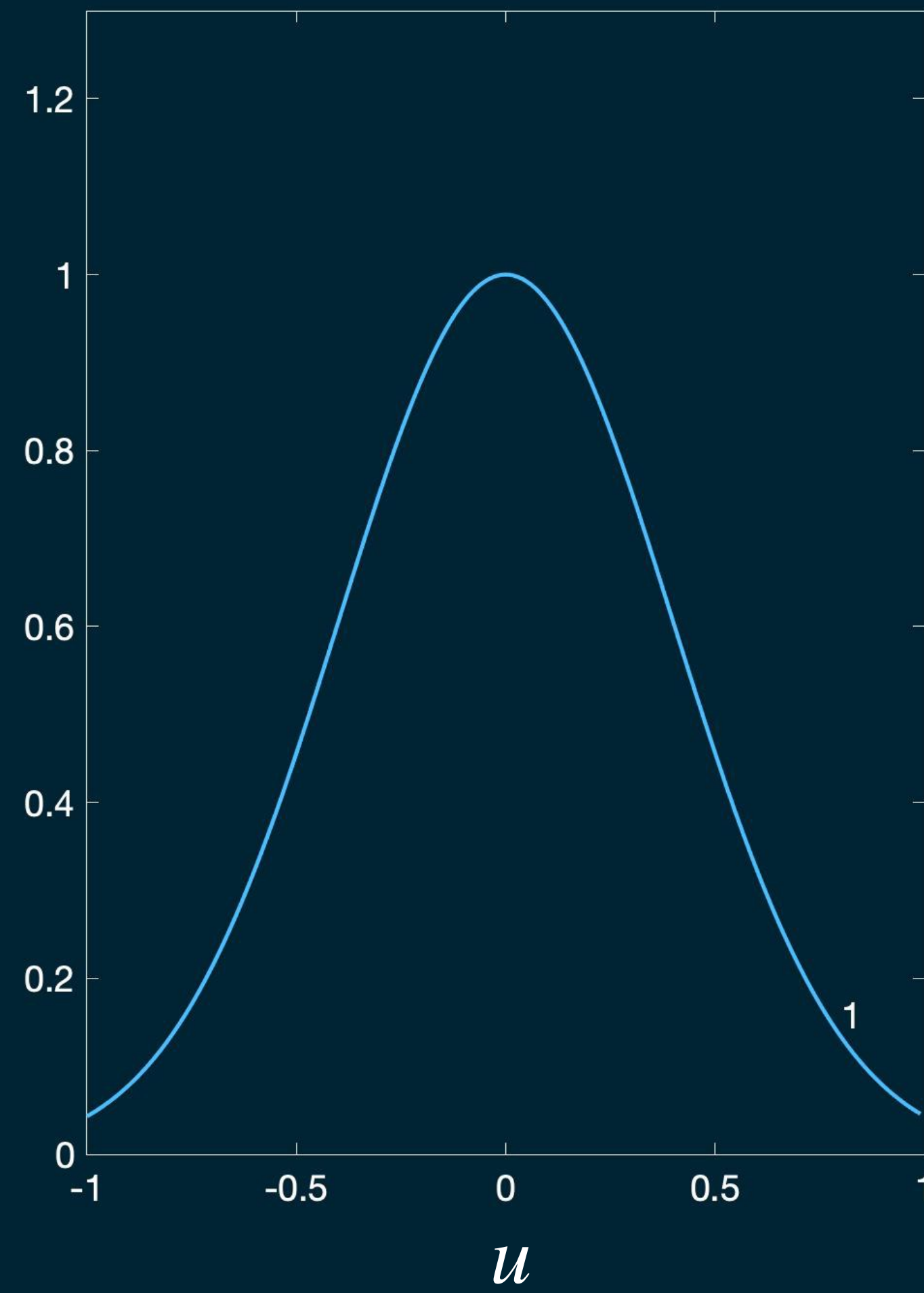
$$\frac{\sin(\pi u)}{\pi u} \text{ is also known as: } \text{sinc}(u)$$

Reciprocal scaling of FT pairs

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

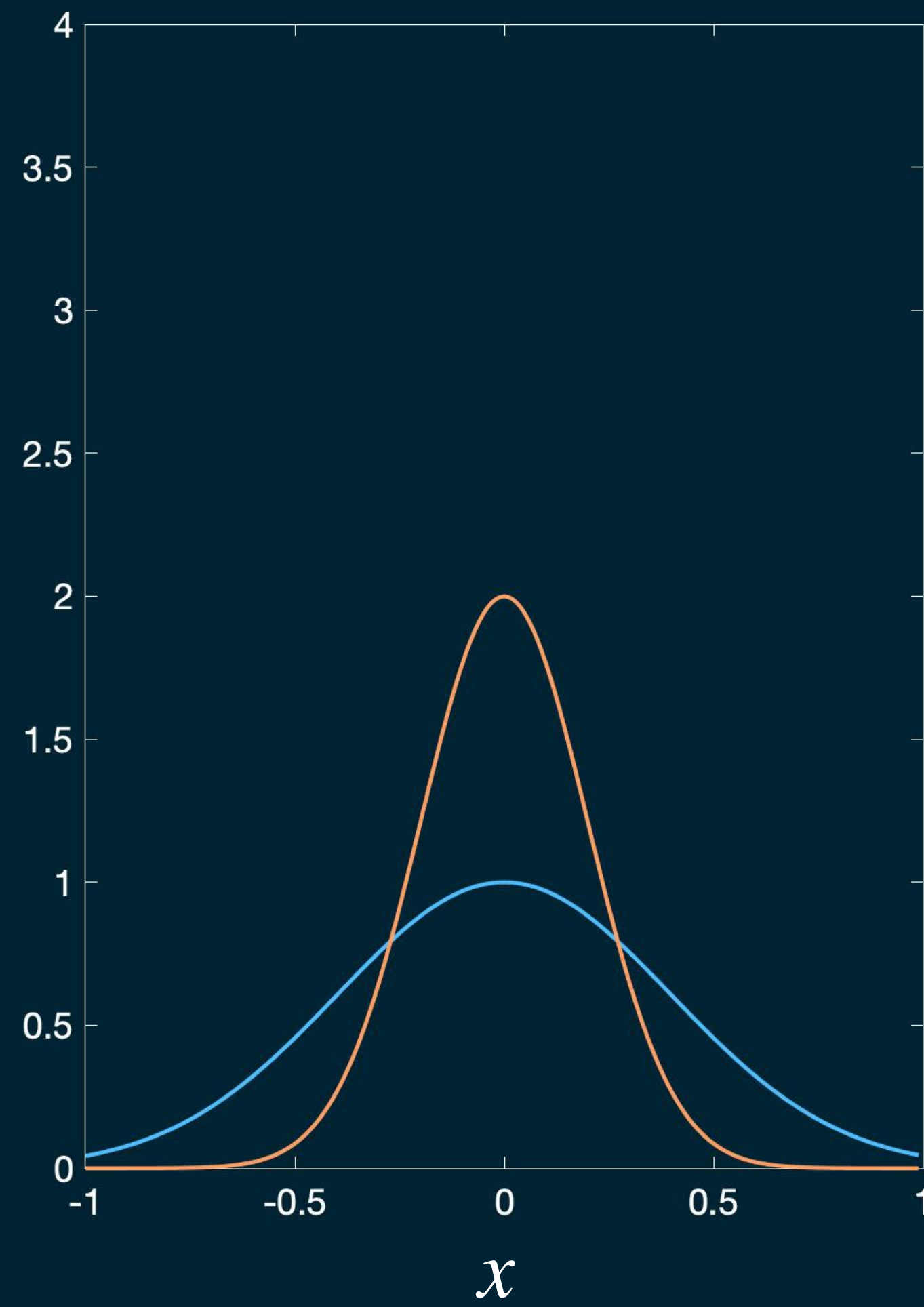


$$G(u) = e^{-\pi(u/a)^2}$$

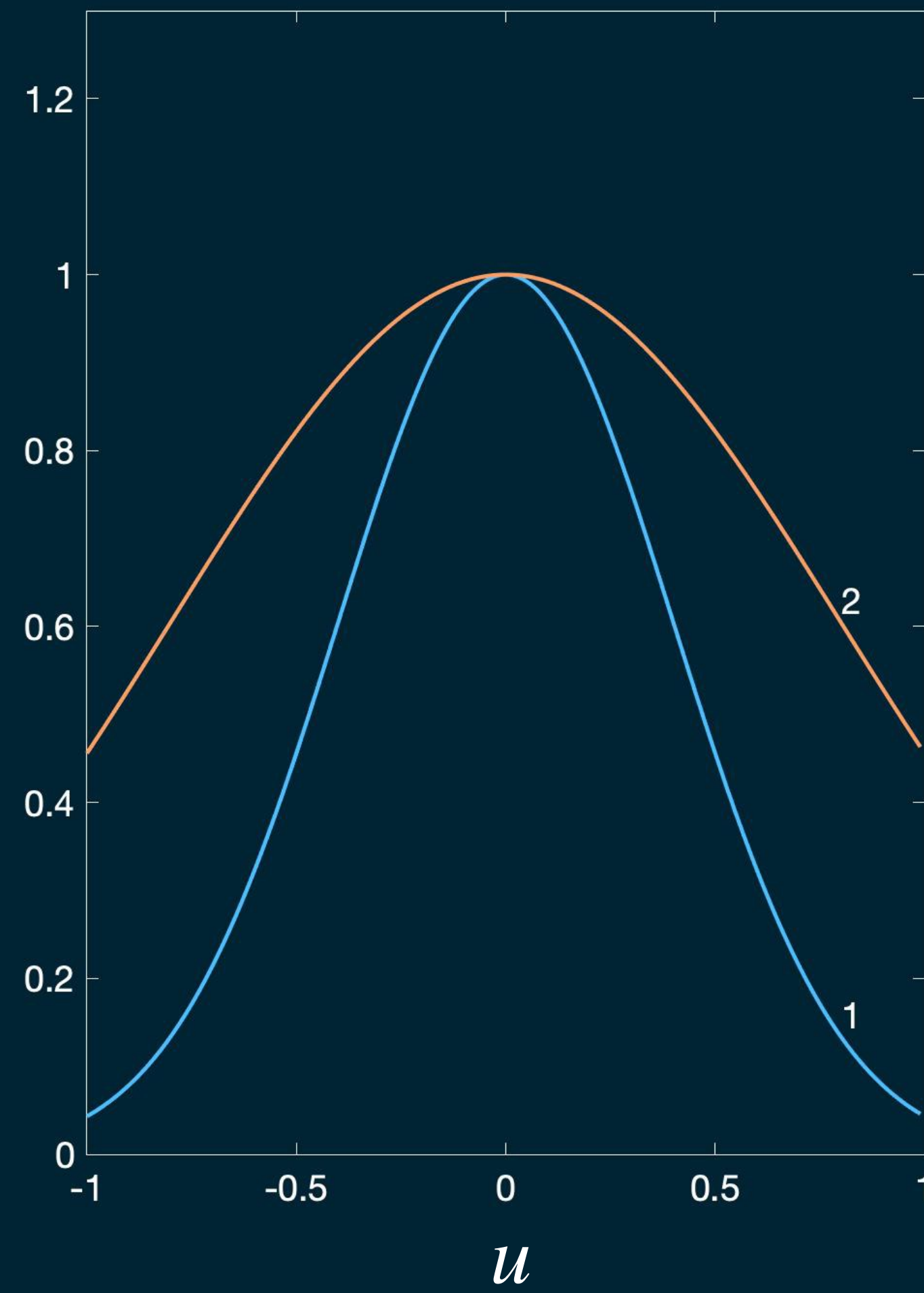


Reciprocal scaling of FT pairs

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

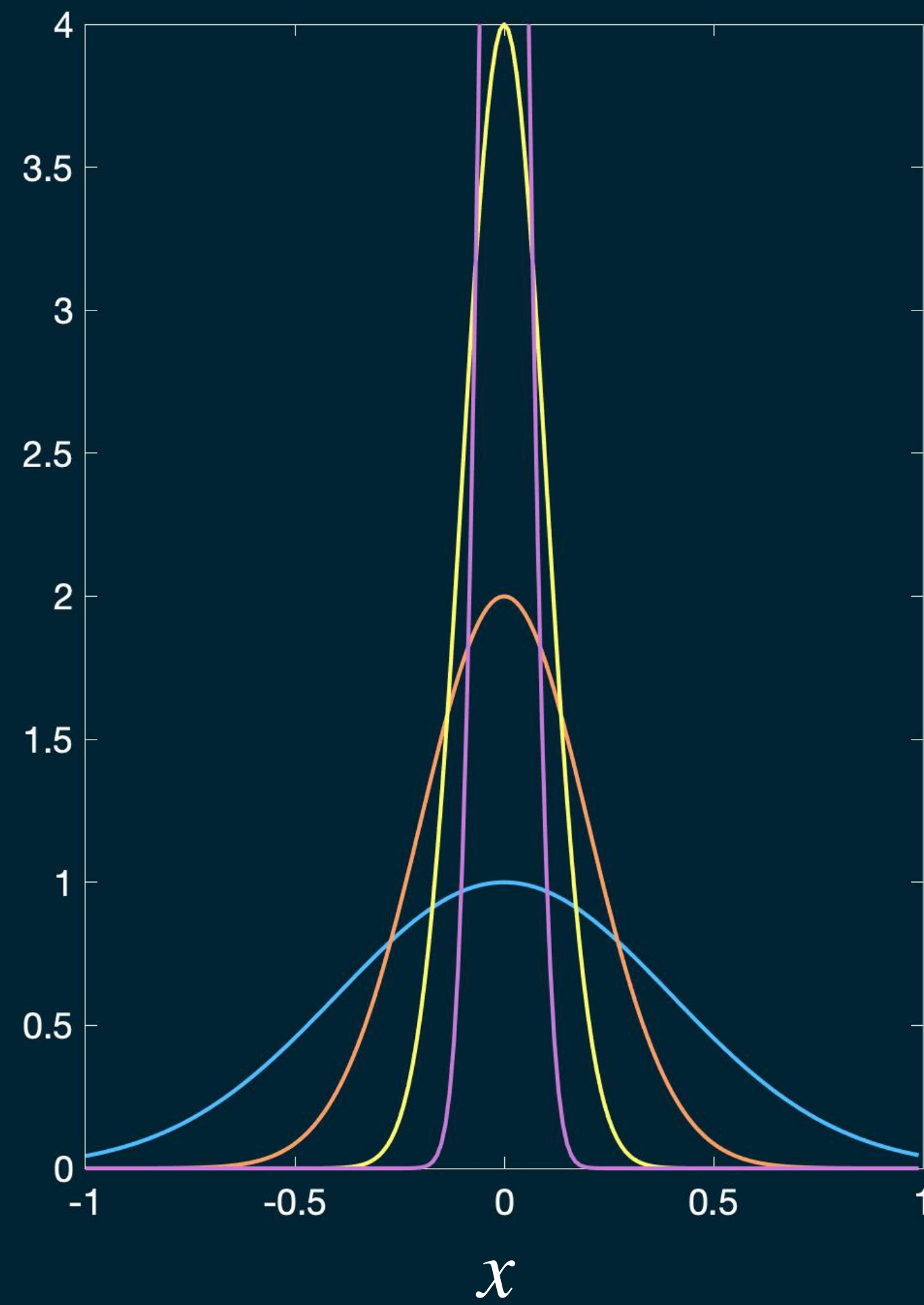


$$G(u) = e^{-\pi(u/a)^2}$$

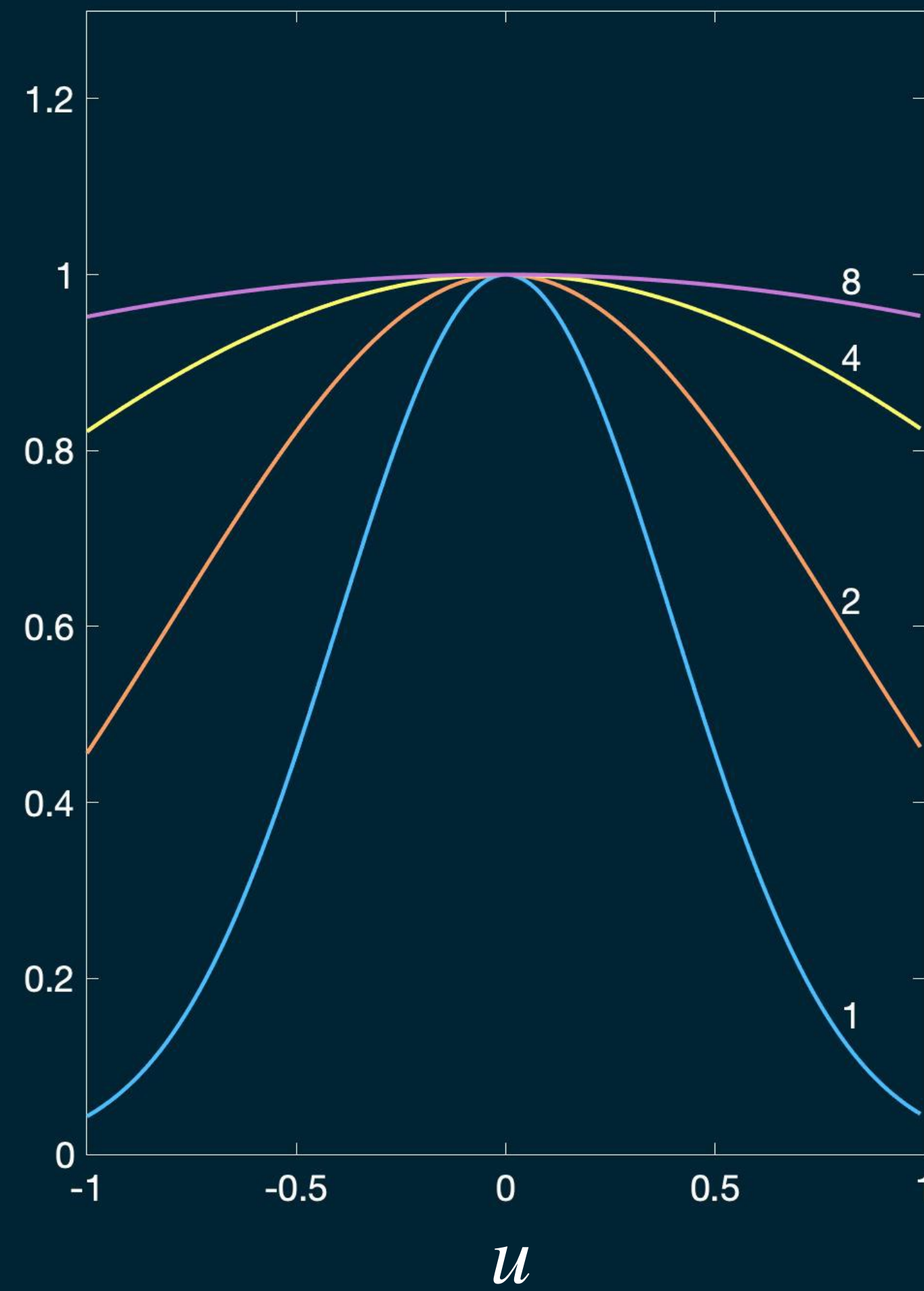


Reciprocal scaling of FT pairs

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



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

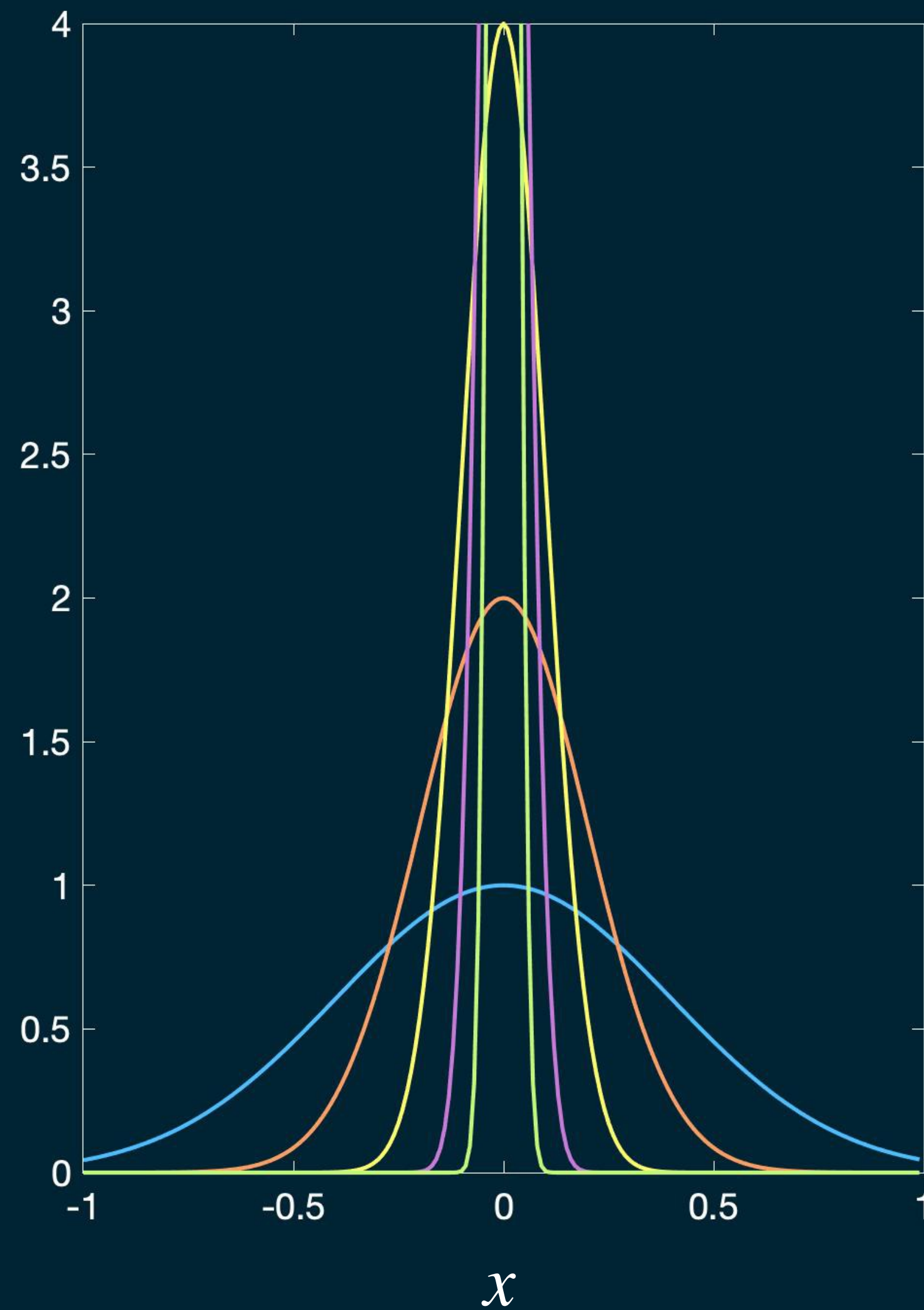


Scale property

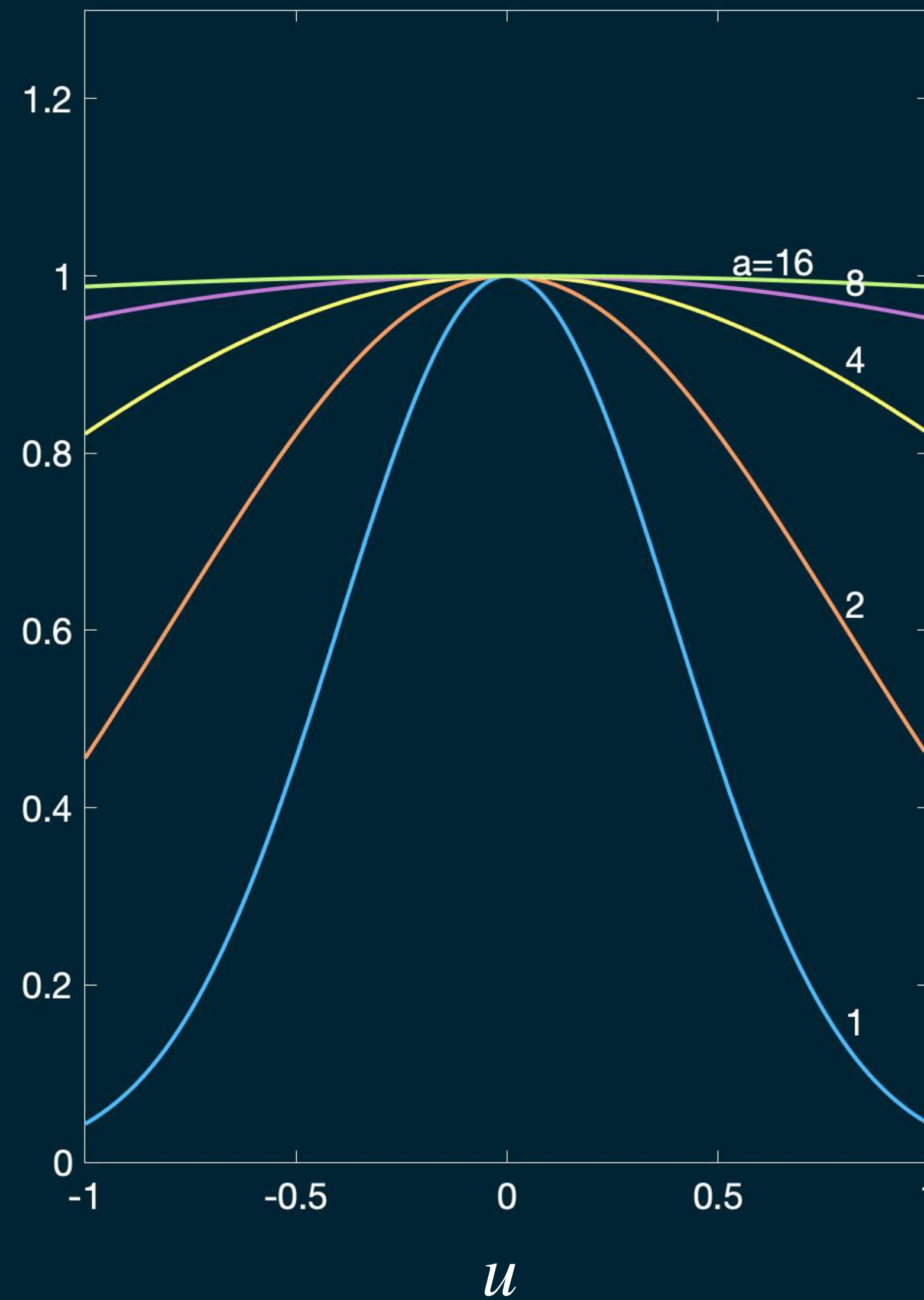
$$ag(ax) \rightarrow G(u/a)$$

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

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

FT Pair

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

Fourier transform pairs

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

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

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

1D Fourier transform properties

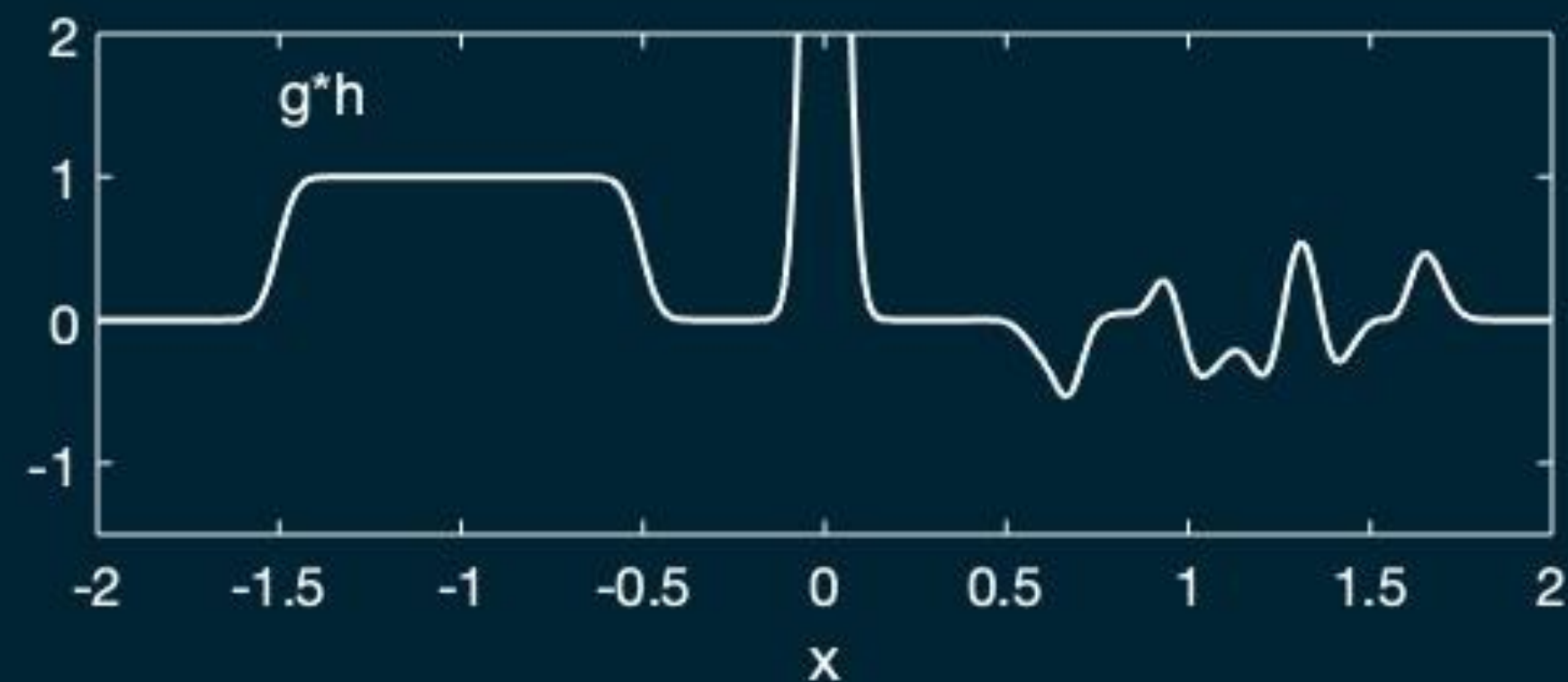
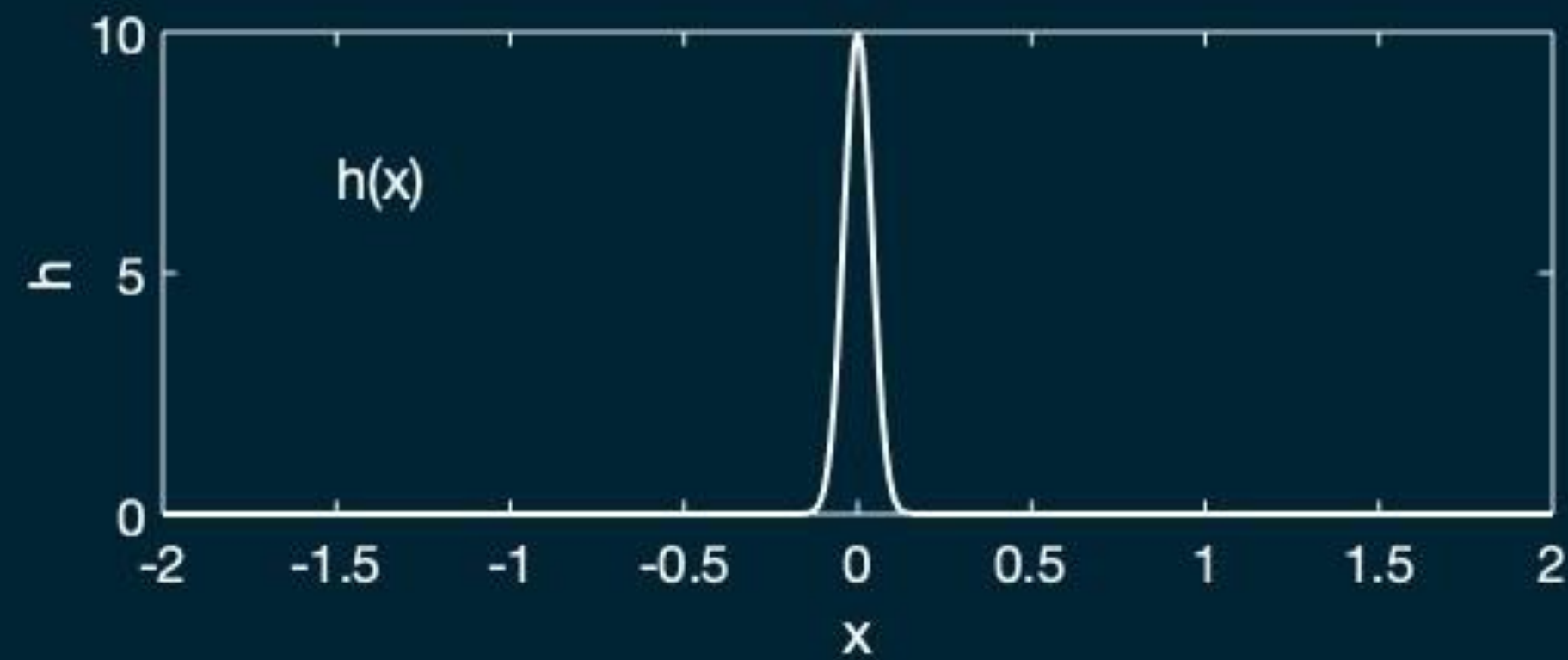
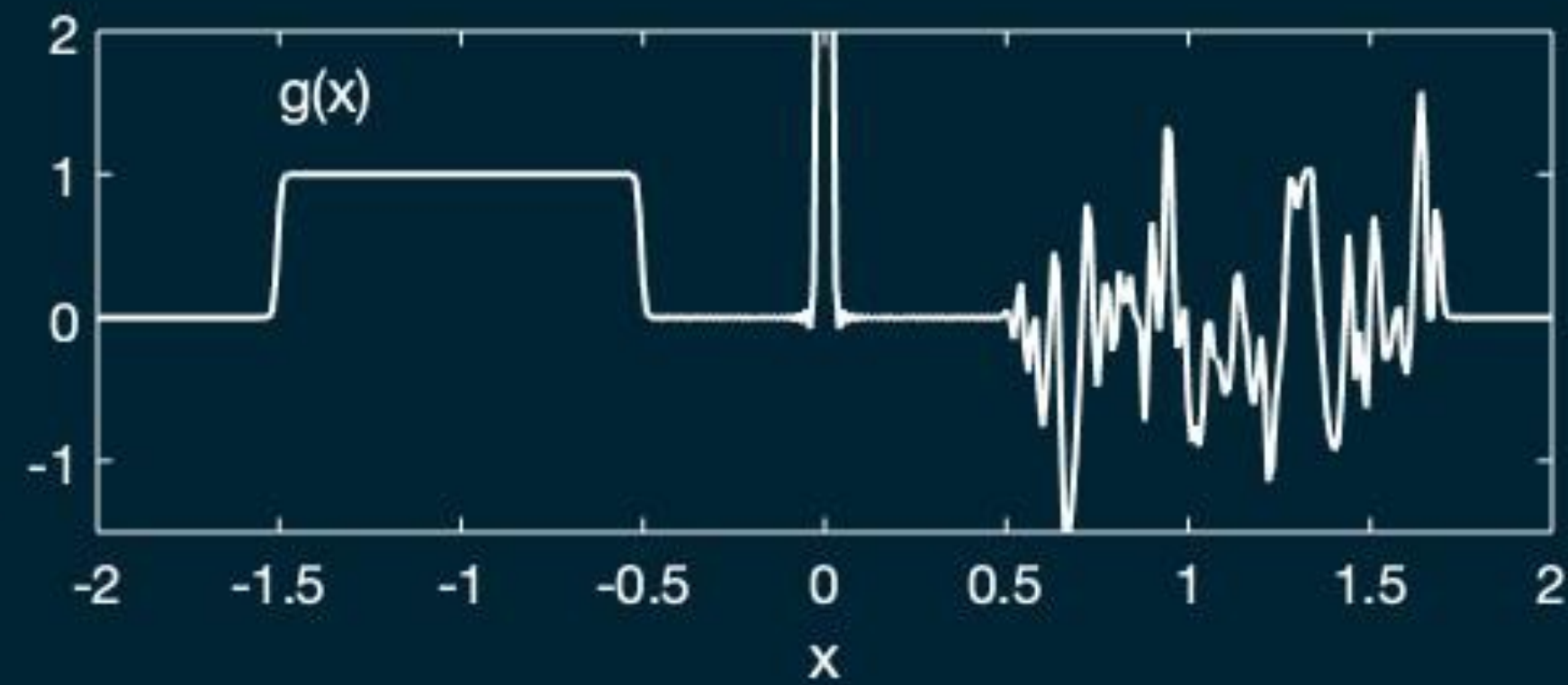
$$g(x) + h(x) \rightarrow G(x) + H(x) \quad \text{Linearity}$$

$$ag(ax) \rightarrow G(u/a) \quad \text{Scale}$$

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

$$g \star h \rightarrow G(u)H(u) \quad \text{Convolution}$$

Convolution with a Gaussian kernel



Convolution

$f(x) = g \star h$ means:

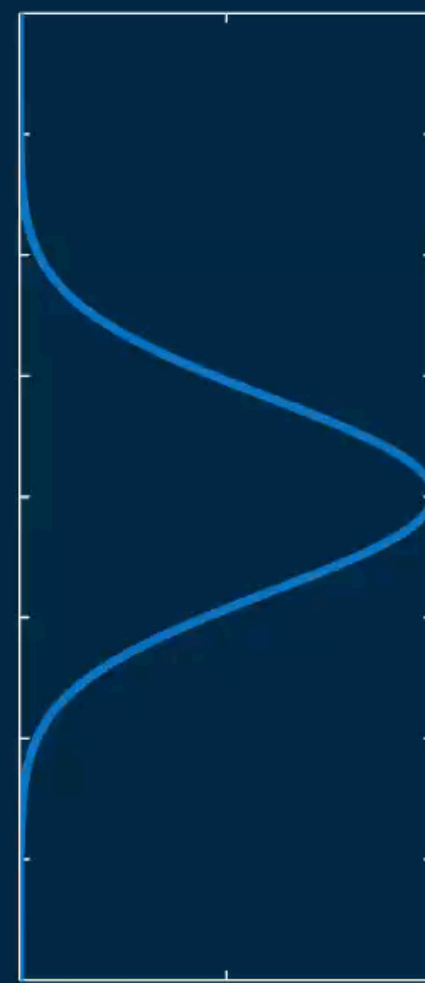
$$f(x) = \int g(x - s)h(s)ds$$

II. Fourier transforms and their properties

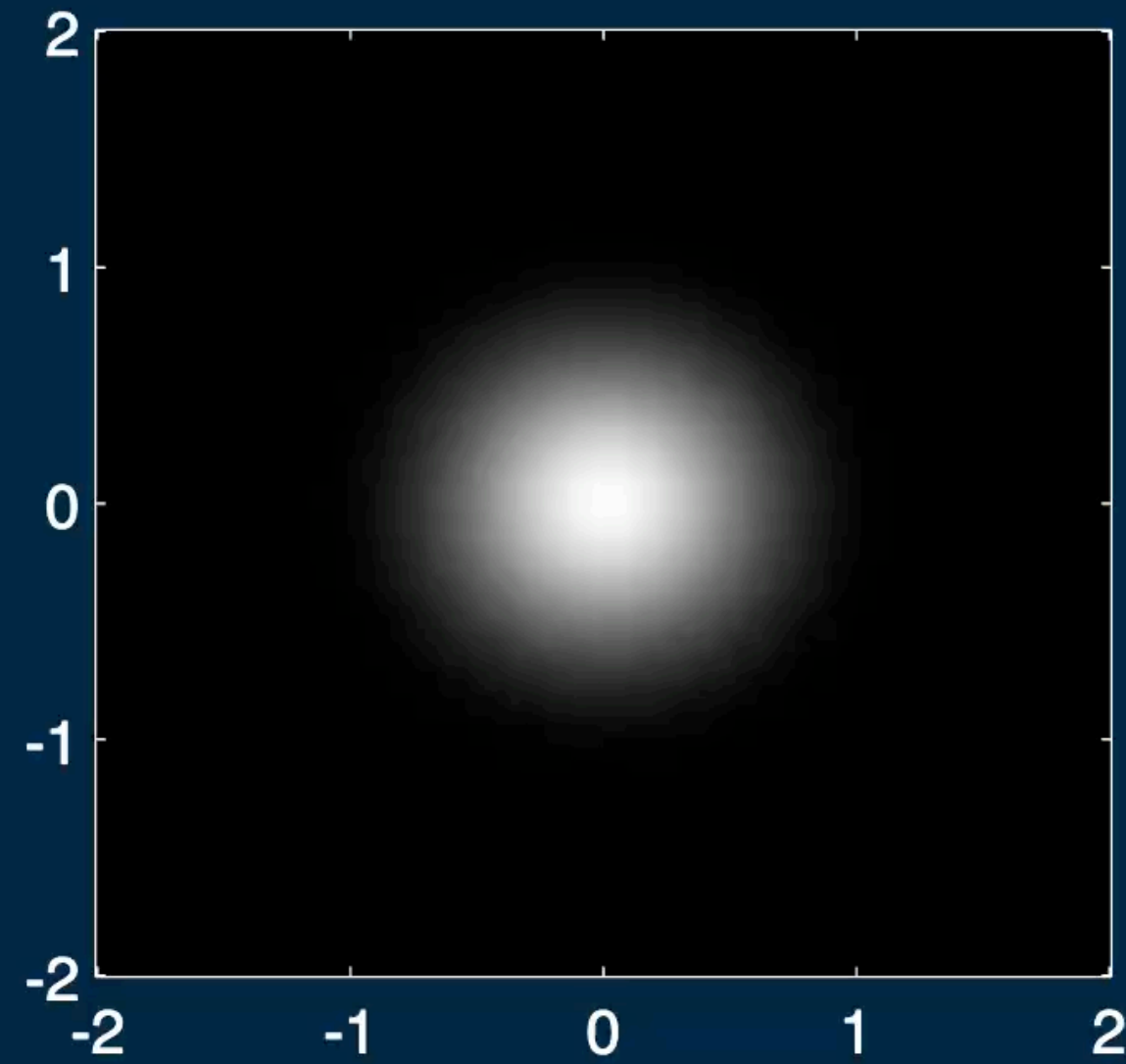
1. Fourier transform in 1D
2. Fourier transform in 2D
3. The Fourier slice theorem and reconstruction

Fourier reconstruction of a 2D Gaussian function

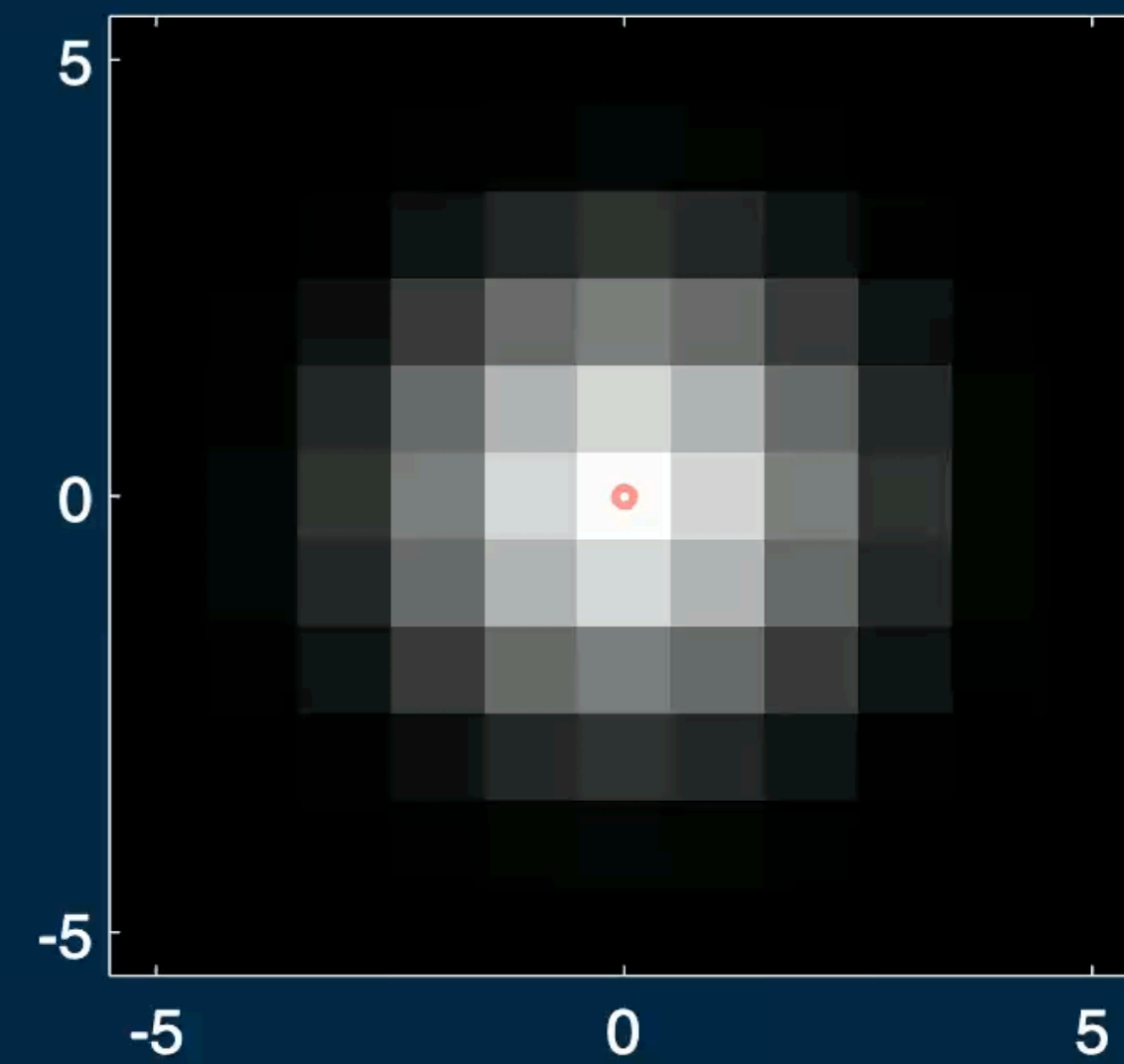
Projection



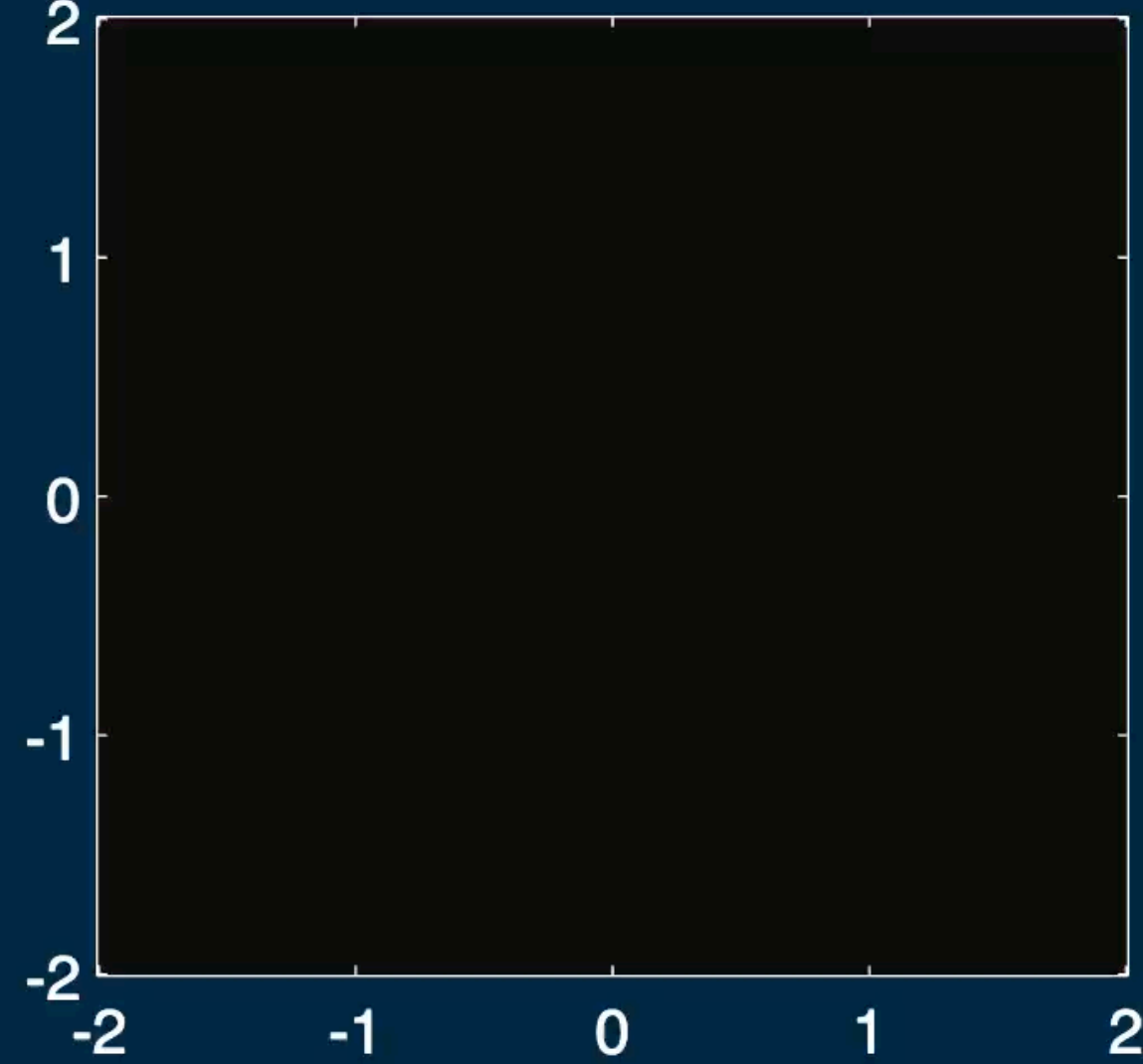
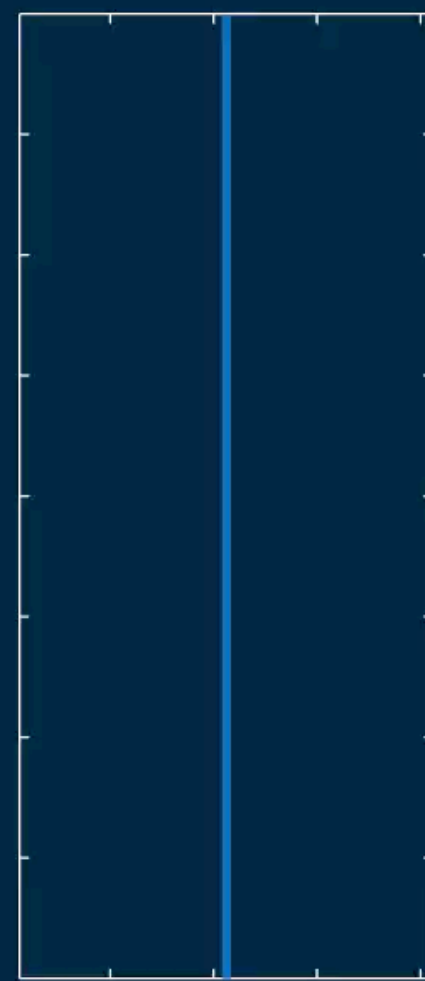
$g(x, y)$



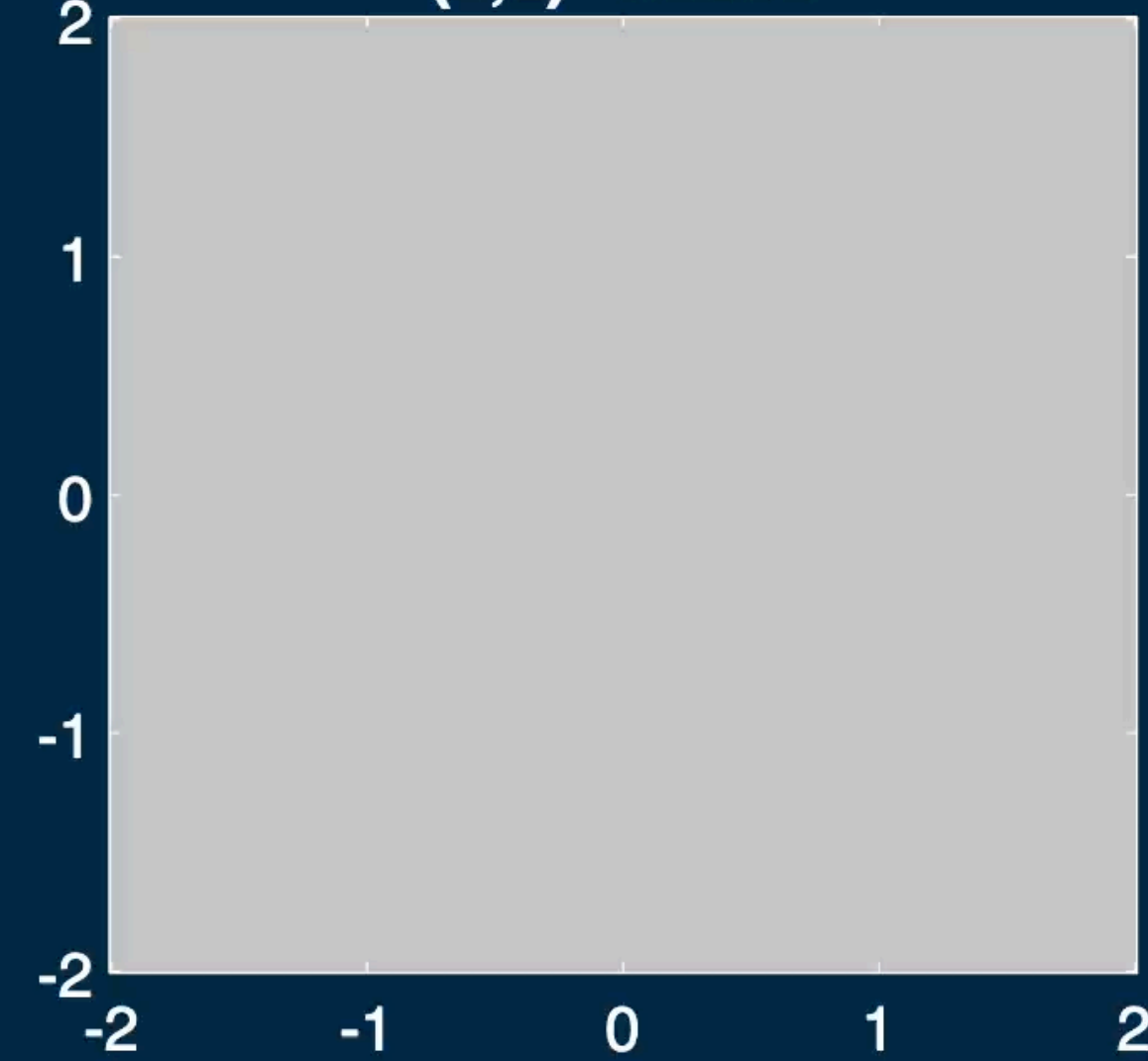
$G(u, v)$



$\hat{g}(x, y)$

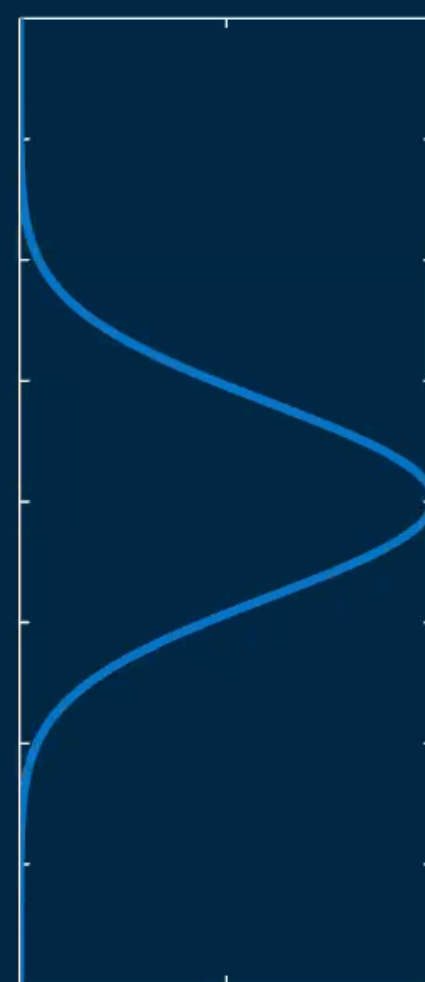


$G(0,0)=1.0000$

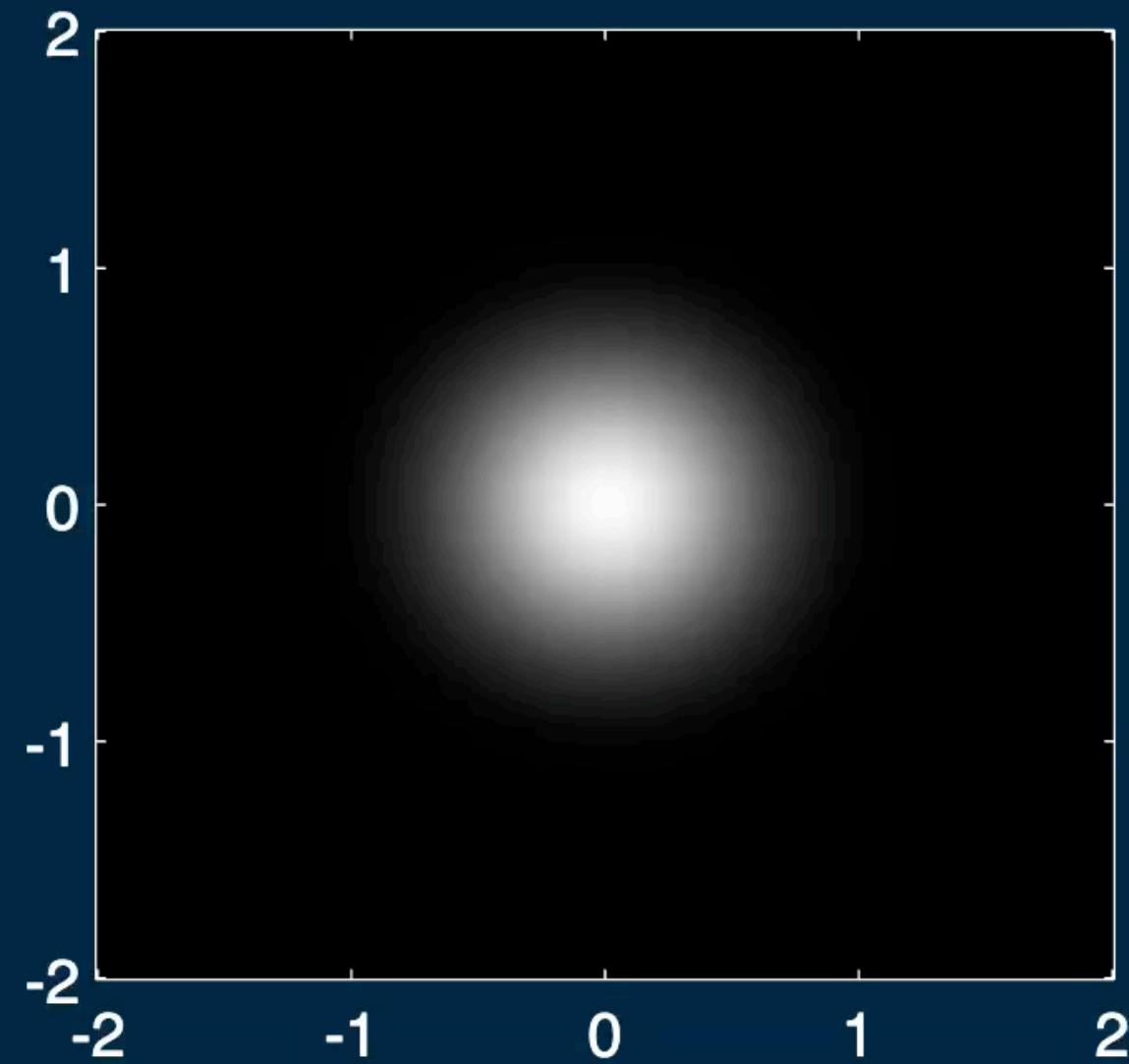


Fourier reconstruction of a 2D Gaussian function

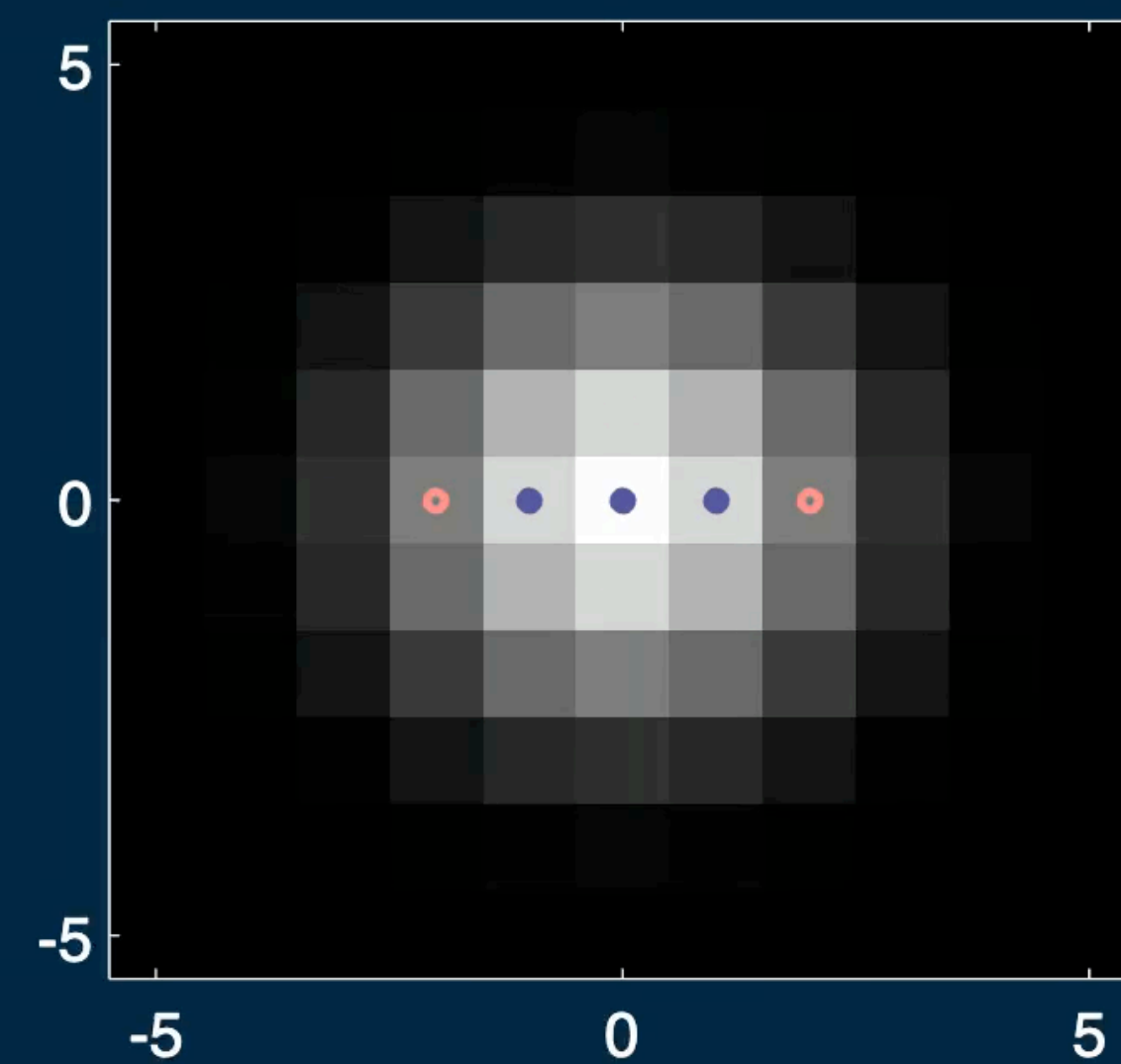
Projection



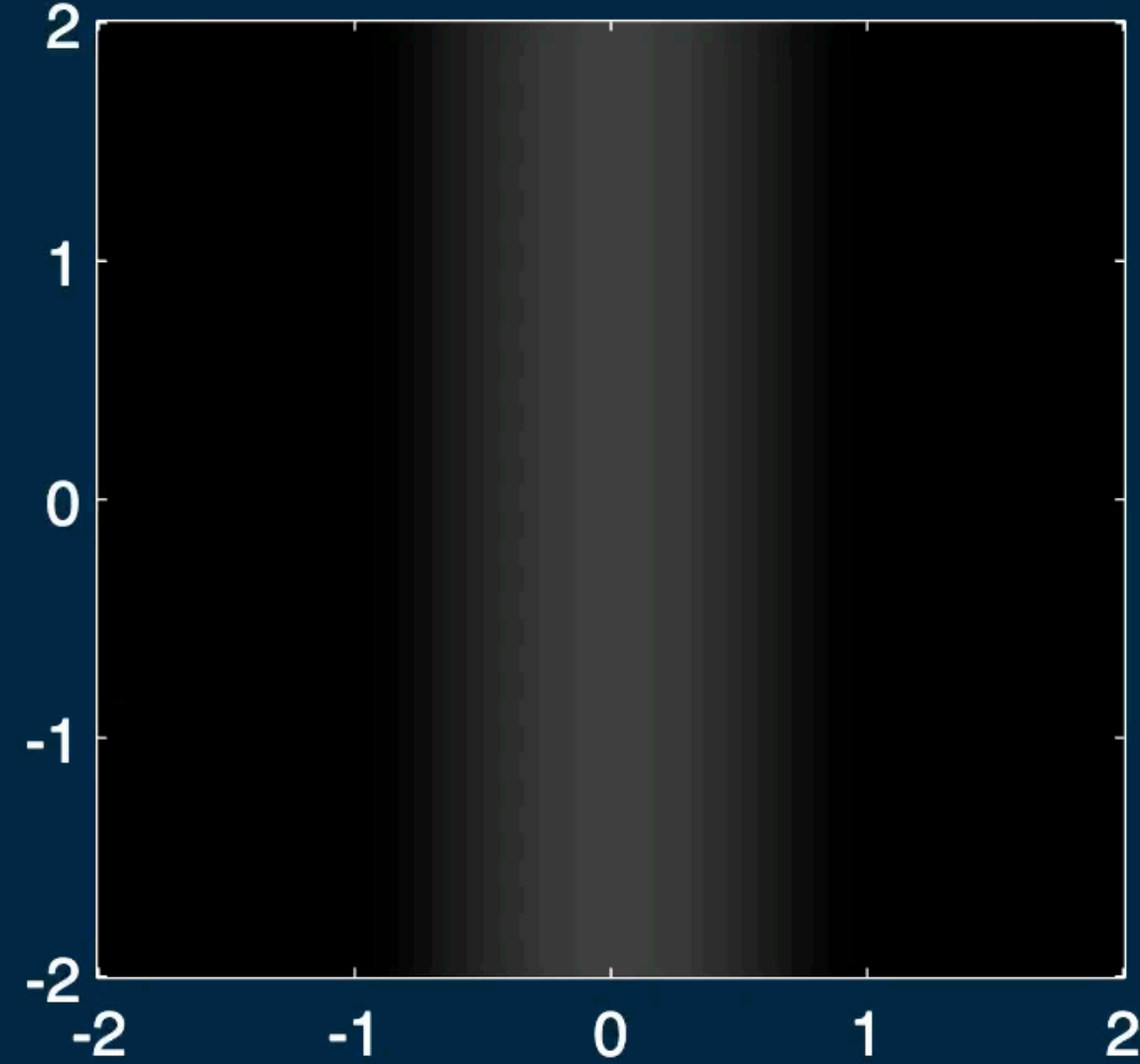
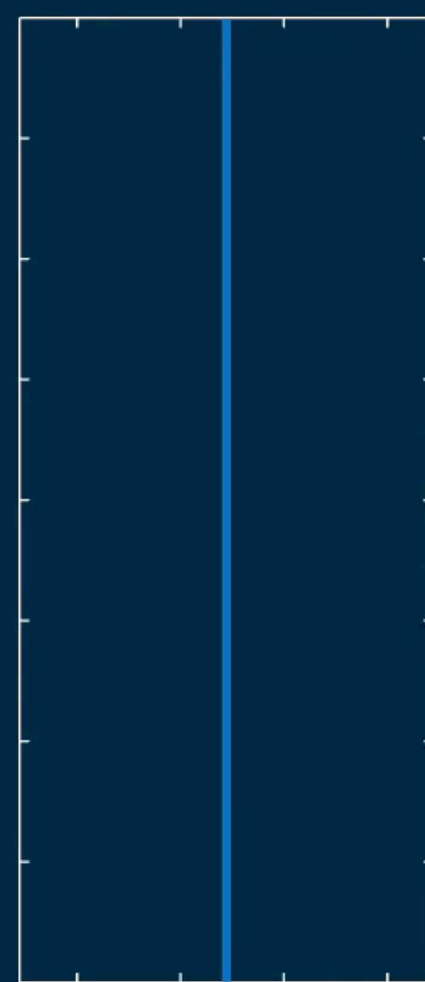
$g(x, y)$



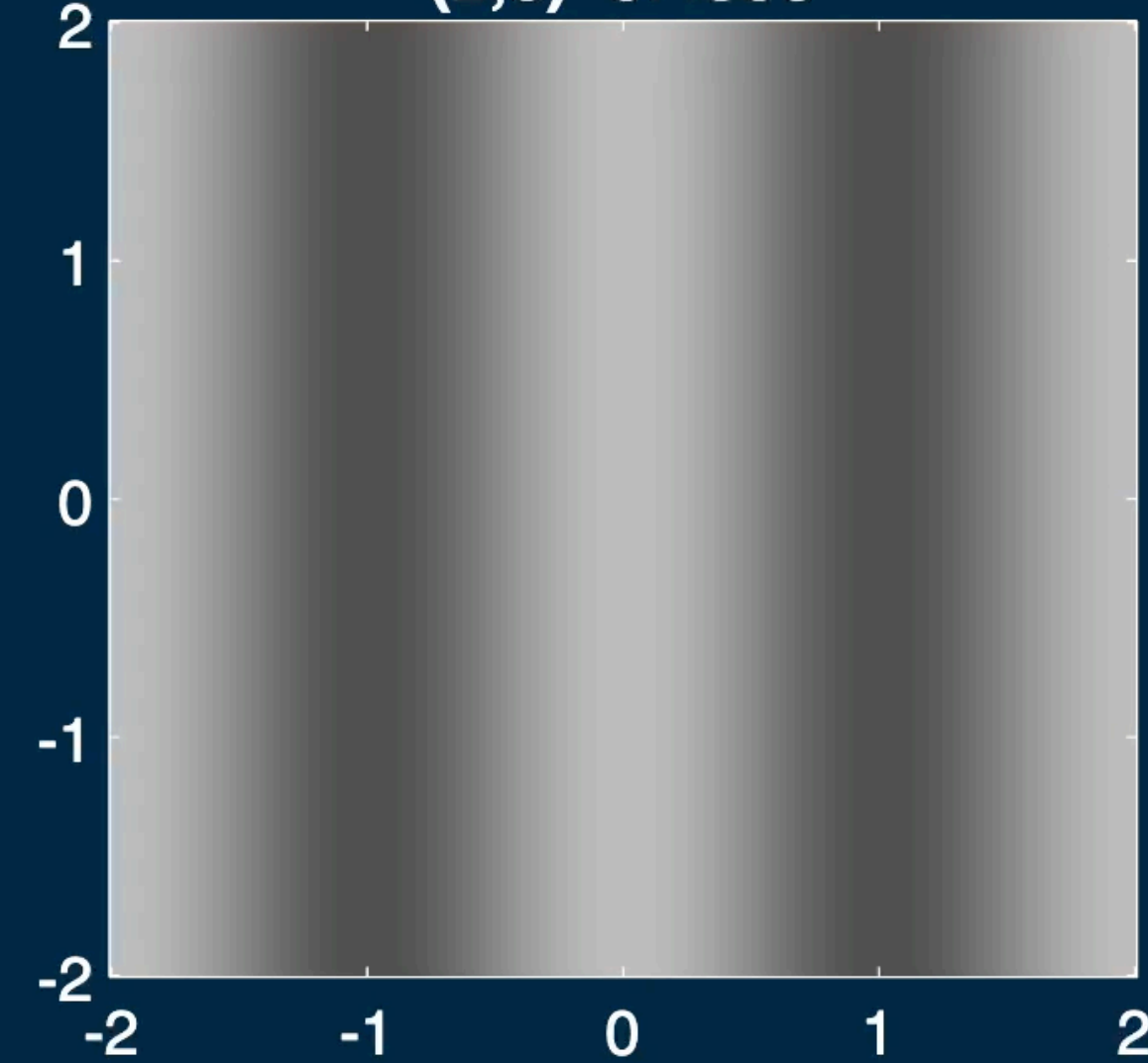
$G(u, v)$



$\hat{g}(x, y)$

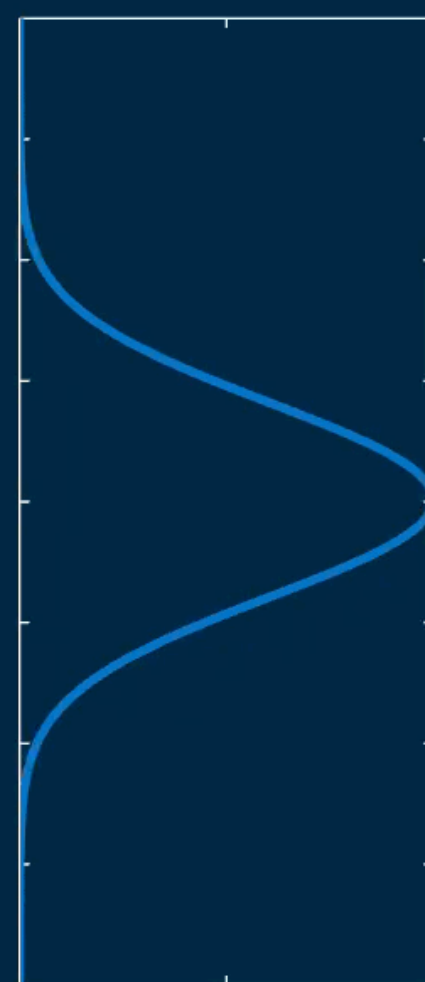


$G(2,0)=0.4559$

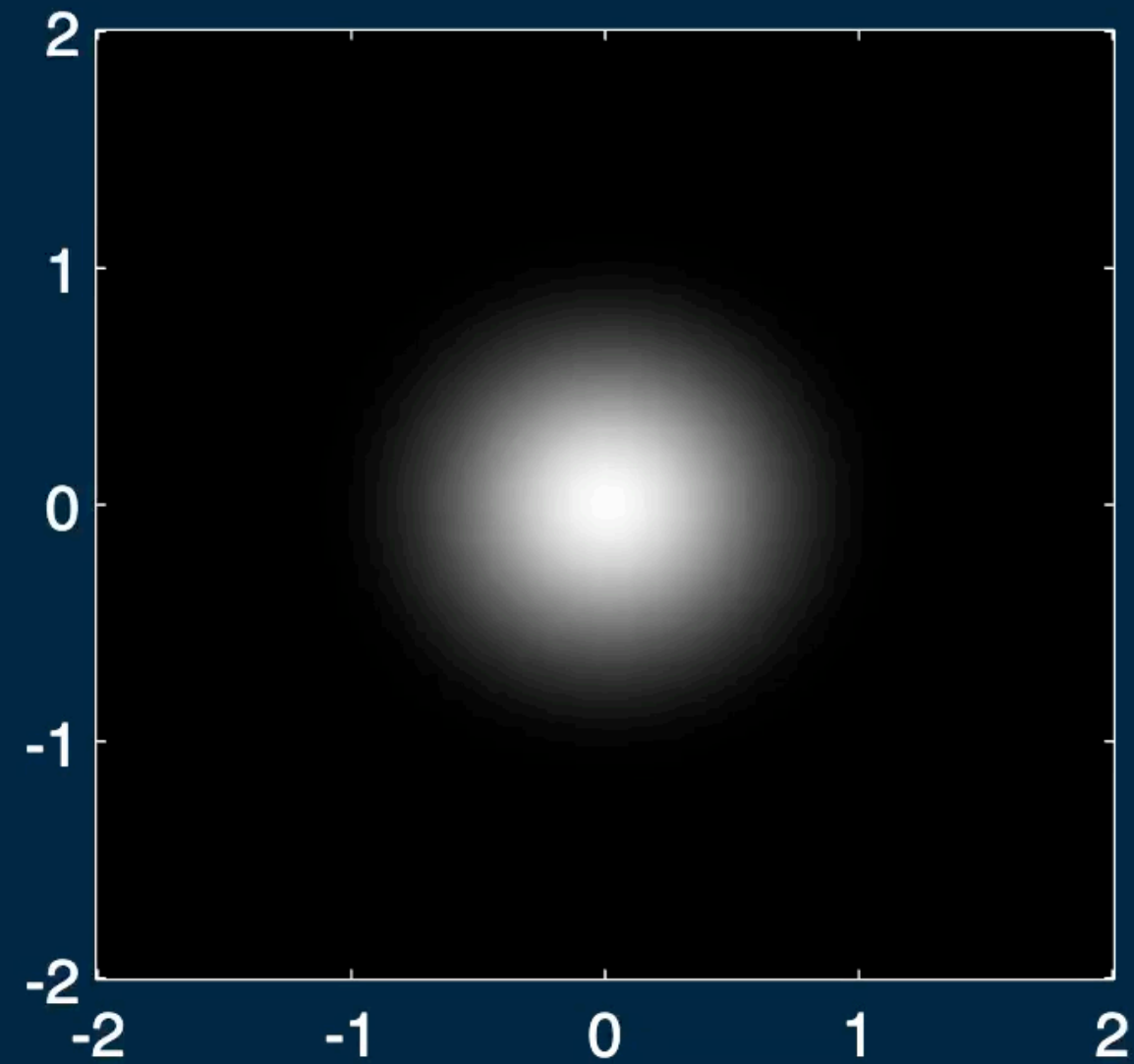


Fourier reconstruction of a 2D Gaussian function

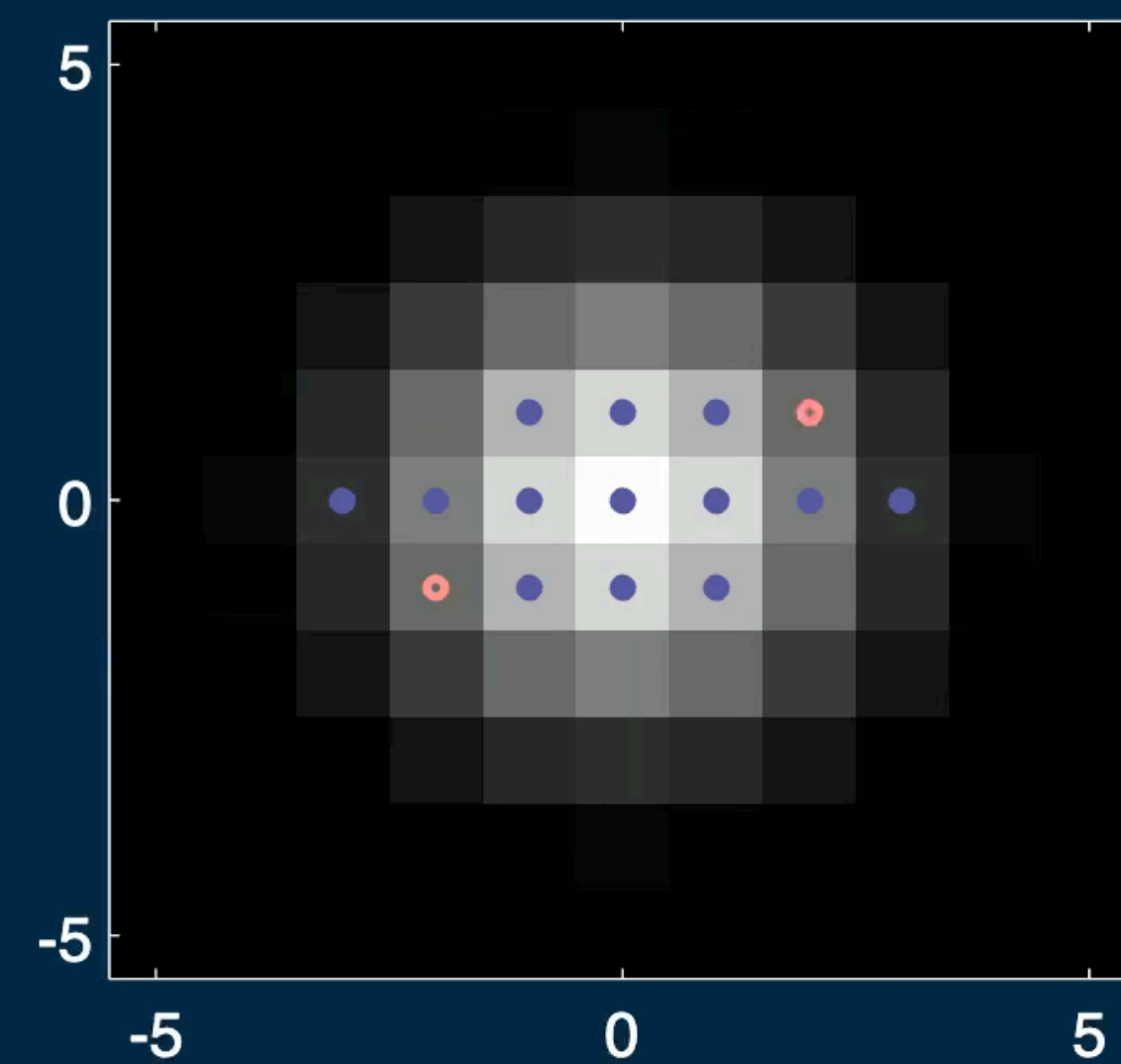
Projection



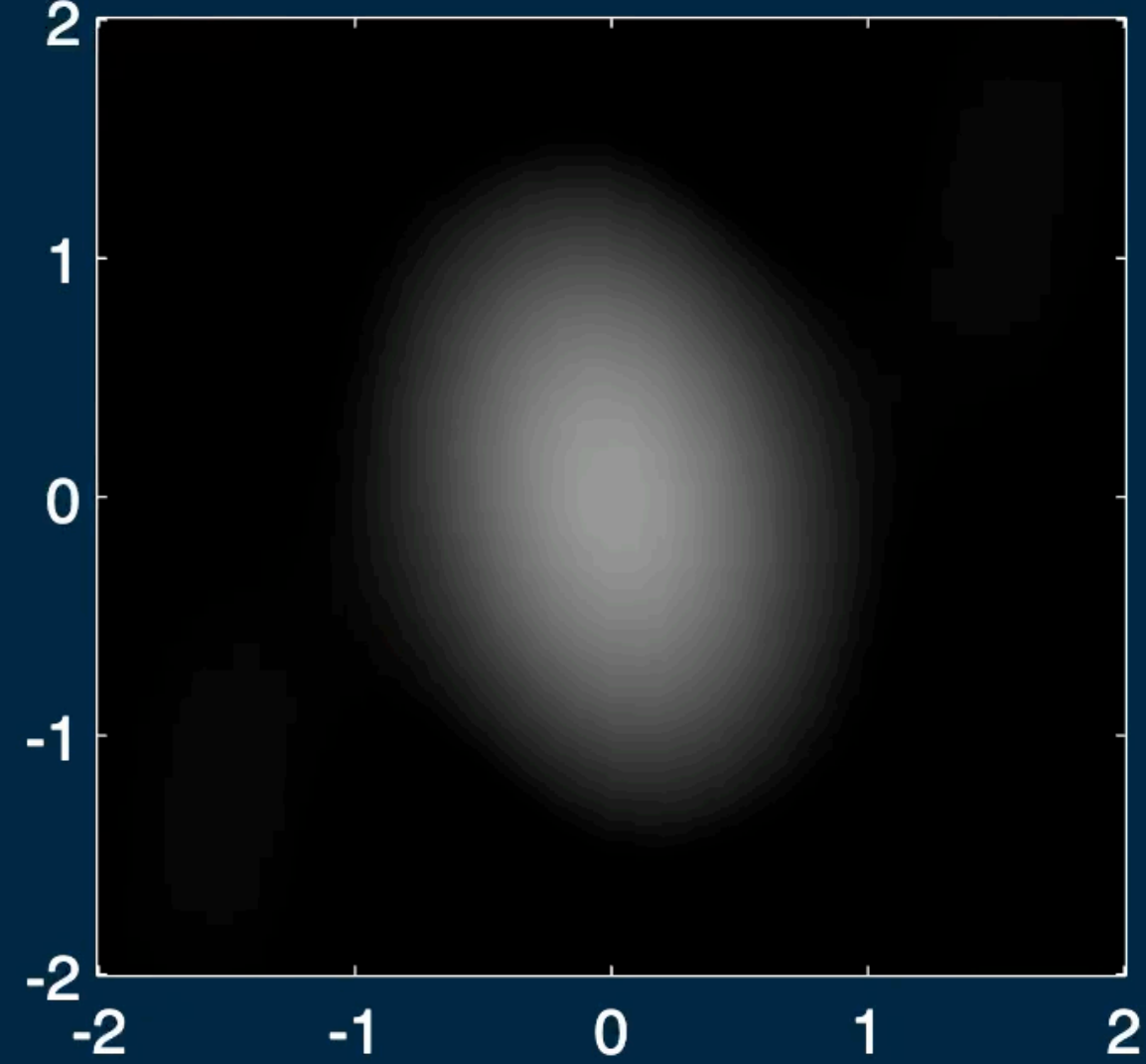
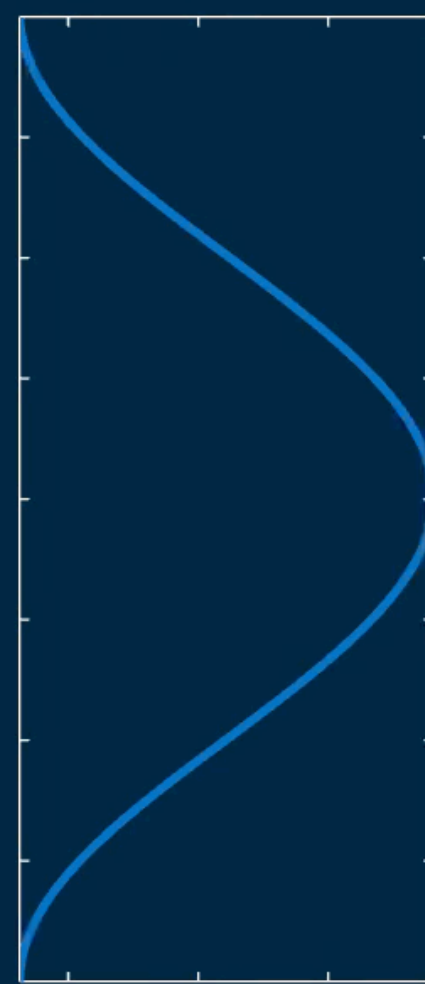
$g(x, y)$



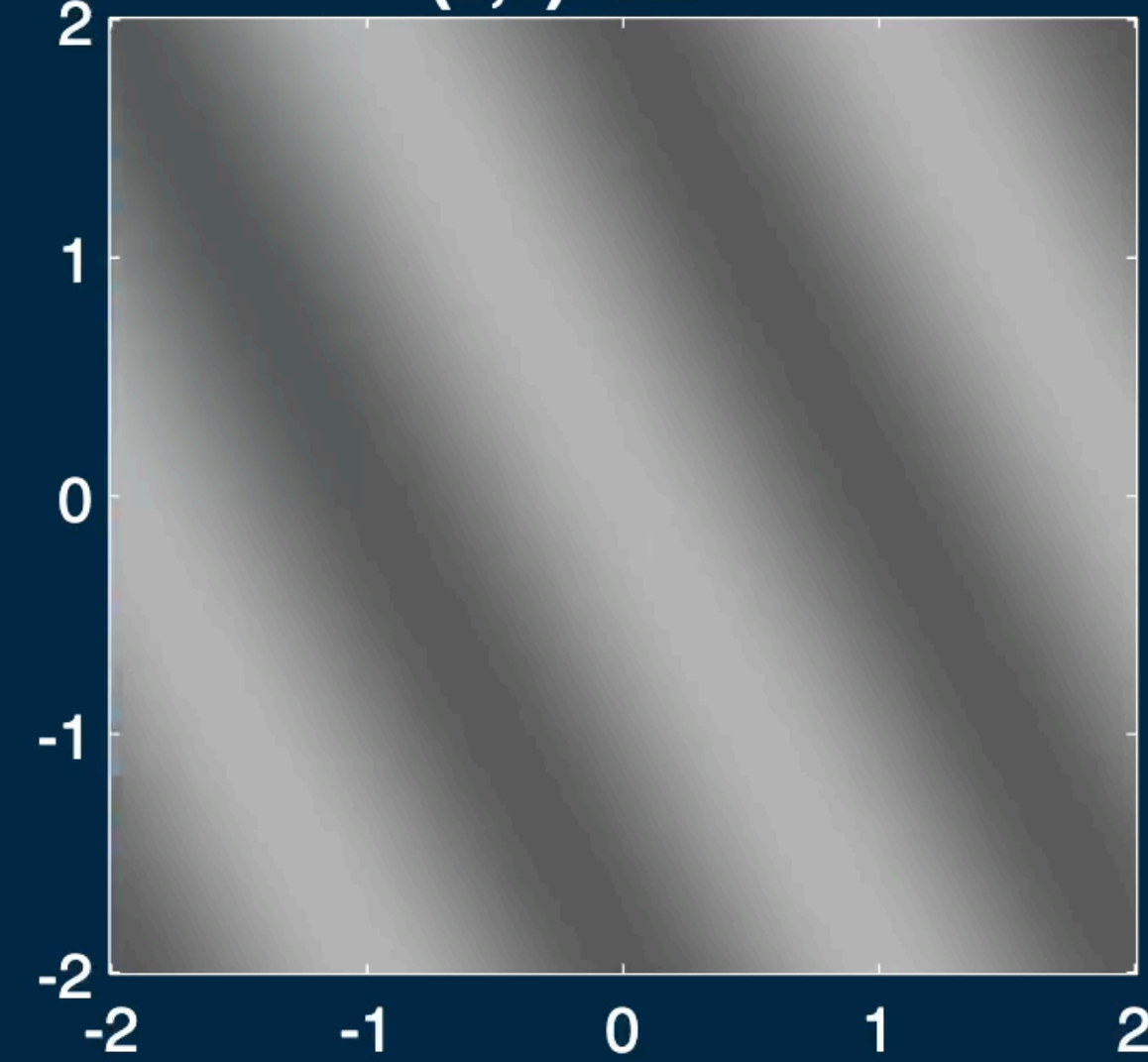
$G(u, v)$



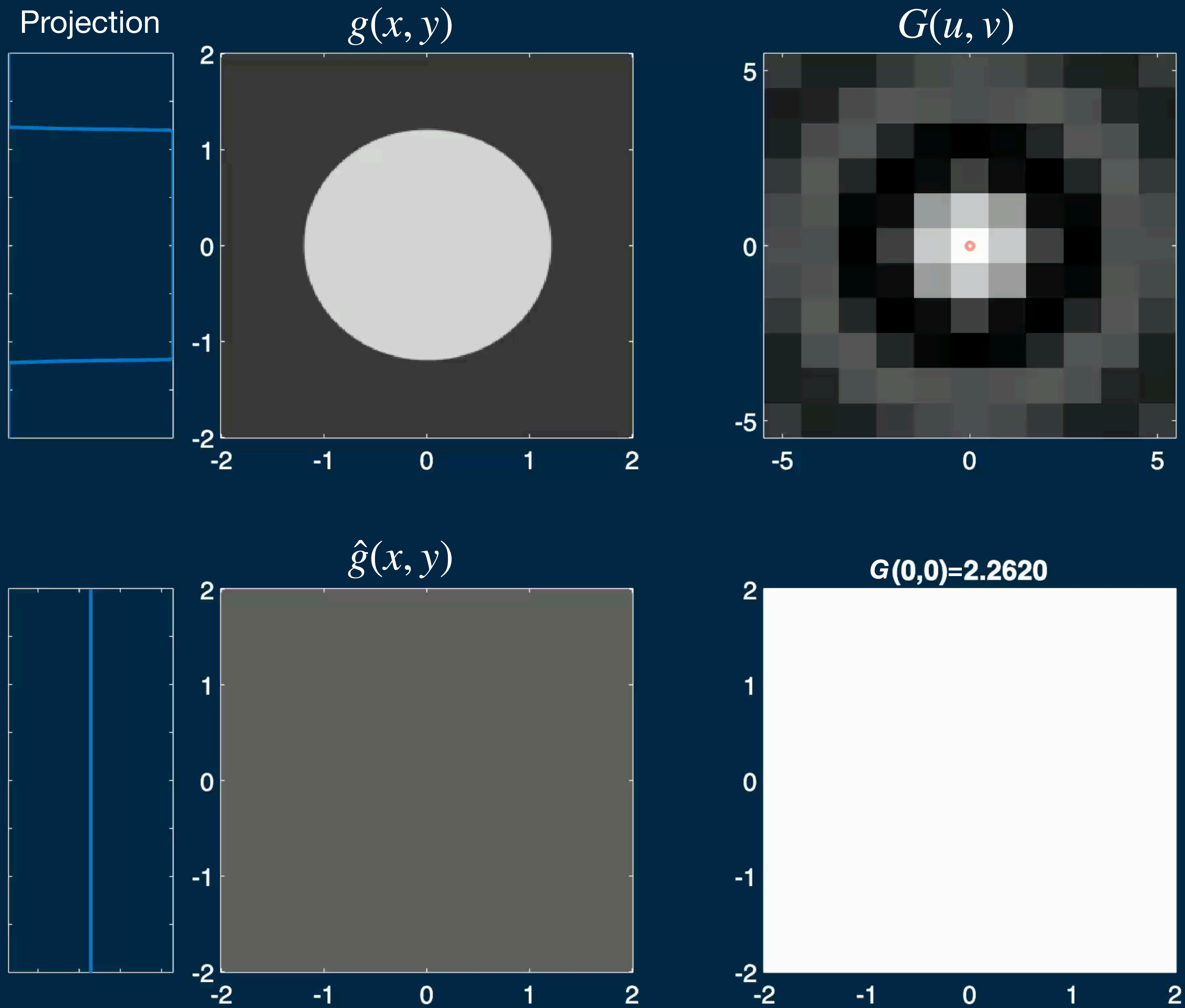
$\hat{g}(x, y)$



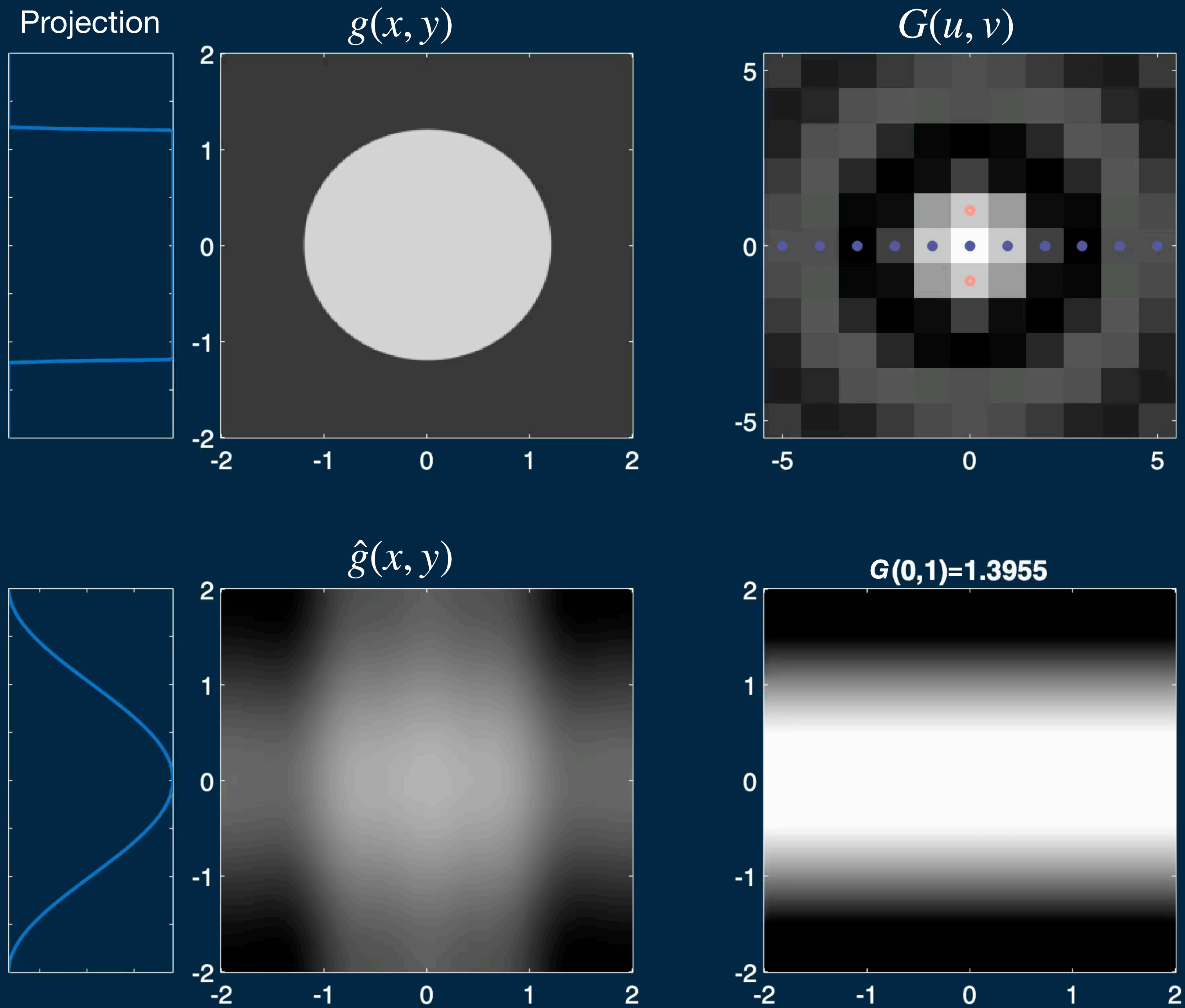
$G(2,1)=0.3747$



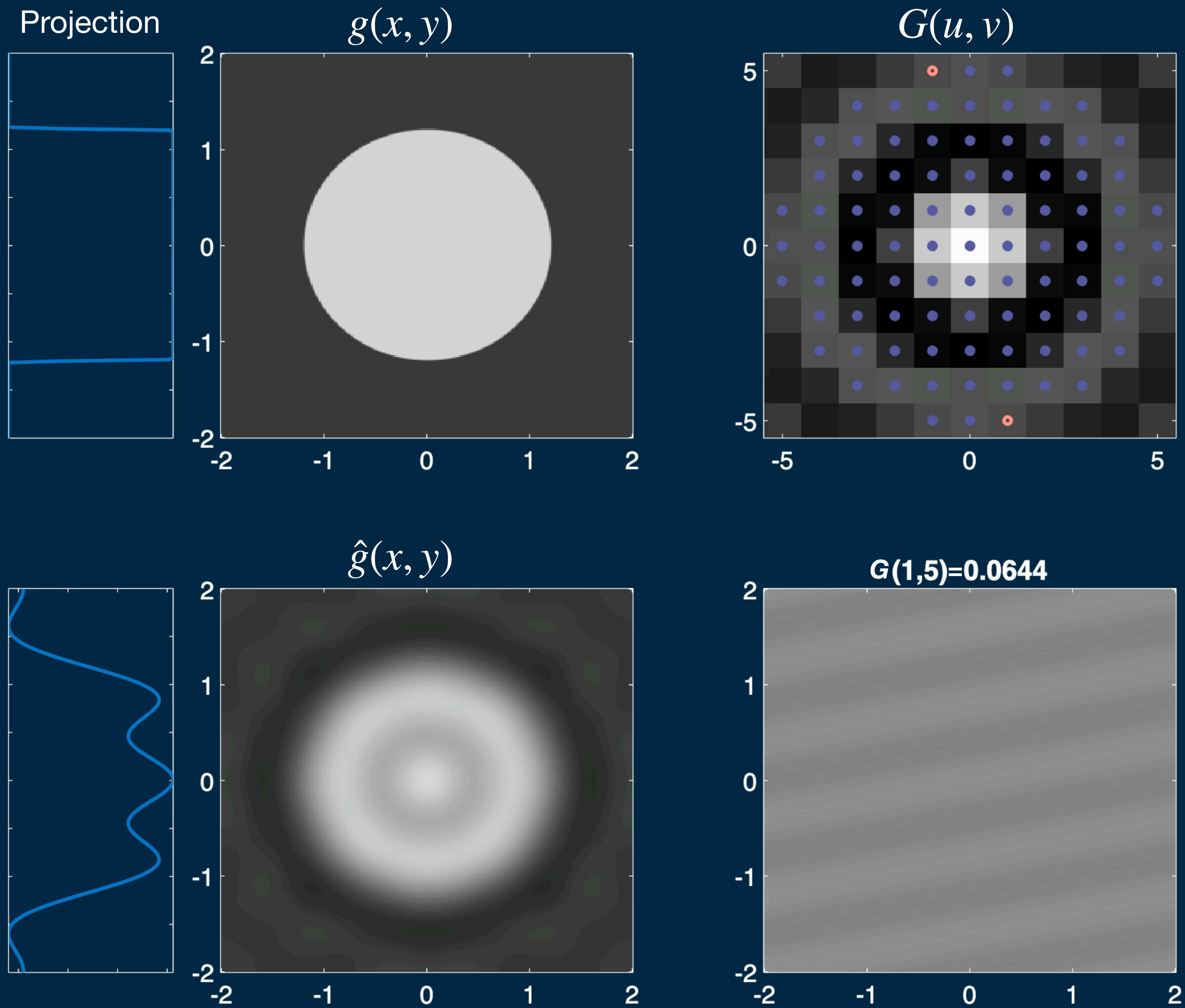
Fourier reconstruction of a 2D circ function



Fourier reconstruction of a 2D circ function



Fourier reconstruction of a 2D circ function



2D transform pairs

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

$$\text{circ}(x, y) \rightarrow \frac{J_1(2\pi\rho)}{\pi\rho}, \quad \rho = \sqrt{u^2 + v^2}$$

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

2D Fourier transform 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

$$g * h \rightarrow GH$$

Convolution

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

Rotation

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

Projection

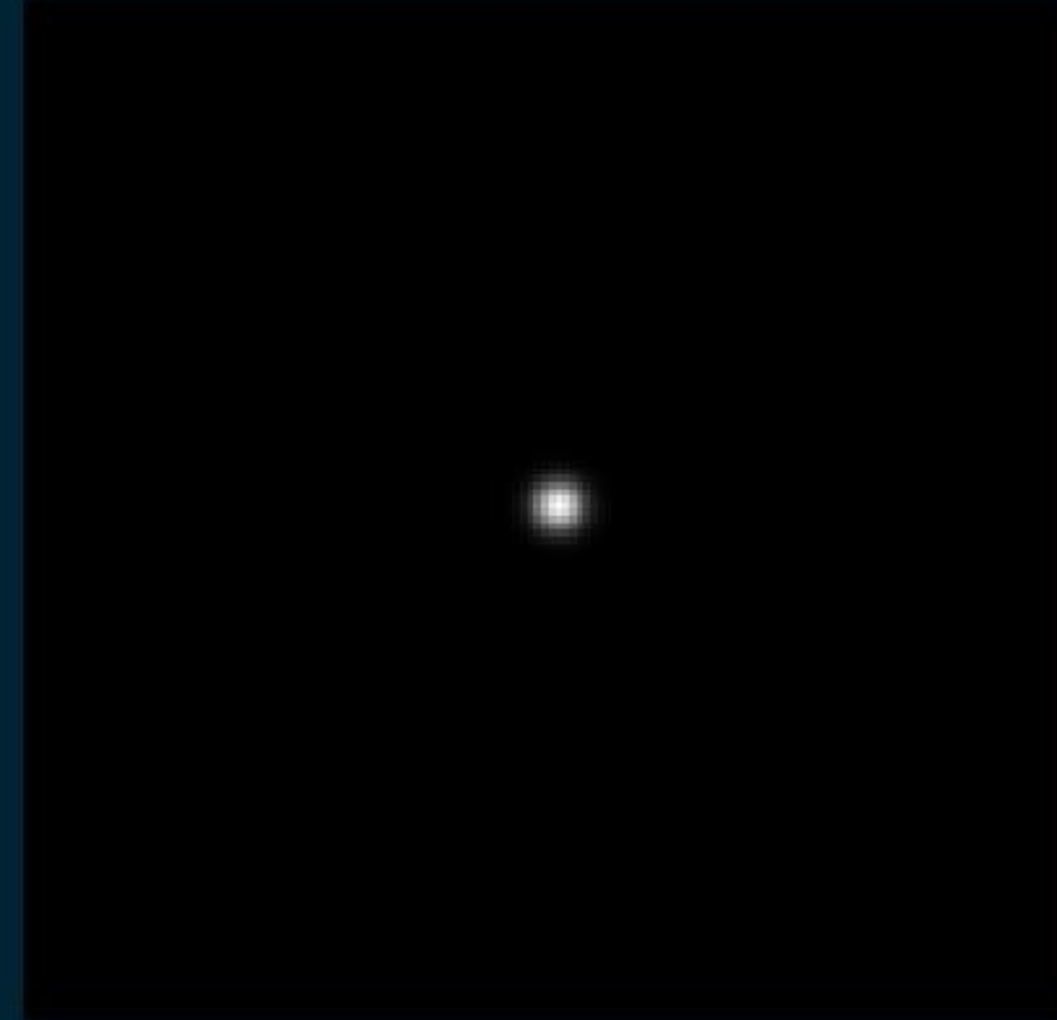
$$g * h = \iint g(x - s, y - t) h(s, t) ds dt$$

Convolution with a Gaussian

$g(x,y)$



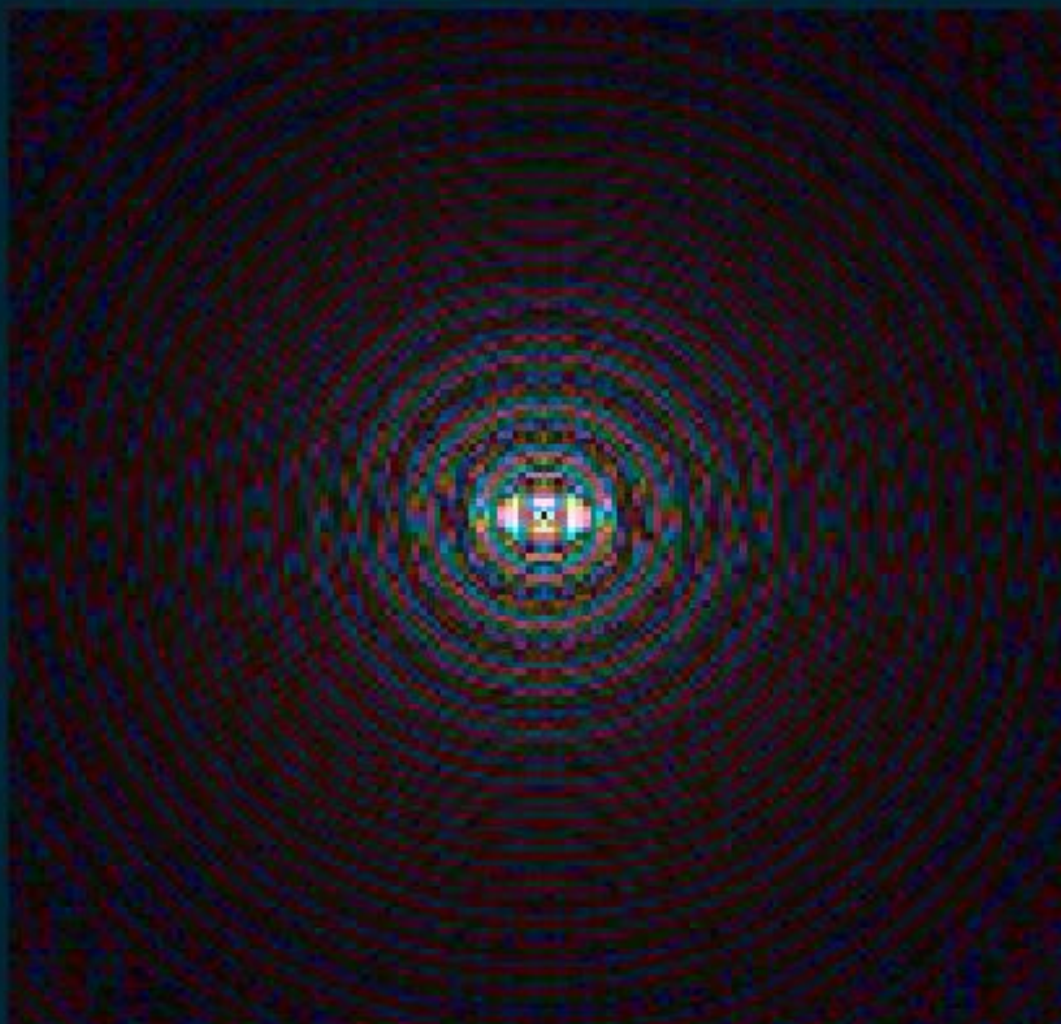
$h(x,y)$



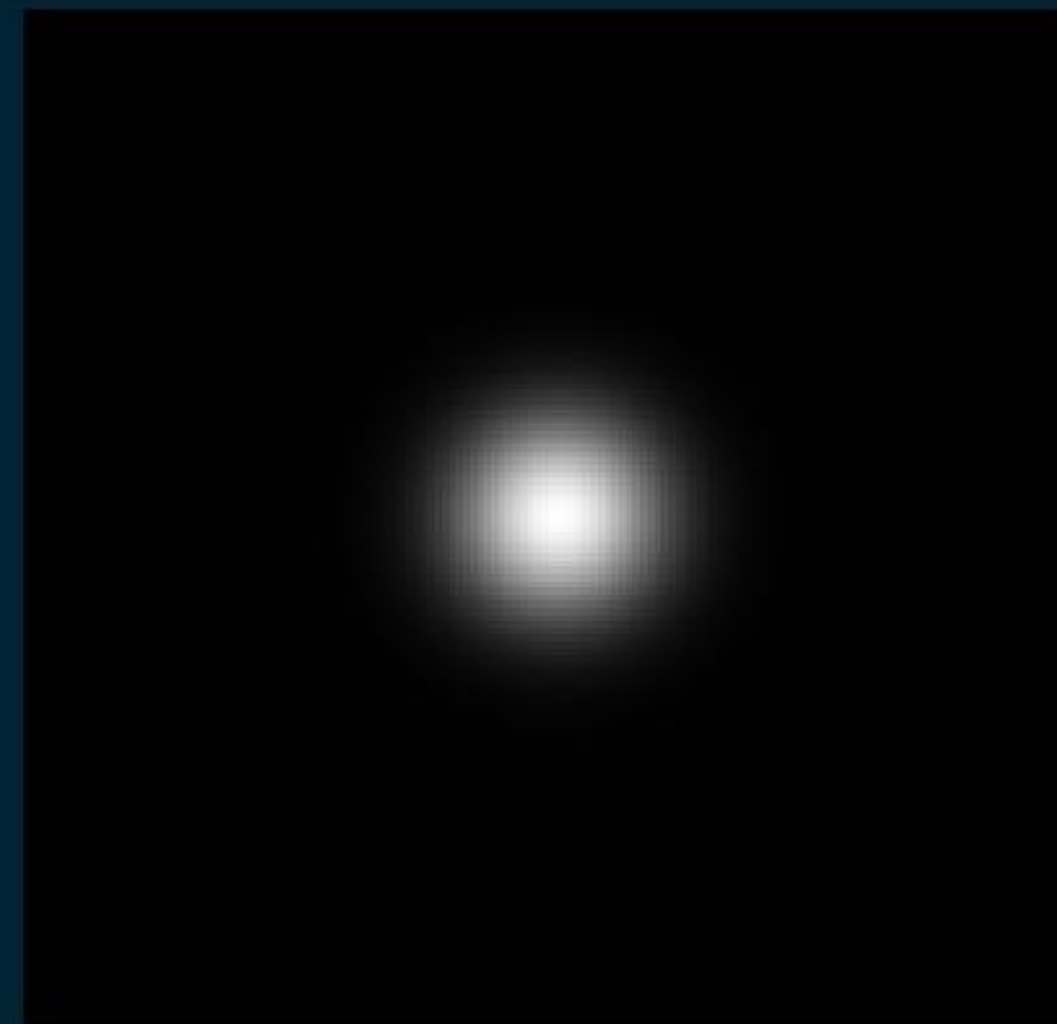
$g*h$



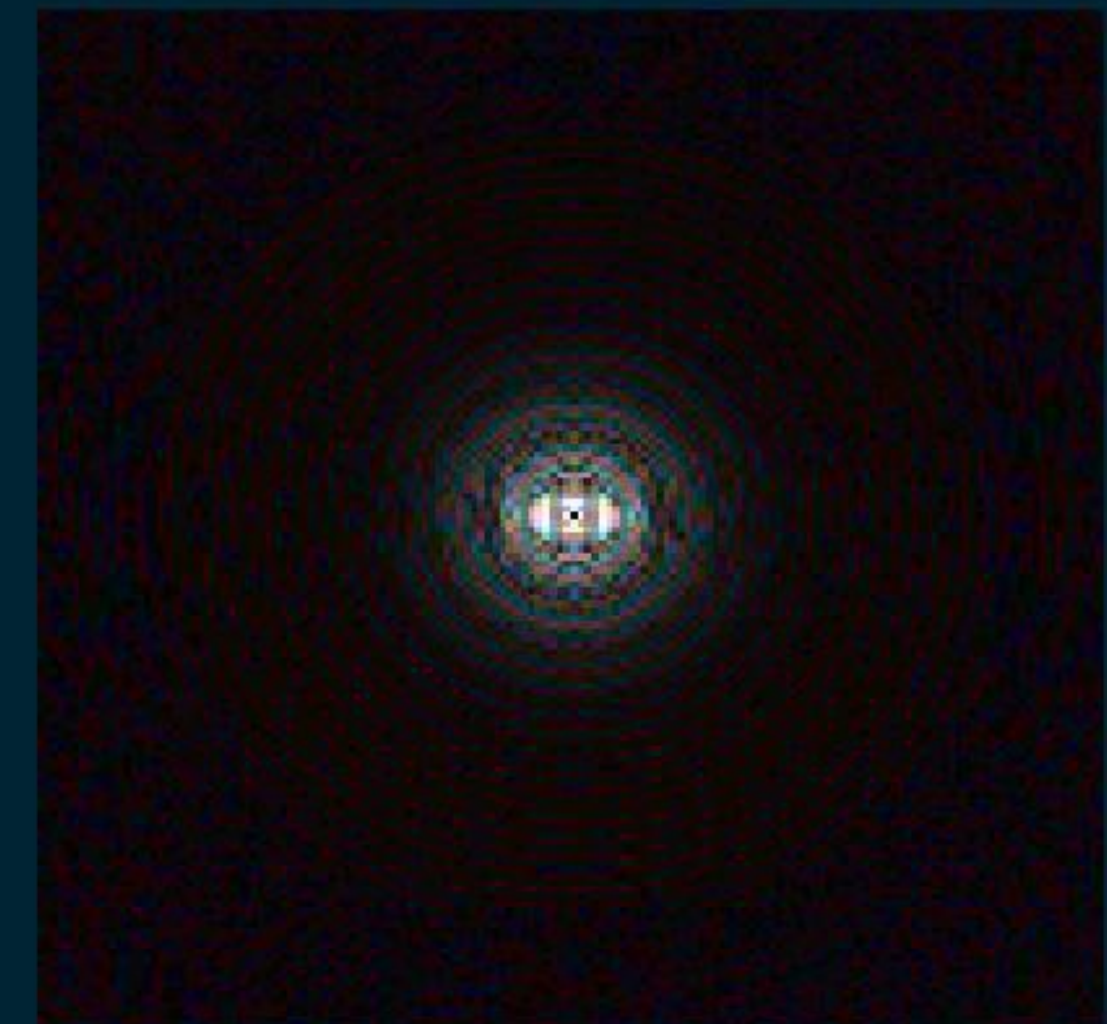
$G(u,v)$



$H(u,v)$

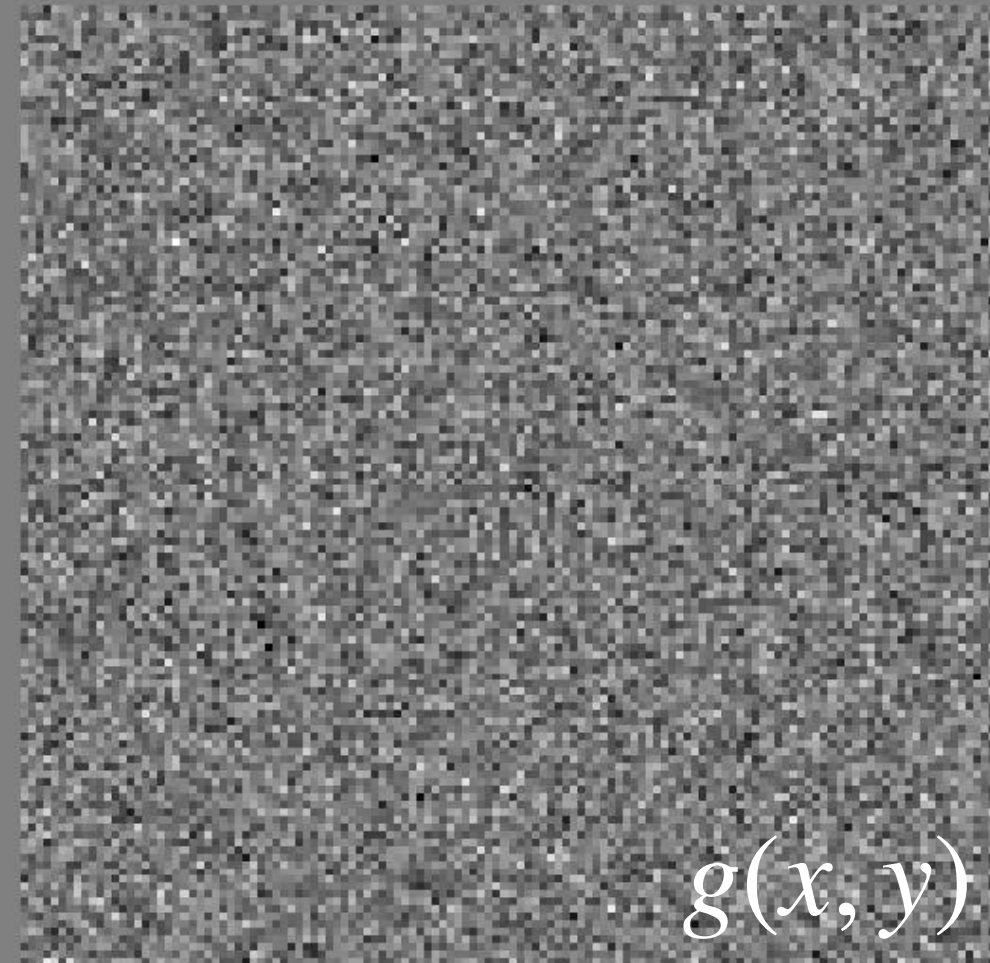


$G(u,v) H(u,v)$

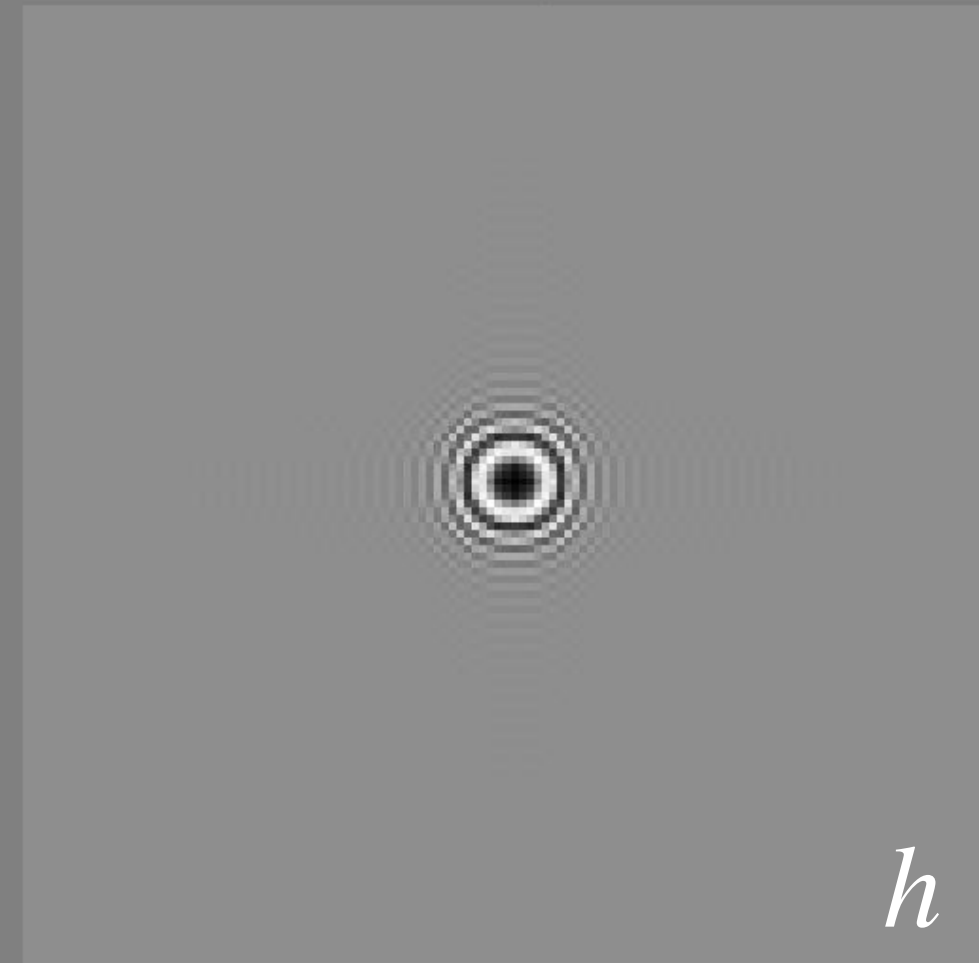


Visualizing the contrast transfer function

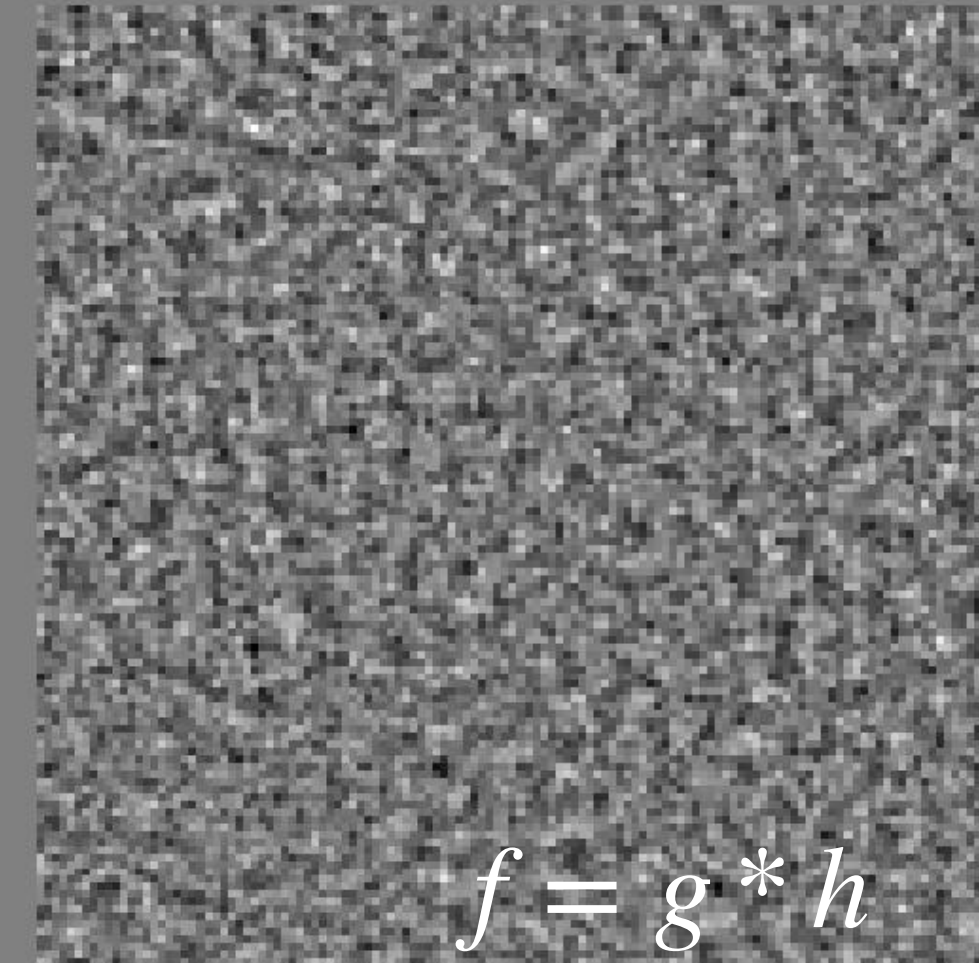
Random object



Point-spread



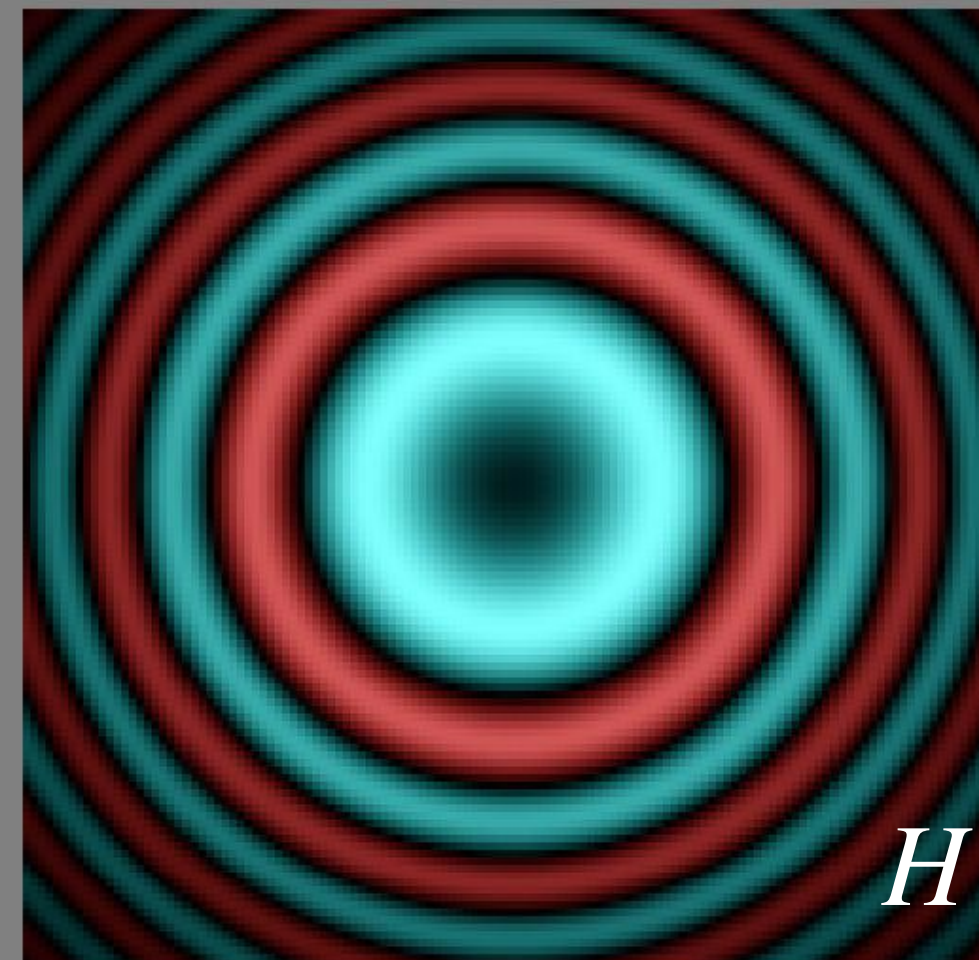
Image



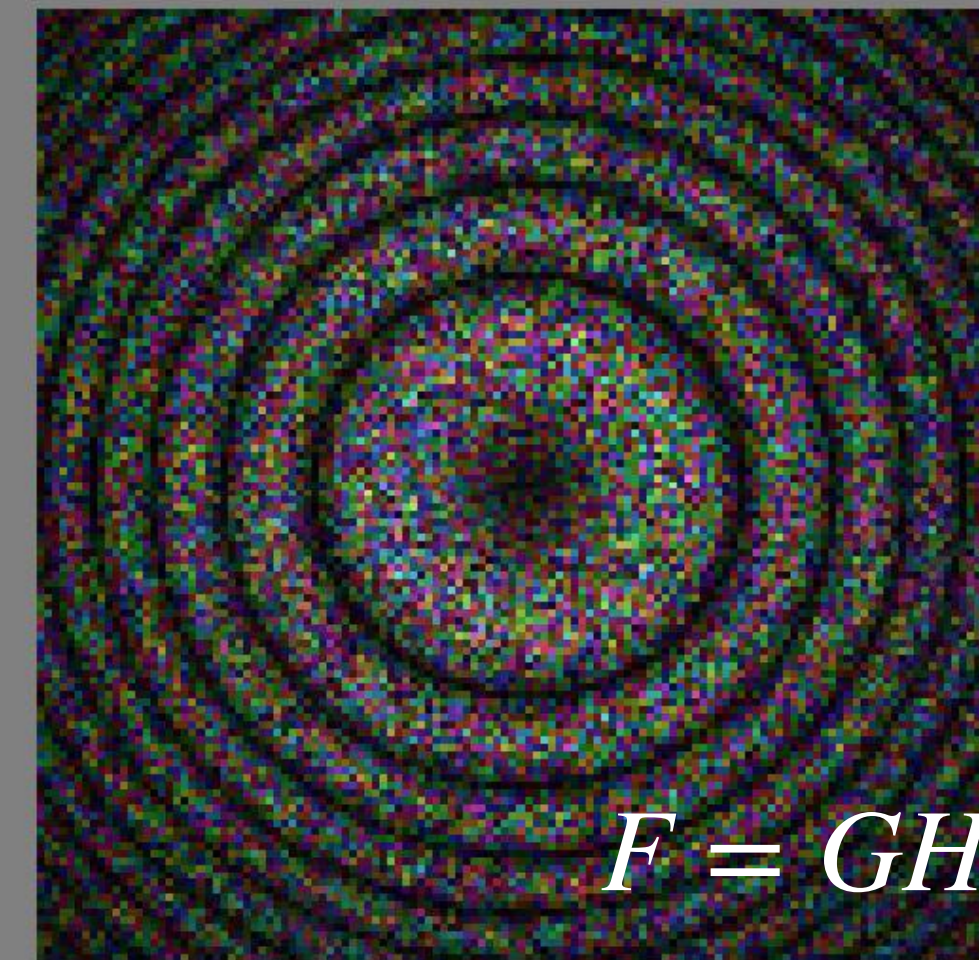
FT of object



CTF

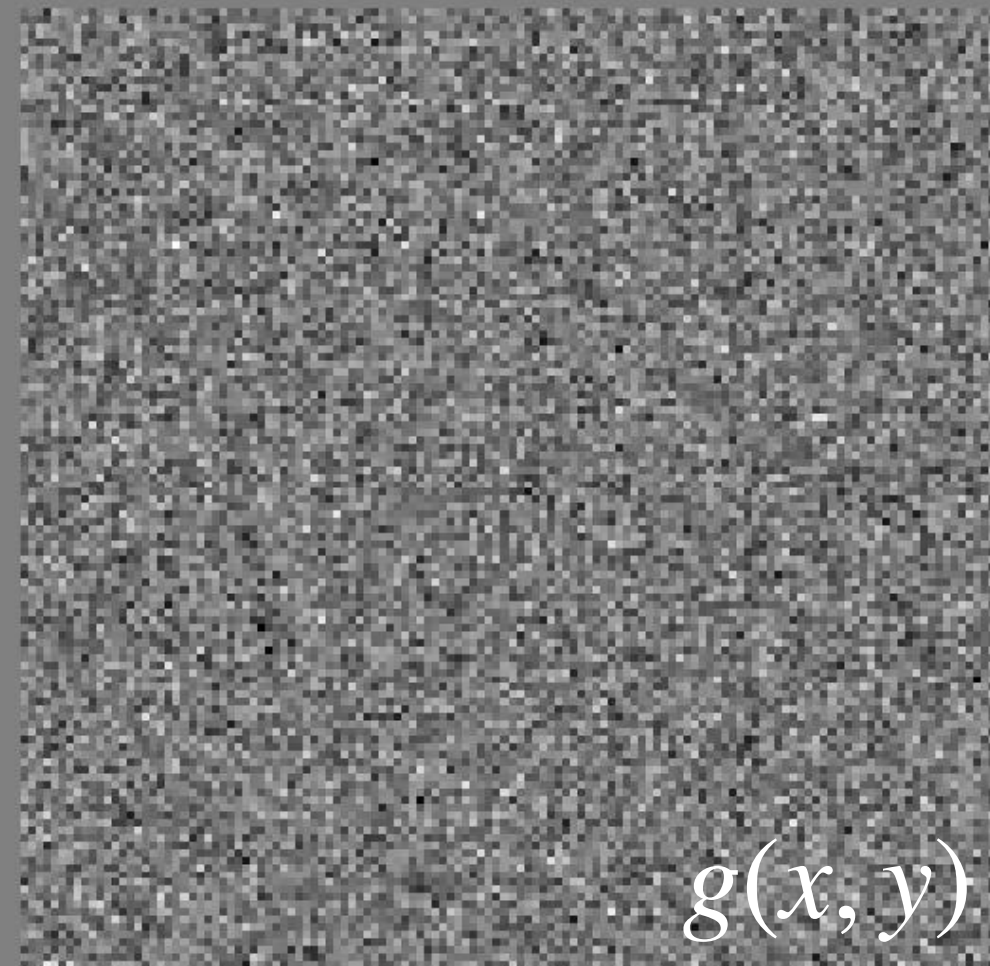


FT of image

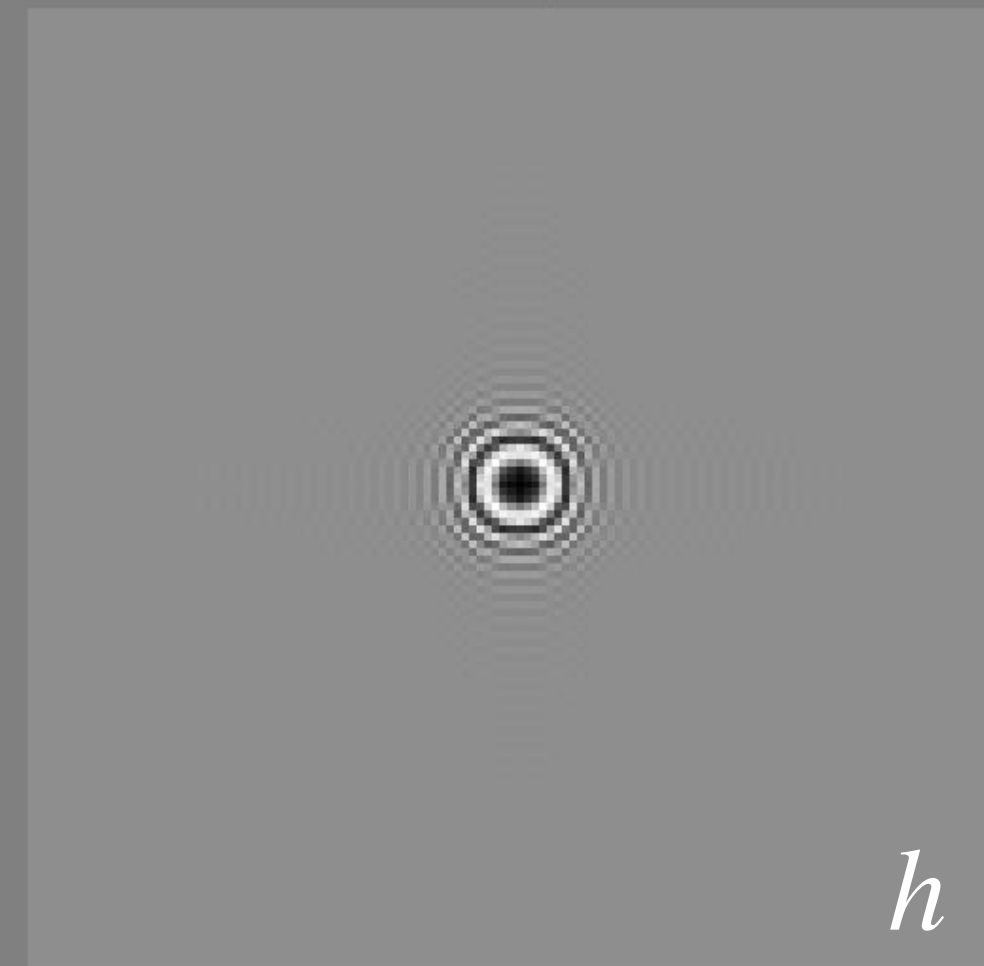


Visualizing the contrast transfer function

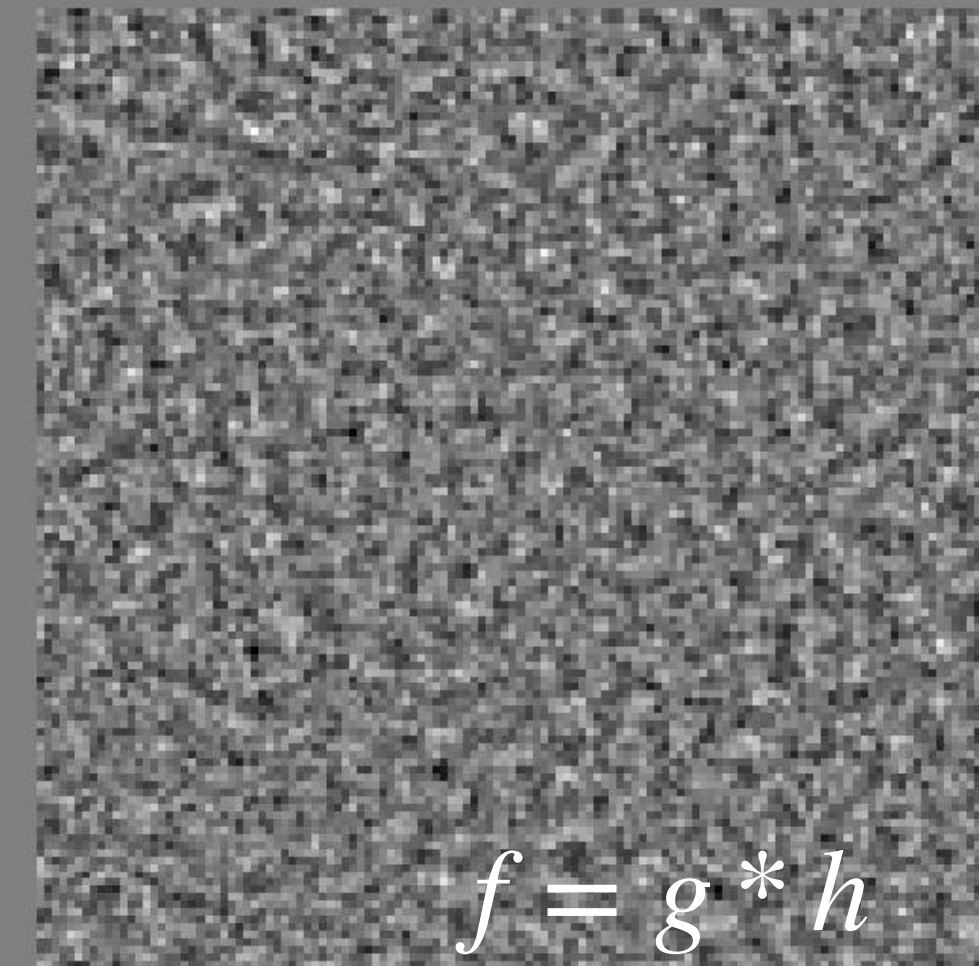
Random object



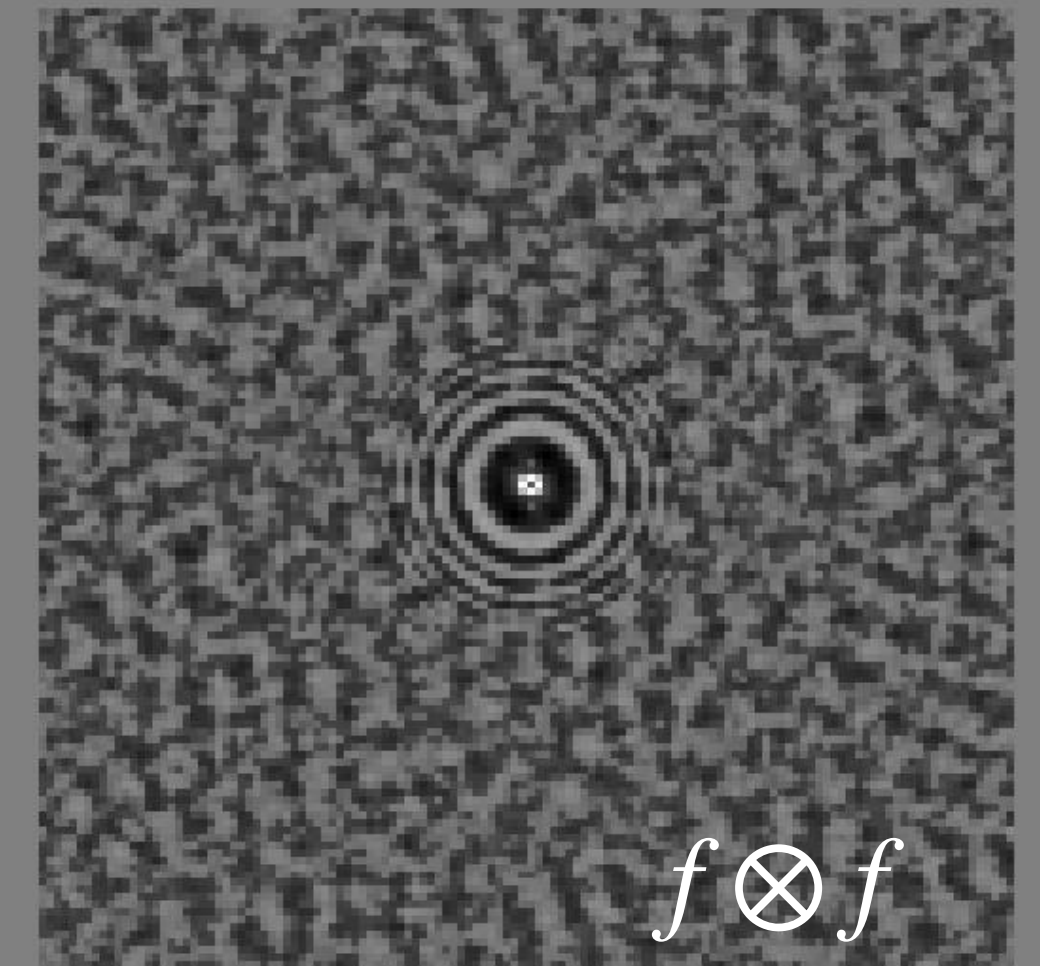
Point-spread



Image



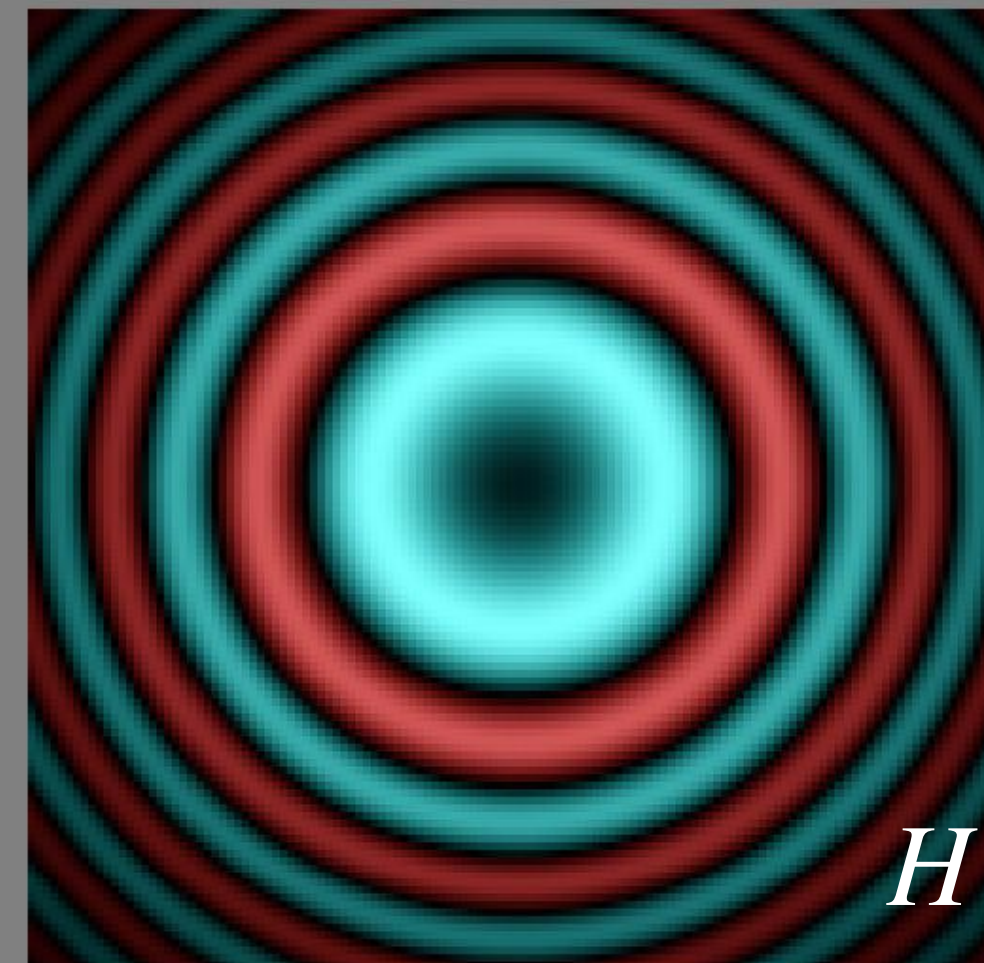
Autocorrelation



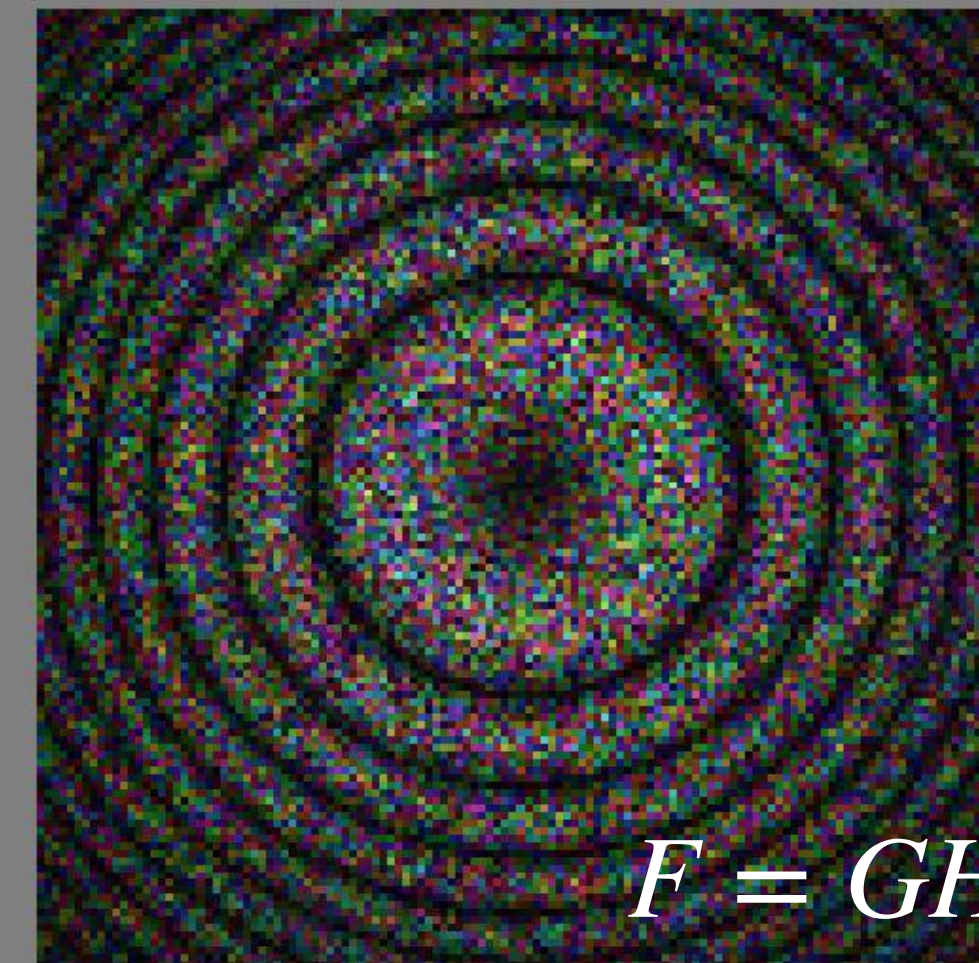
FT of object



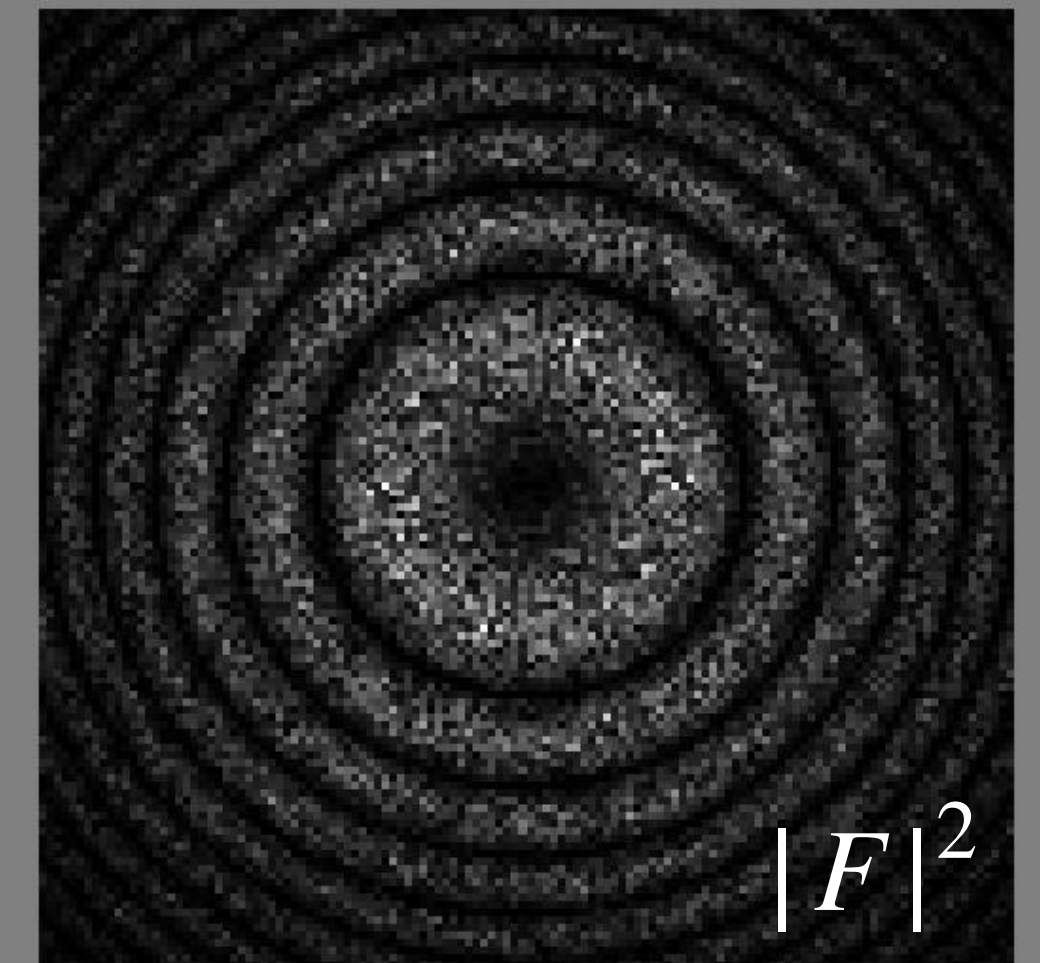
CTF



FT of image



Power spectrum



II. Fourier transforms and their properties

1. Fourier transform in 1D
2. Fourier transform in 2D
3. The Fourier slice theorem and reconstruction

The rotation property

2D Fourier Transform

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

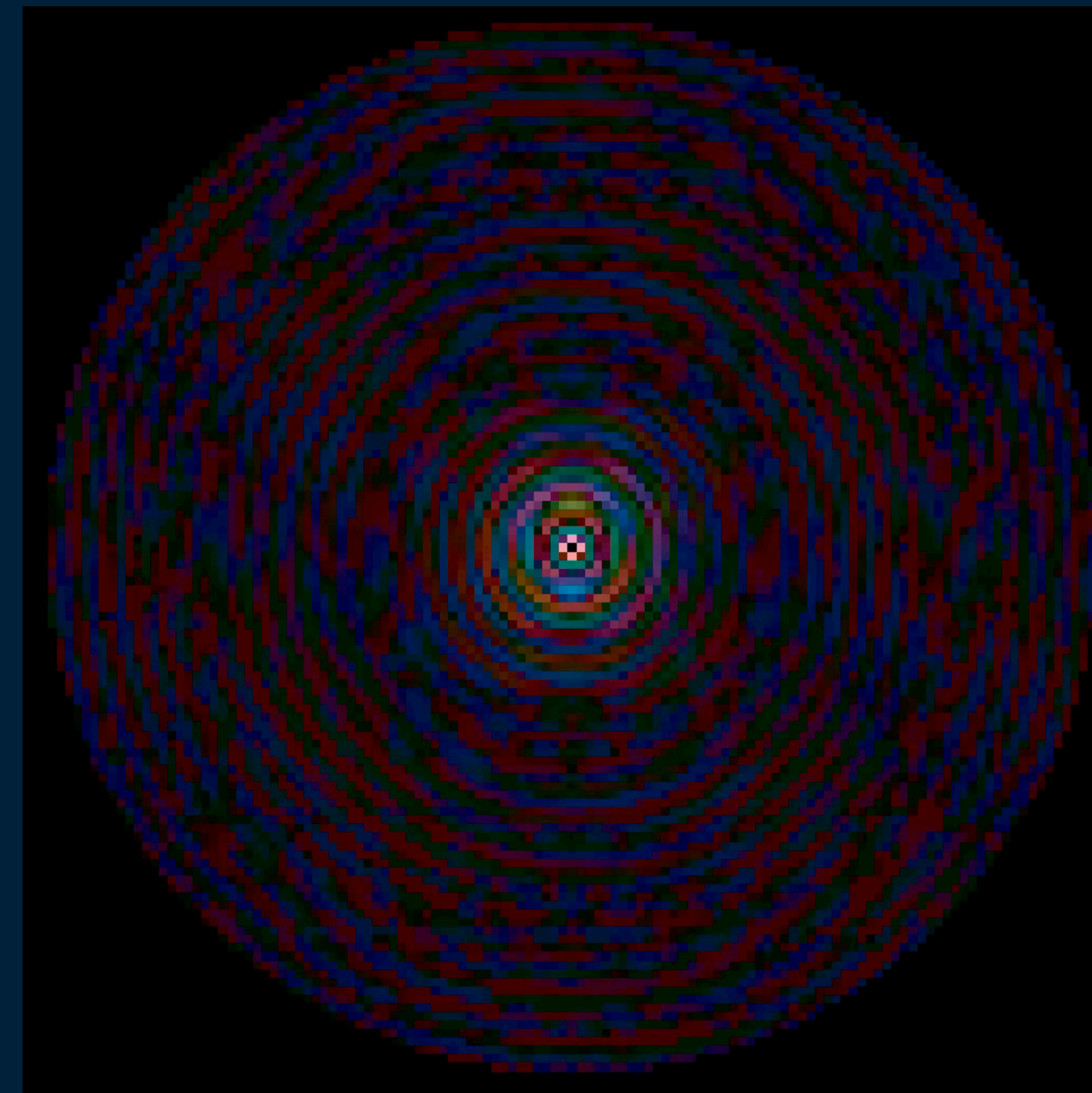
FT using 2D vectors

$$G(\mathbf{u}) = \iint g(\mathbf{x}) e^{-i2\pi(\mathbf{u} \cdot \mathbf{x})} d^2\mathbf{x}$$

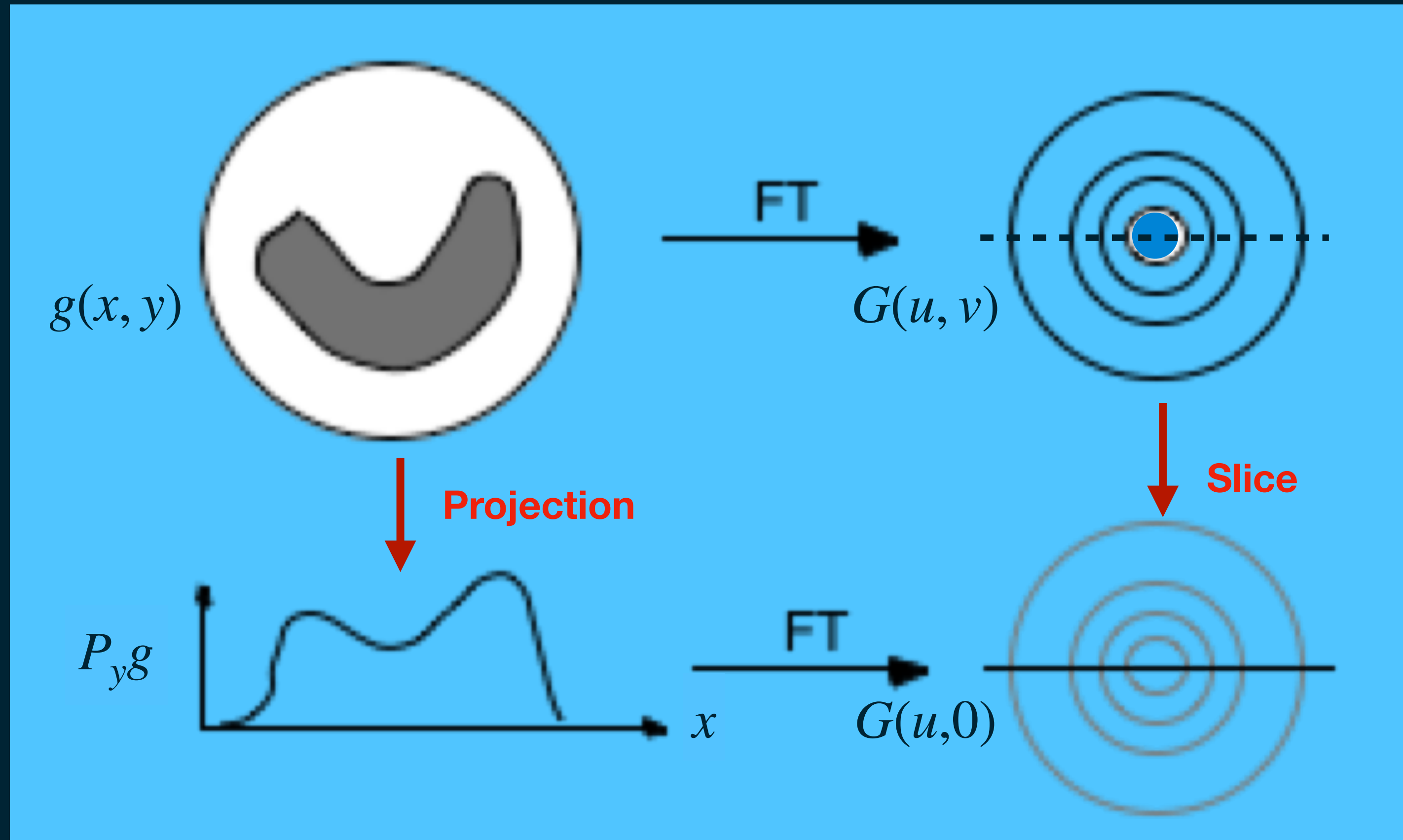
The dot-product is invariant under rotations!



FT
→



The Fourier Slice Theorem in 2D



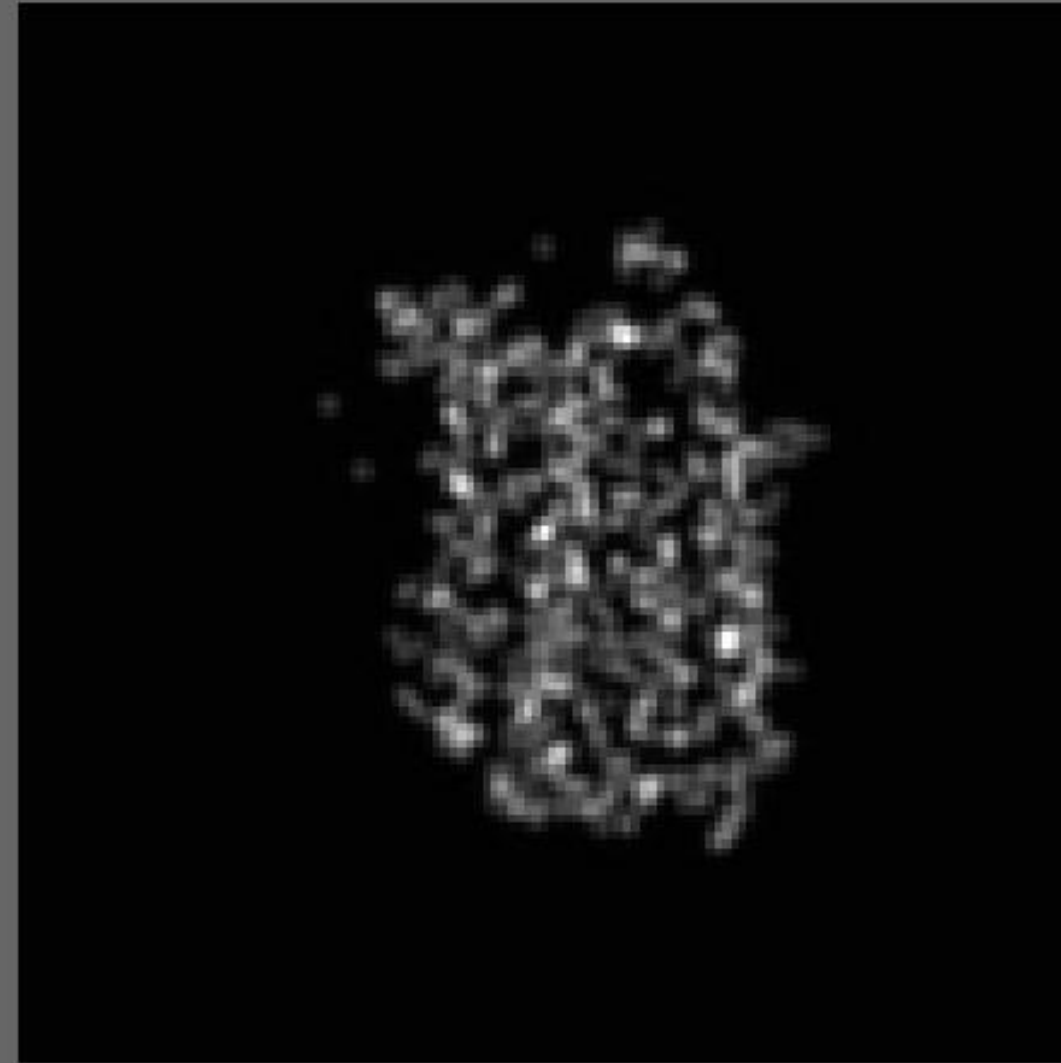
$$G(u, v) = \iint g(x, y) e^{-i2\pi(ux+vy)} dx dy$$

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

$$= \mathcal{F}\{P_y g\}$$

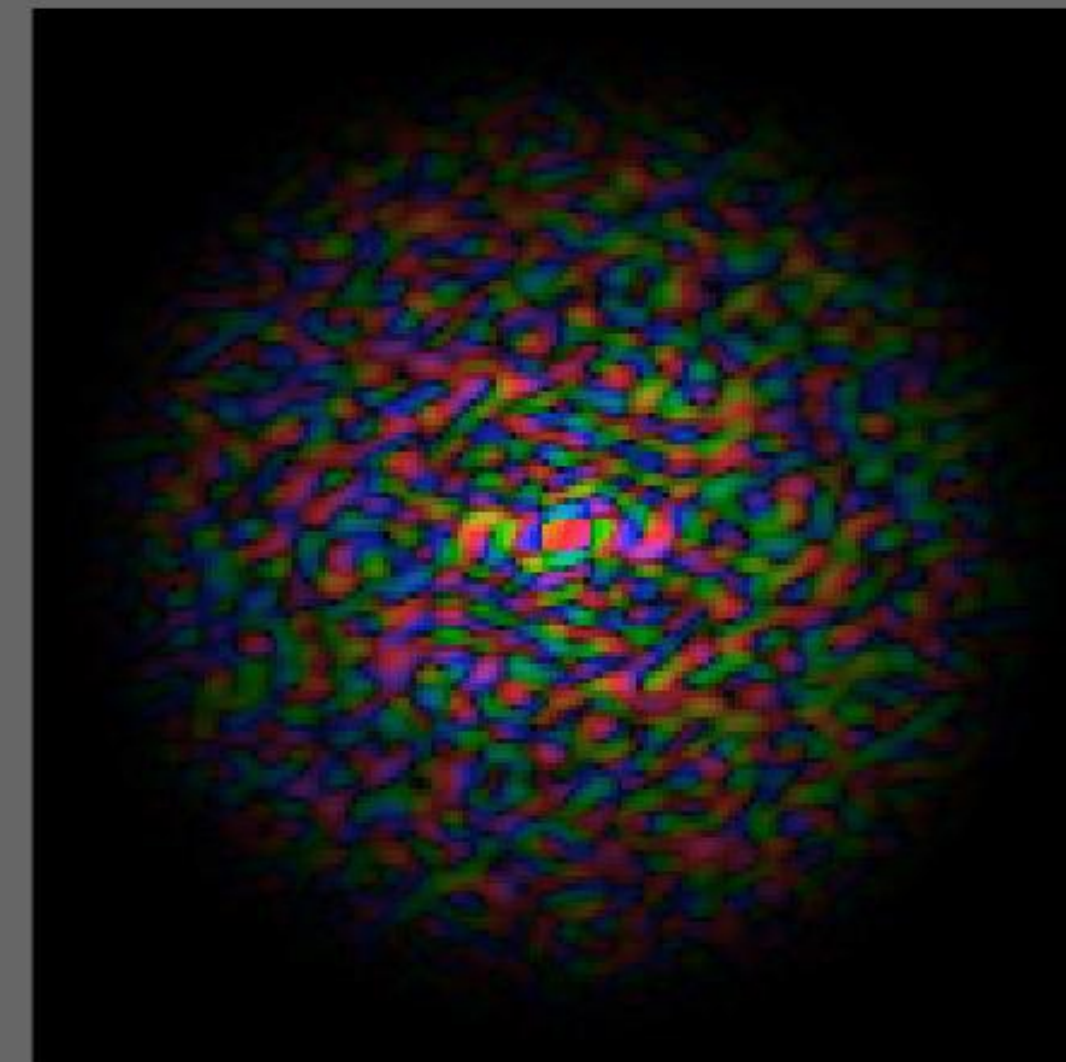
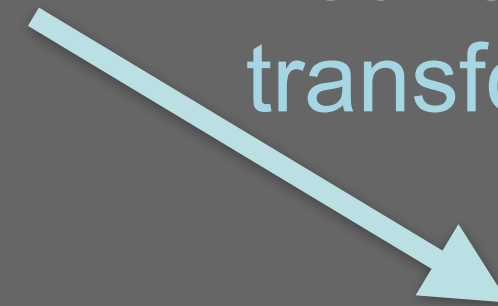
$$P_y g(x, y) = \int g(x, y) dy$$

Tomographic reconstruction using the Fourier slice theorem

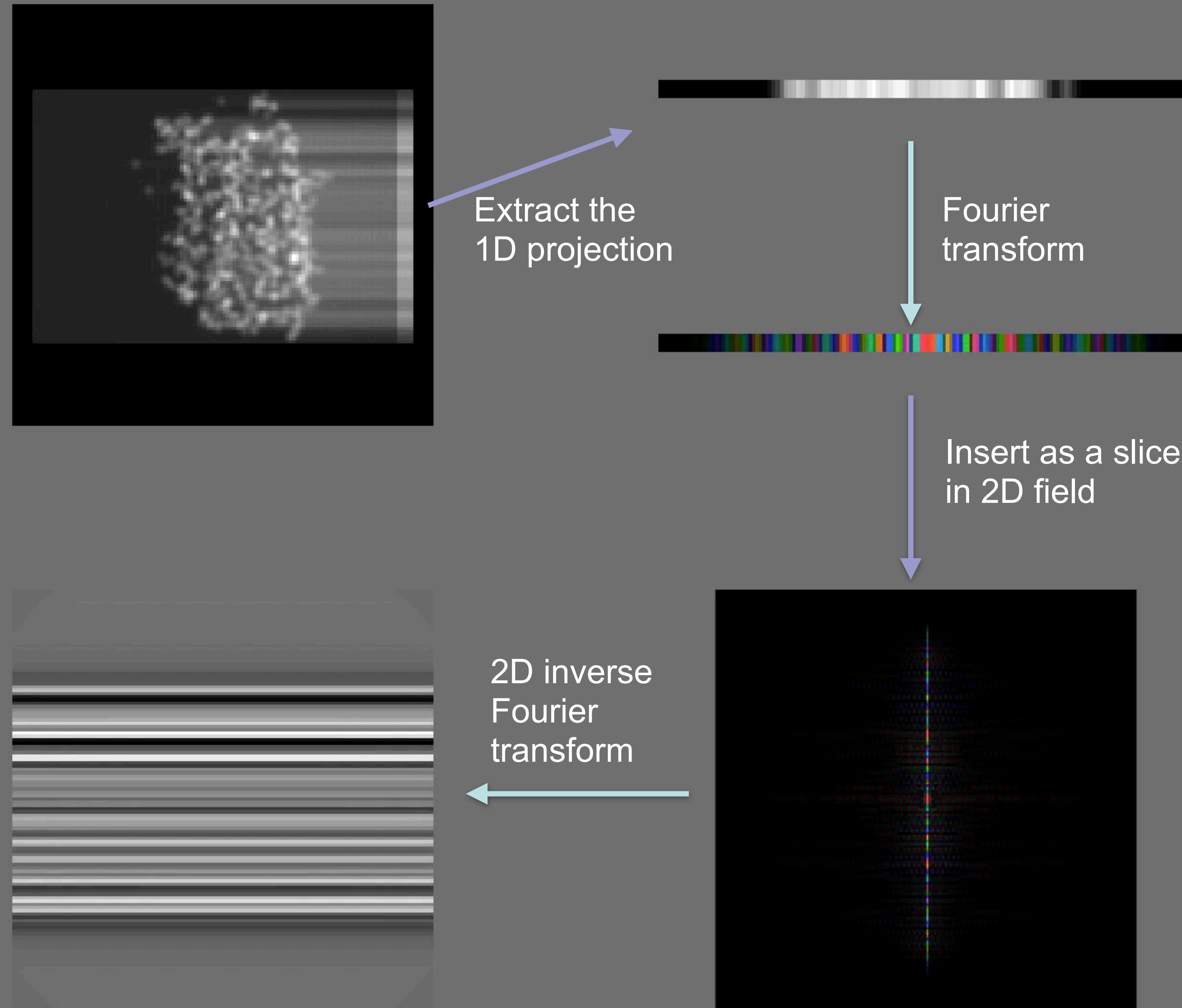


Here we'll demonstrate
building up a 2D structure
from 1D projections.

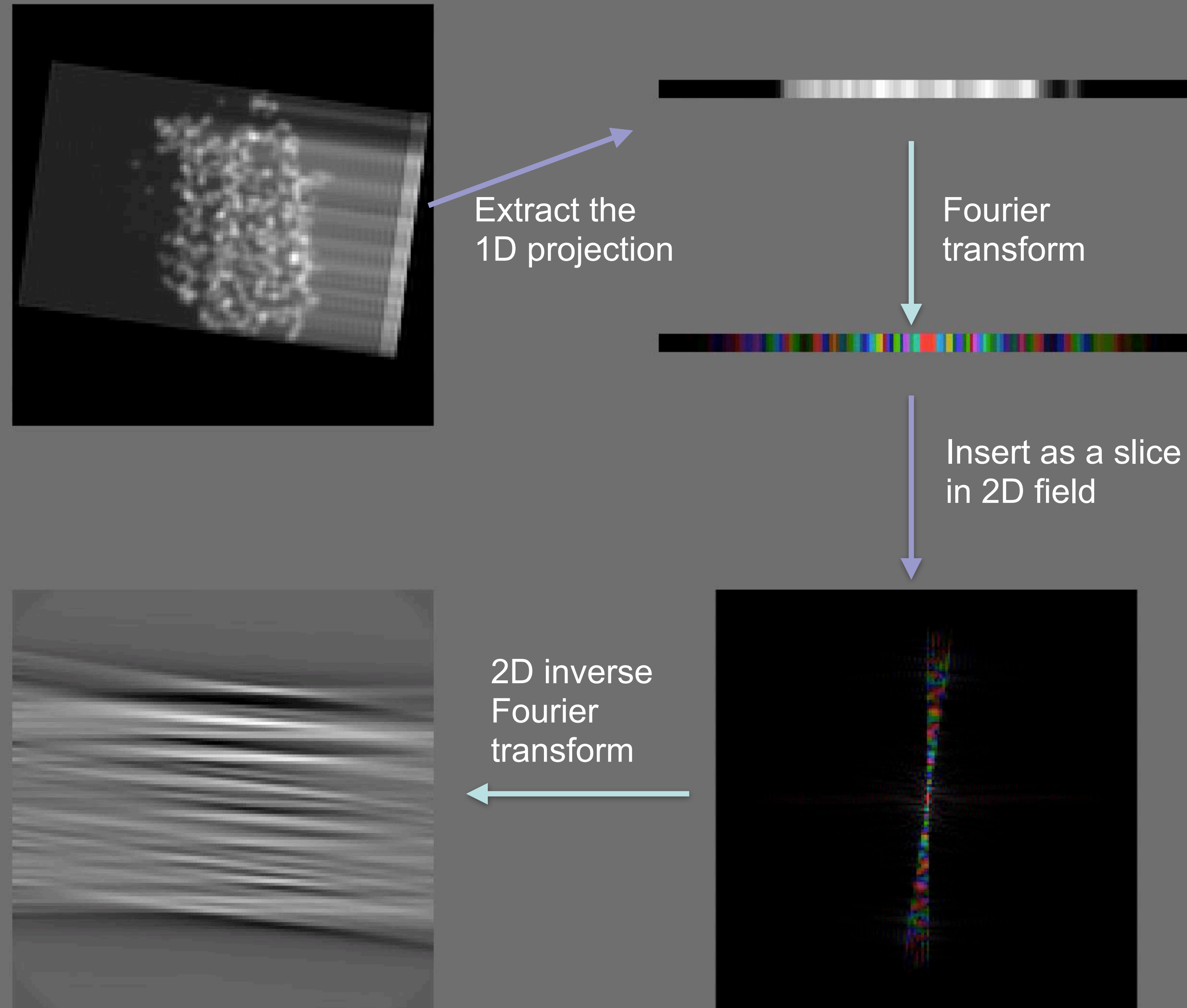
Fourier
transform



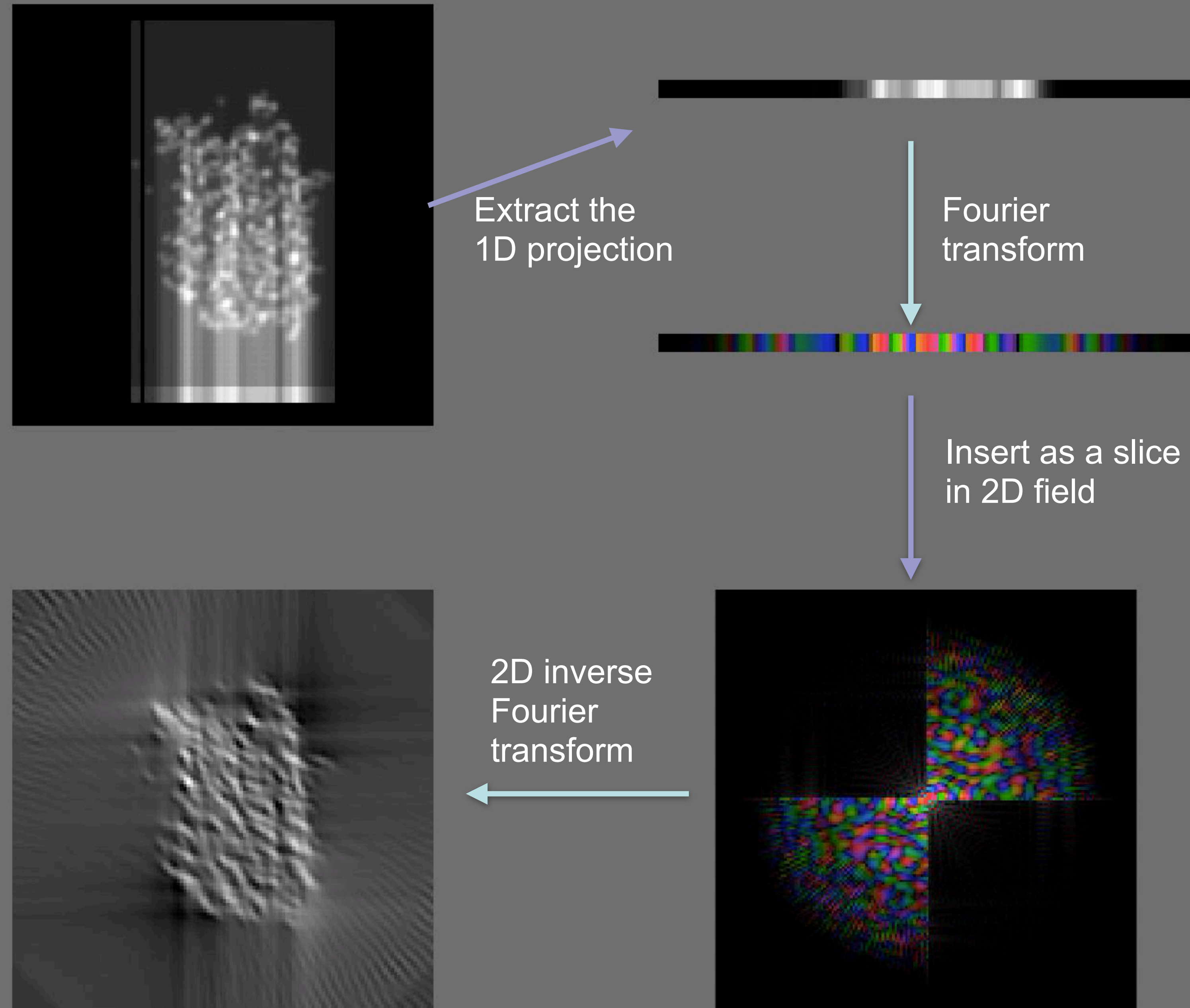
Tomographic reconstruction: 2D image from 1D projections



Tomographic reconstruction: 2D image from 1D projections



Tomographic reconstruction: 2D image from 1D projections



The discrete FT is what is calculated on a computer

2D Fourier transform

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

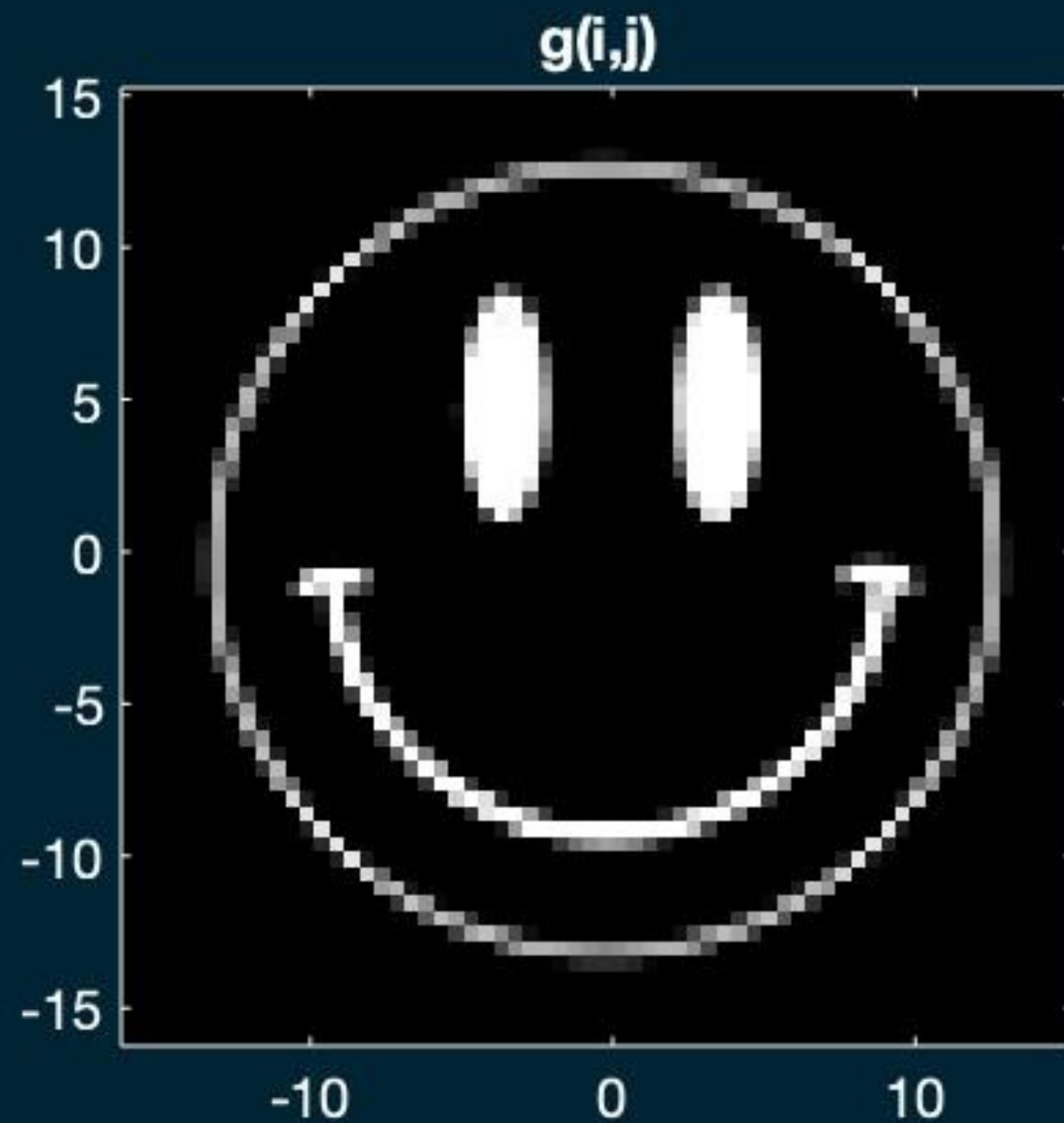
u, v are real numbers

2D discrete Fourier transform

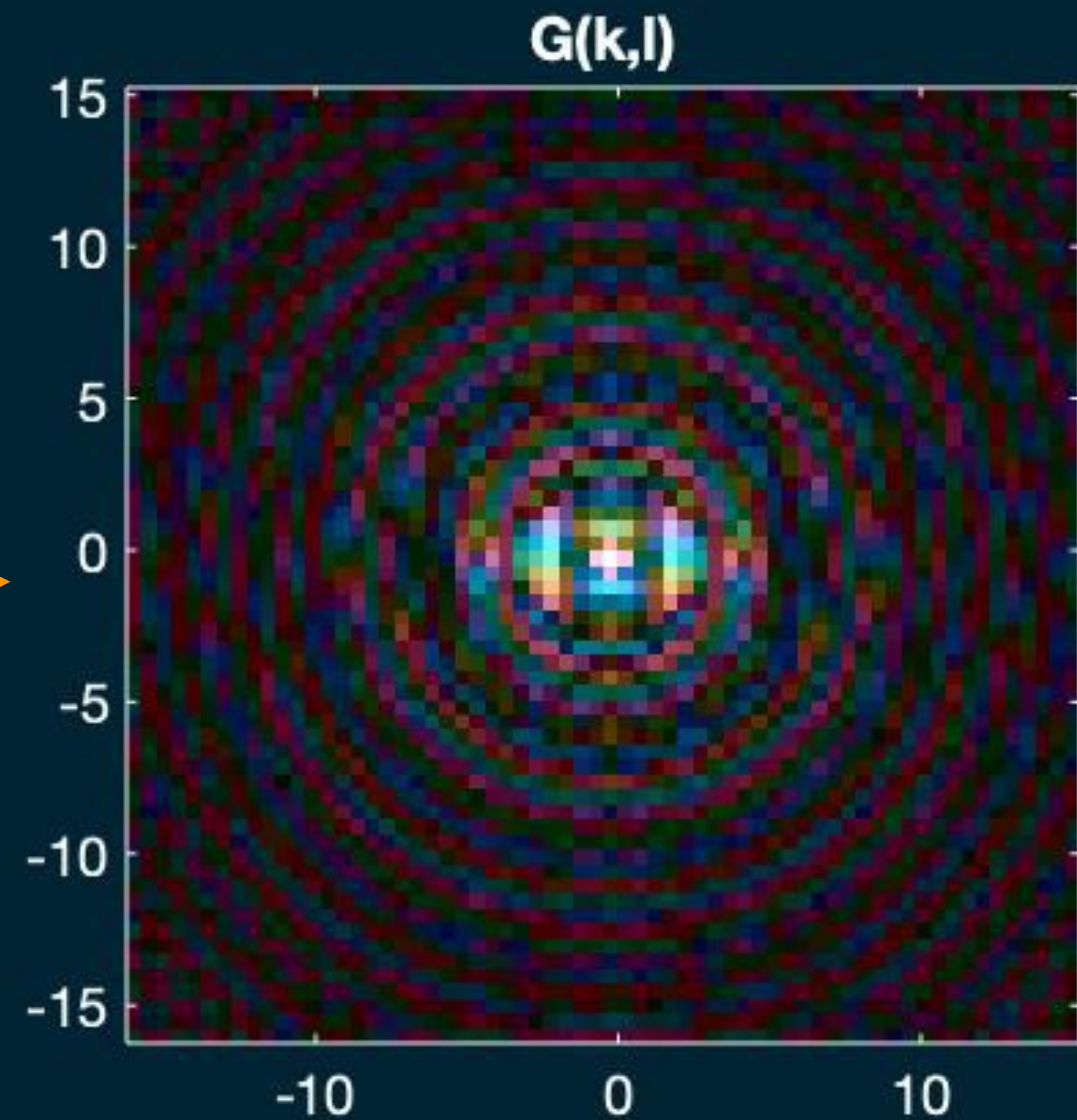
$$G(k, l) = \frac{1}{N} \sum_{i,j=-N/2}^{N/2-1} g(i, j) e^{-i2\pi(ik+jl)/N}$$

k, l are integers

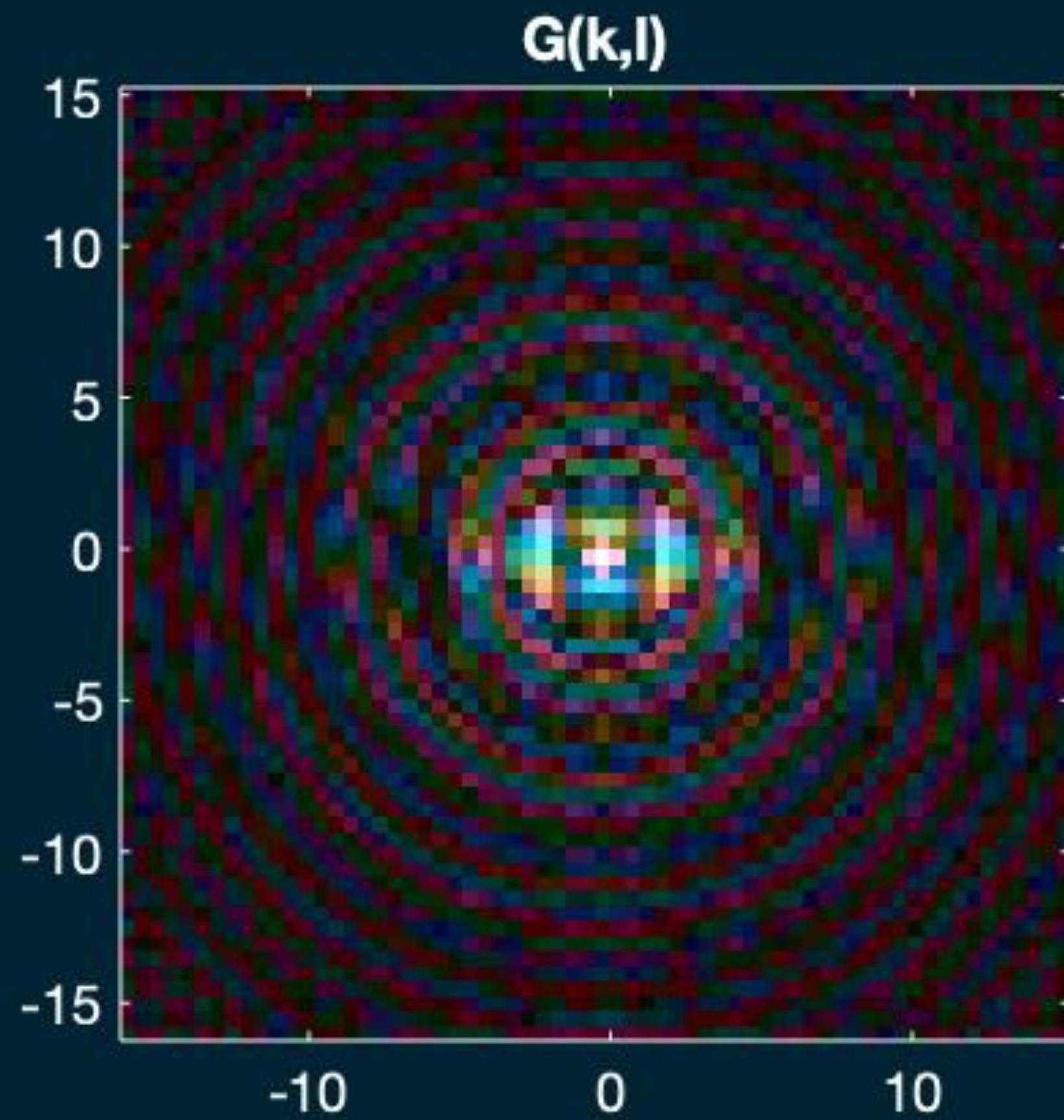
The DFT of a 32 x 32 pixel image has 32 x 32 complex pixel values



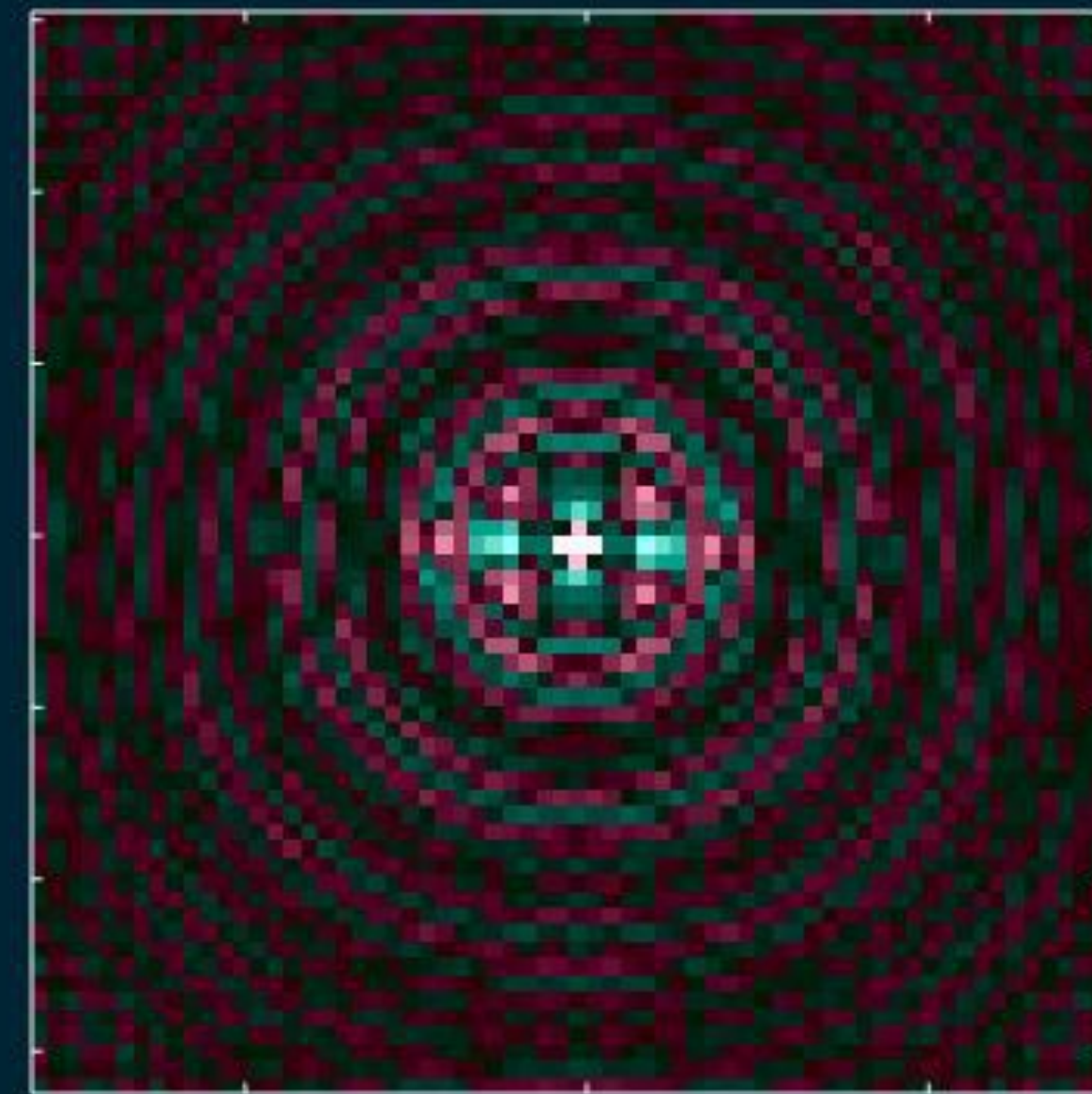
DFT
→



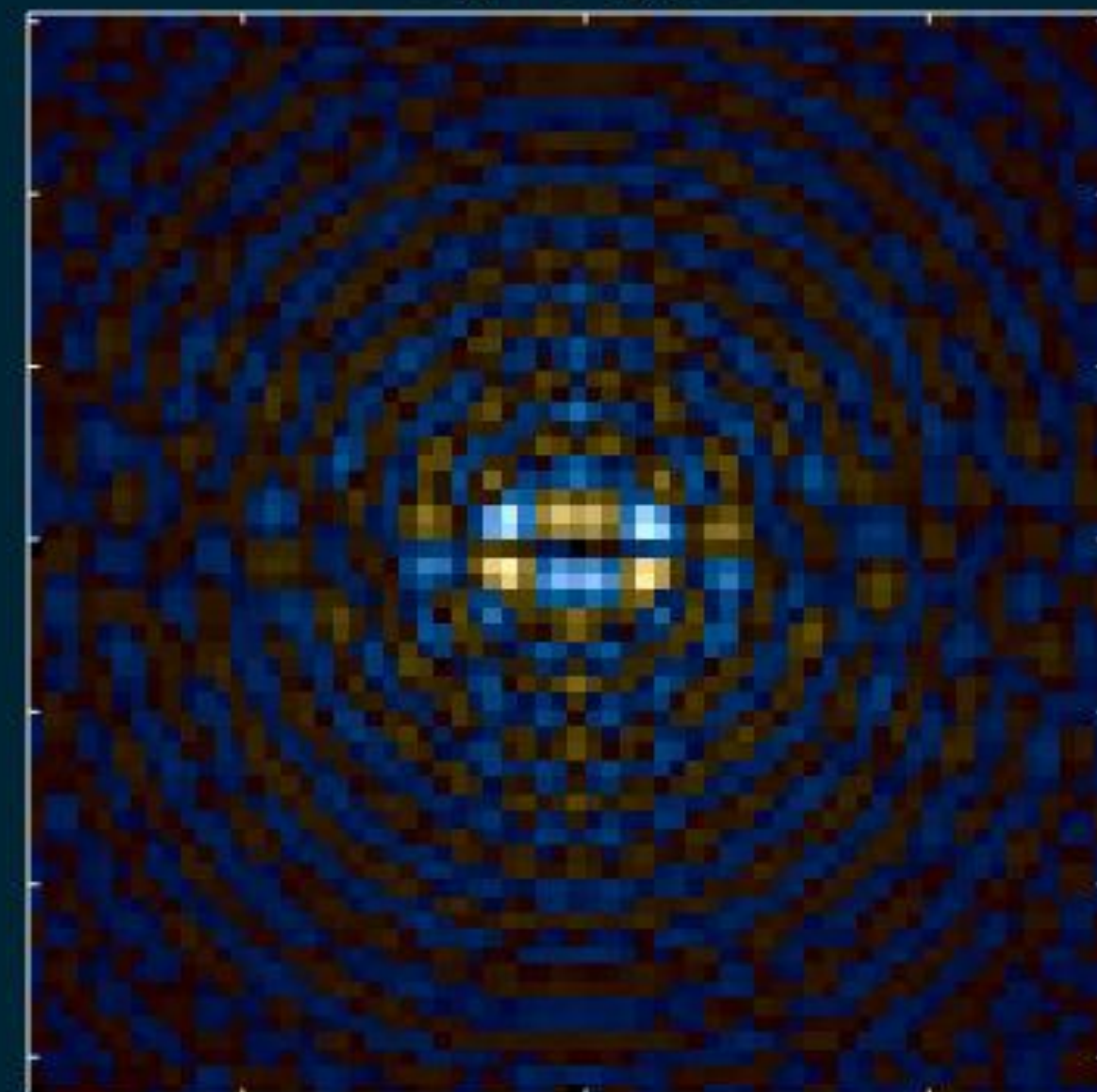
But the DFT of a real image has twofold redundancy



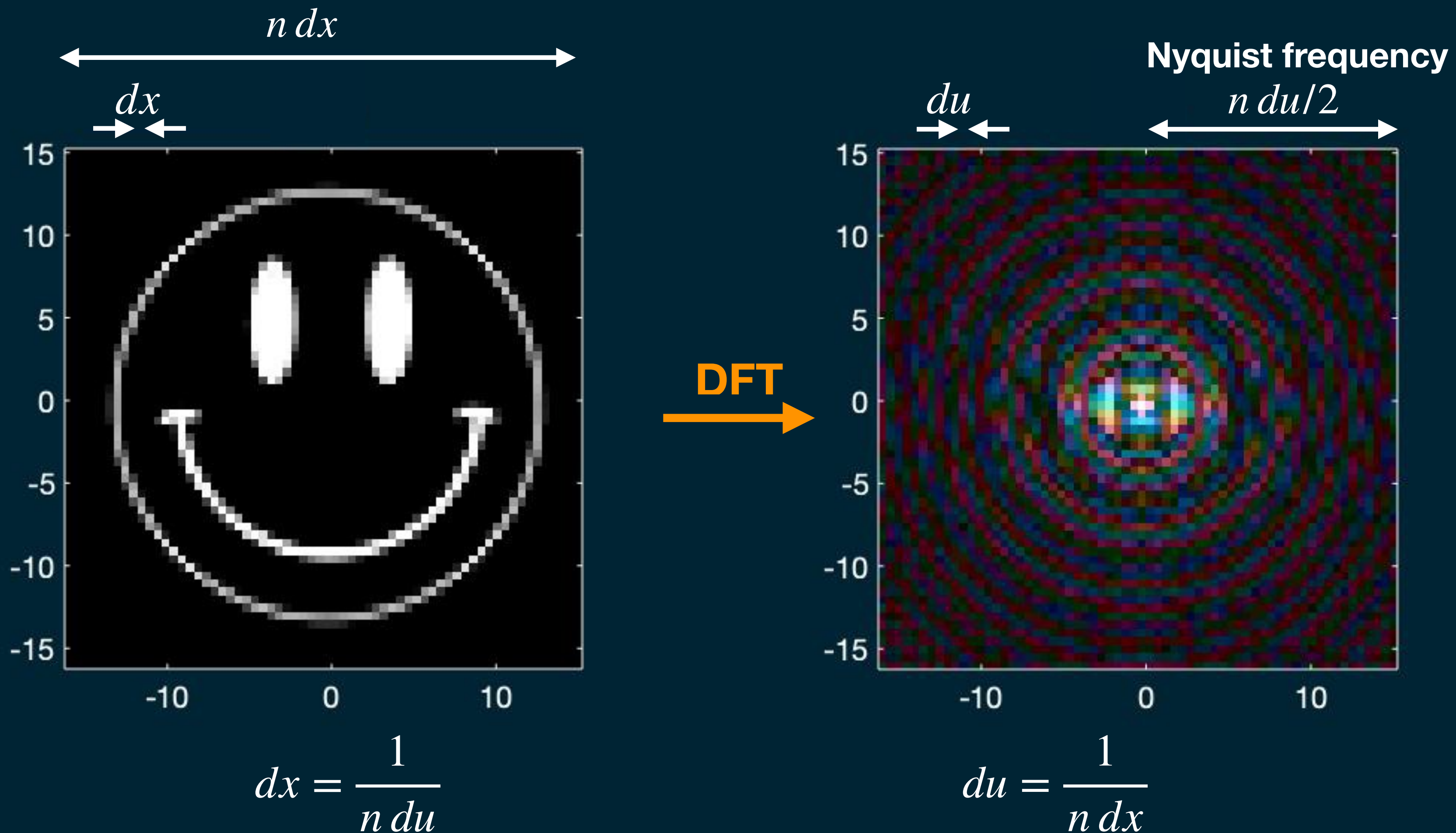
Real part



Imaginary part



What is the pixel size of the transformed image?



Note that the maximum accessible frequency $n du/2$ (the **Nyquist frequency**) corresponds to $2dx$, twice the sampling period.

The Fourier transform in three dimensions

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

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

3D Fourier transform properties

$$abc \, g(ax, by, cz) \rightarrow G(u/a, v/b, w/c)$$

Scale

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

Shift

$$g * h \rightarrow GH$$

Convolution

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

Rotation

$$P_z g(x, y, z) \rightarrow G(u, v, 0)$$

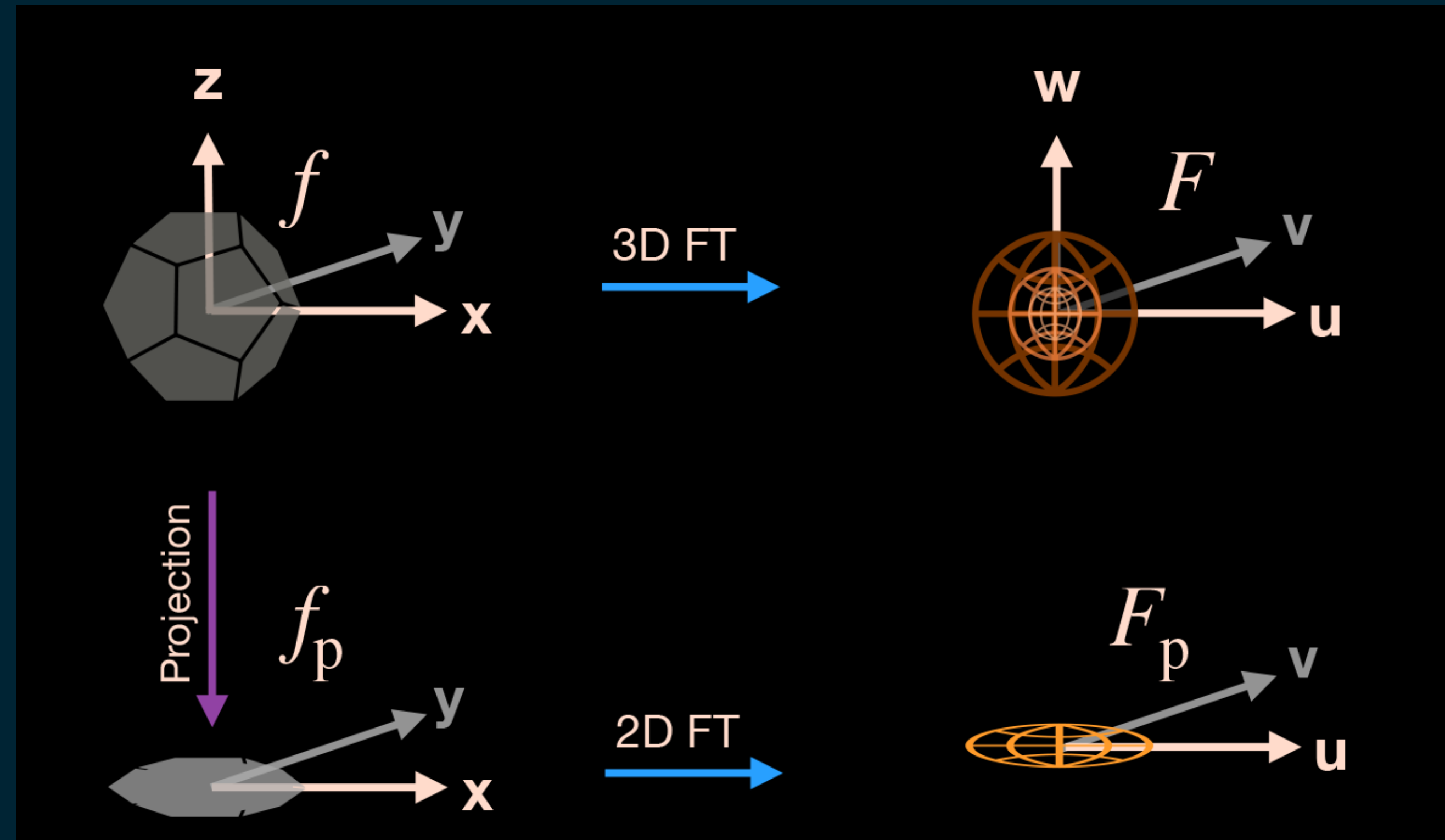
Projection

The 3D Fourier slice theorem

Suppose we have a 3D density $f(x, y, z)$.
The projection along z is a 2D image we'll
call $f_p(x, y)$:

$$f_p(x, y) = \int f(x, y, z) dz$$

Let its Fourier transform be $F_p(u, v)$.



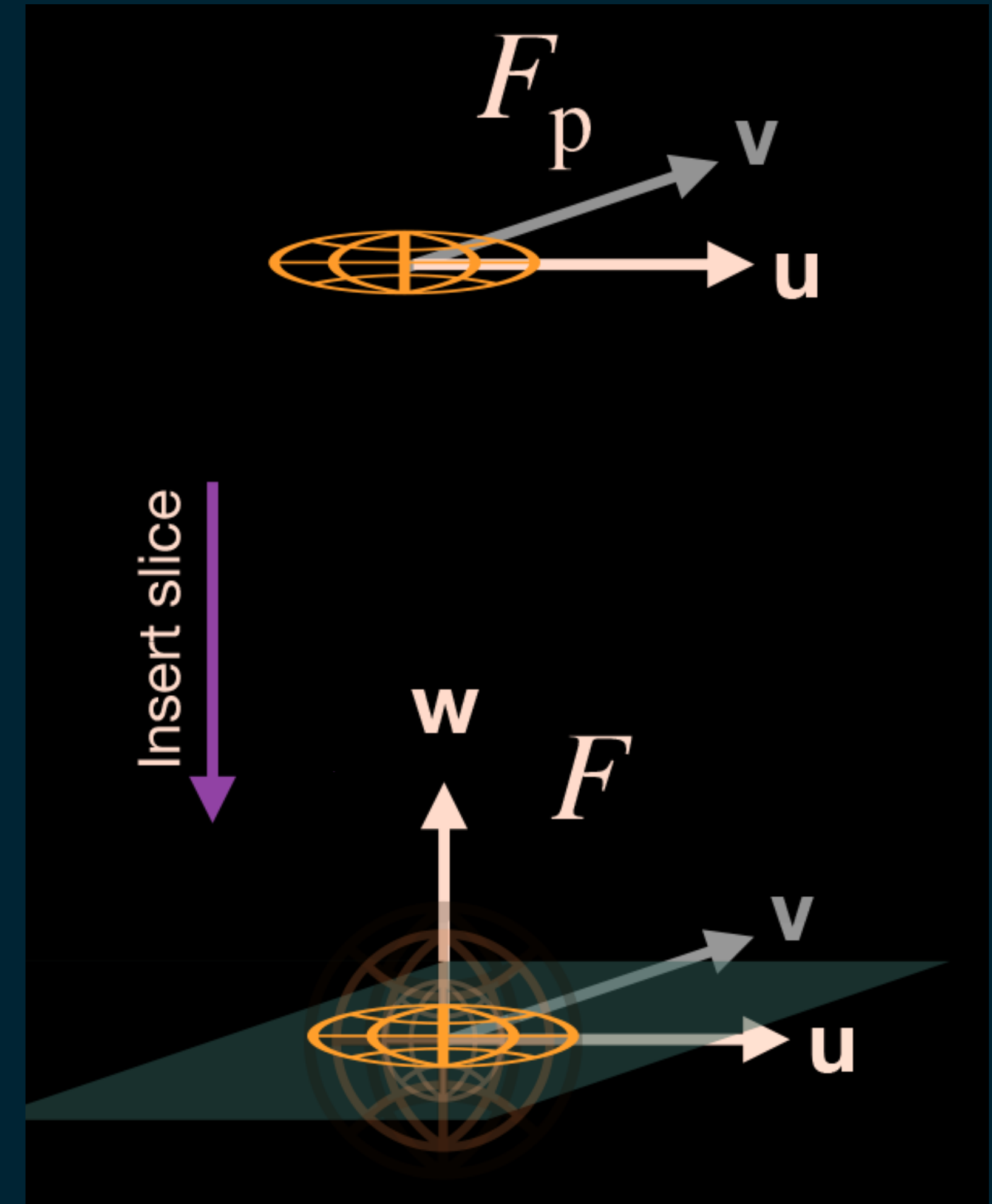
The 3D Fourier slice theorem

$F_p(u, v)$ is actually the same as the FT of the 3D volume, when we evaluate it at $w = 0$. In other words,

$$F_p(u, v) = F(u, v, 0).$$

That's because we can separate out the integral over z to get

$$F(u, v, 0) = \iint \underbrace{\left(\int f(x, y, z) dz \right)}_{f_p(x, y)} e^{-i2\pi(ux+vy)} dx dy$$



Building up a 3D reconstruction

We can make use of the rotation property of the 3D FT to compute projections in many different directions, and insert the planes at the corresponding angles into the 3D Fourier volume.

If we've covered the volume completely then we can transform back to recover the complete 3D volume.

