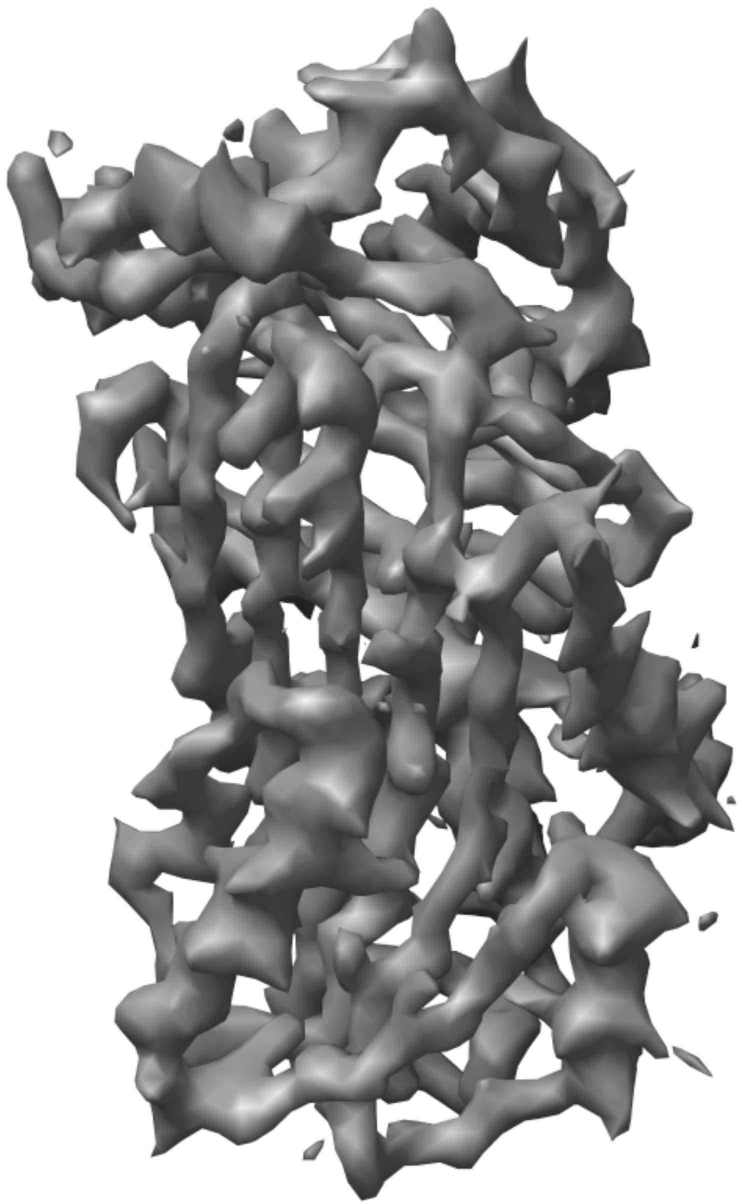
CTF Correction,
FFTs
and Model Bias

NCRR

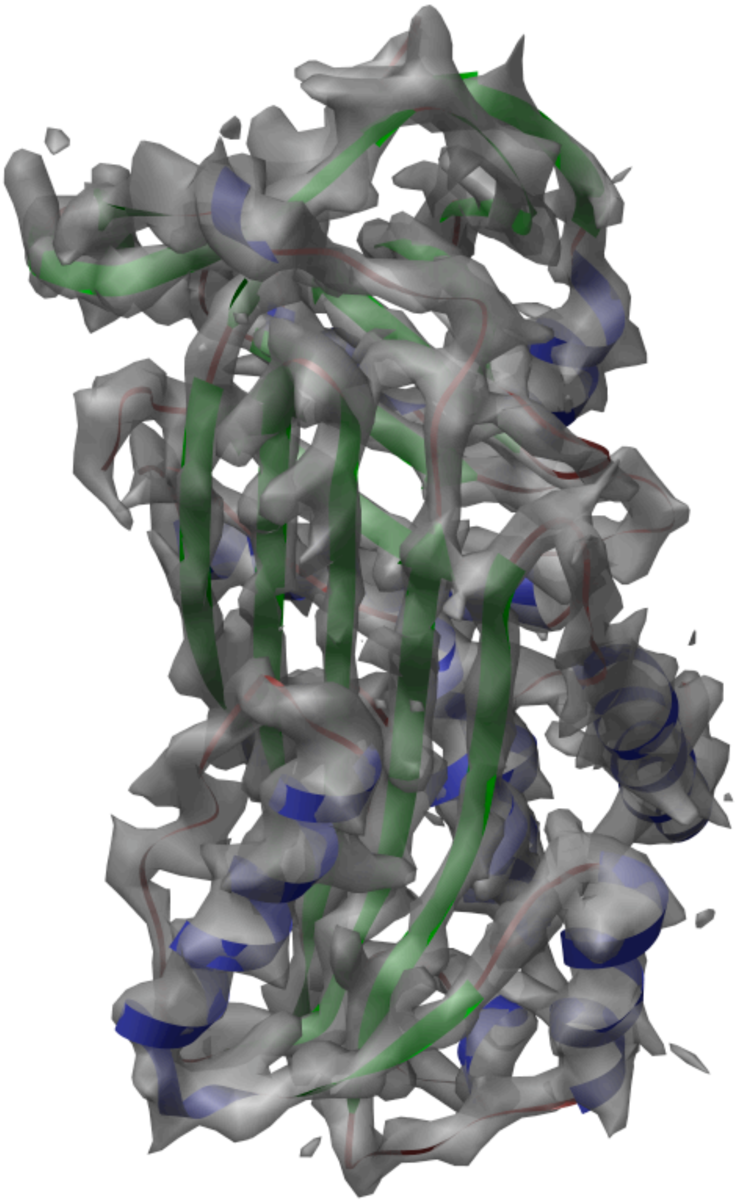
NCMI
National Center for Macromolecular Imaging

4CAA

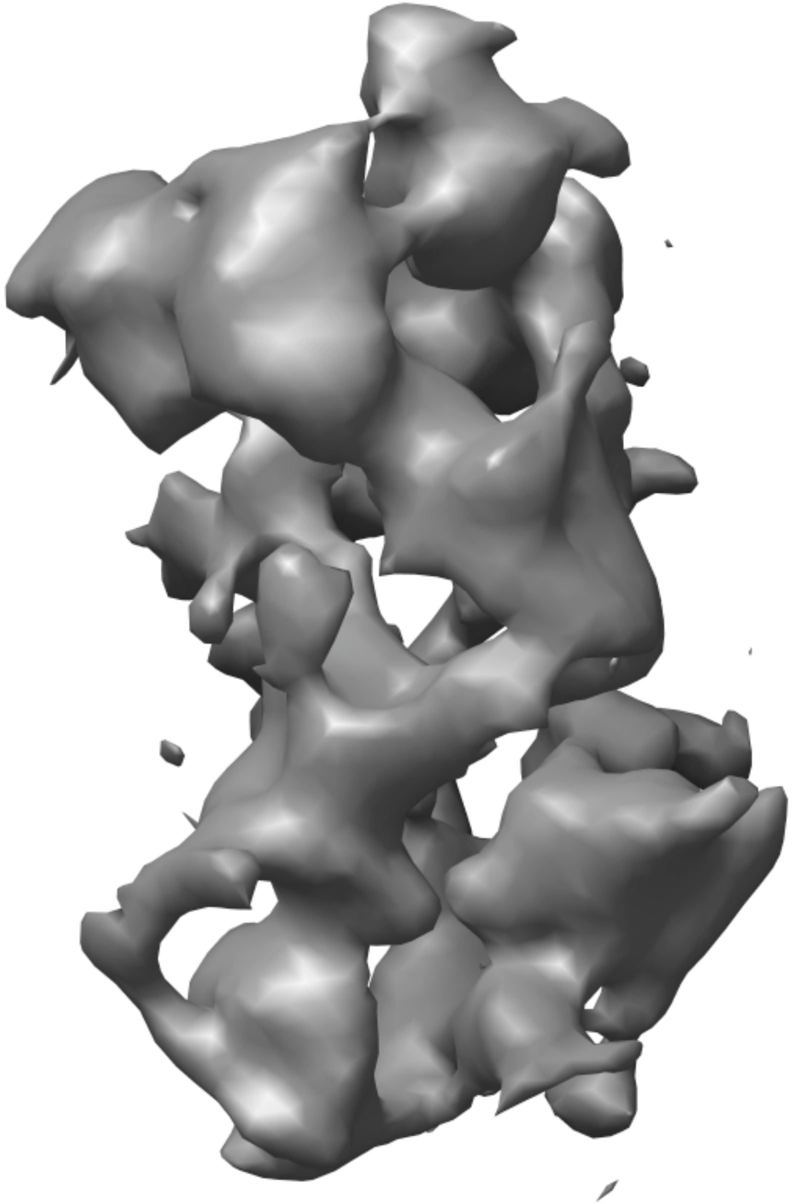
4CAA



4CAA

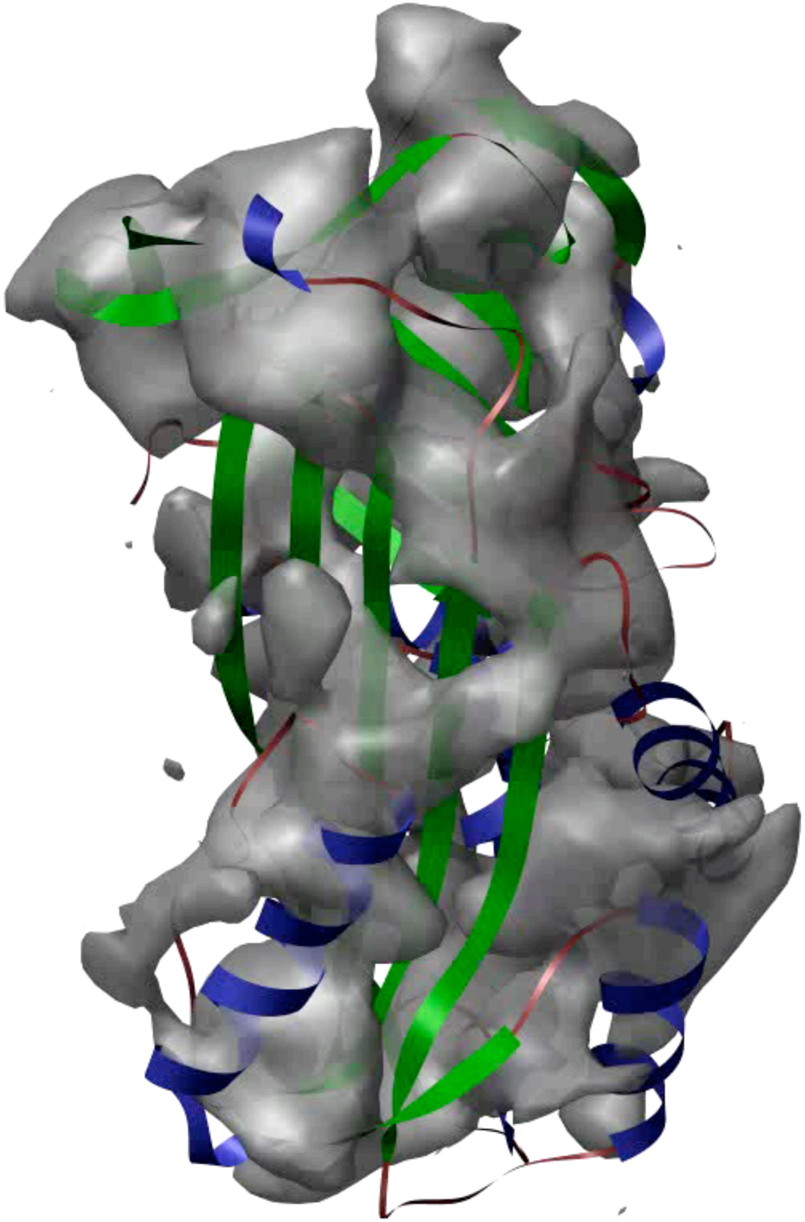


No CTF Corr (1 defocus)

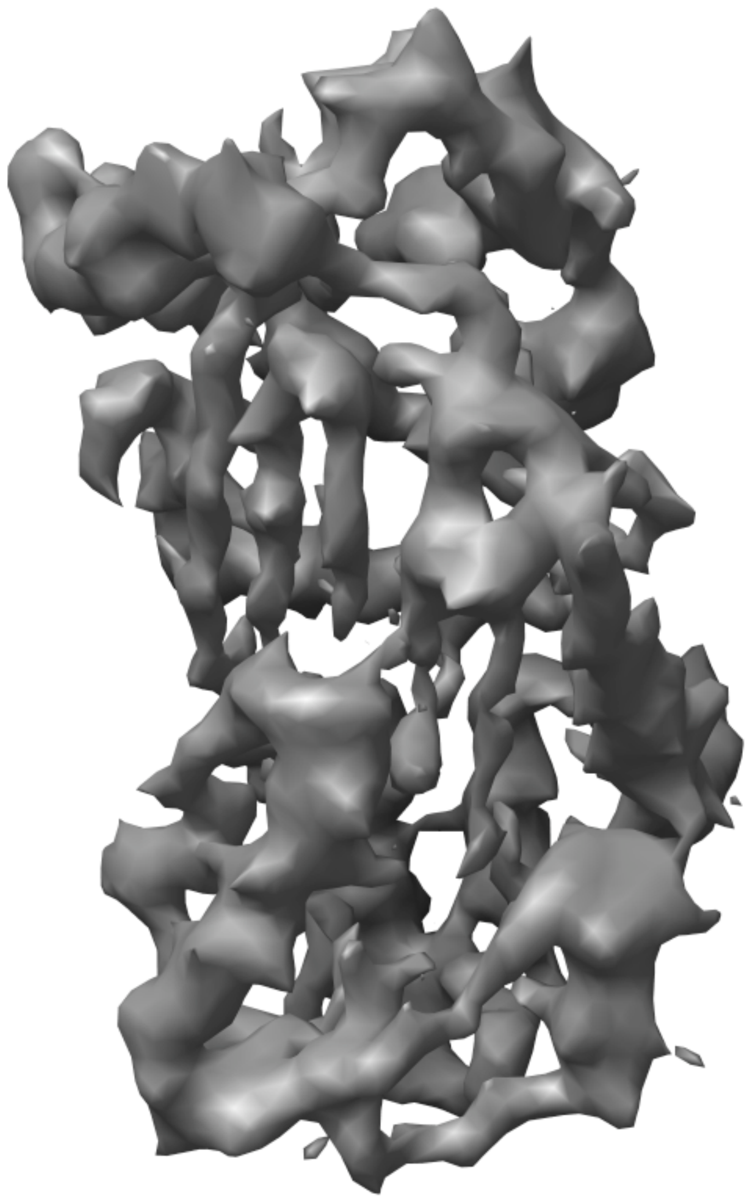


No CTF Corr (1 defocus)

No CTF Corr (1 defocus)



Phase Flipped (1 defocus)



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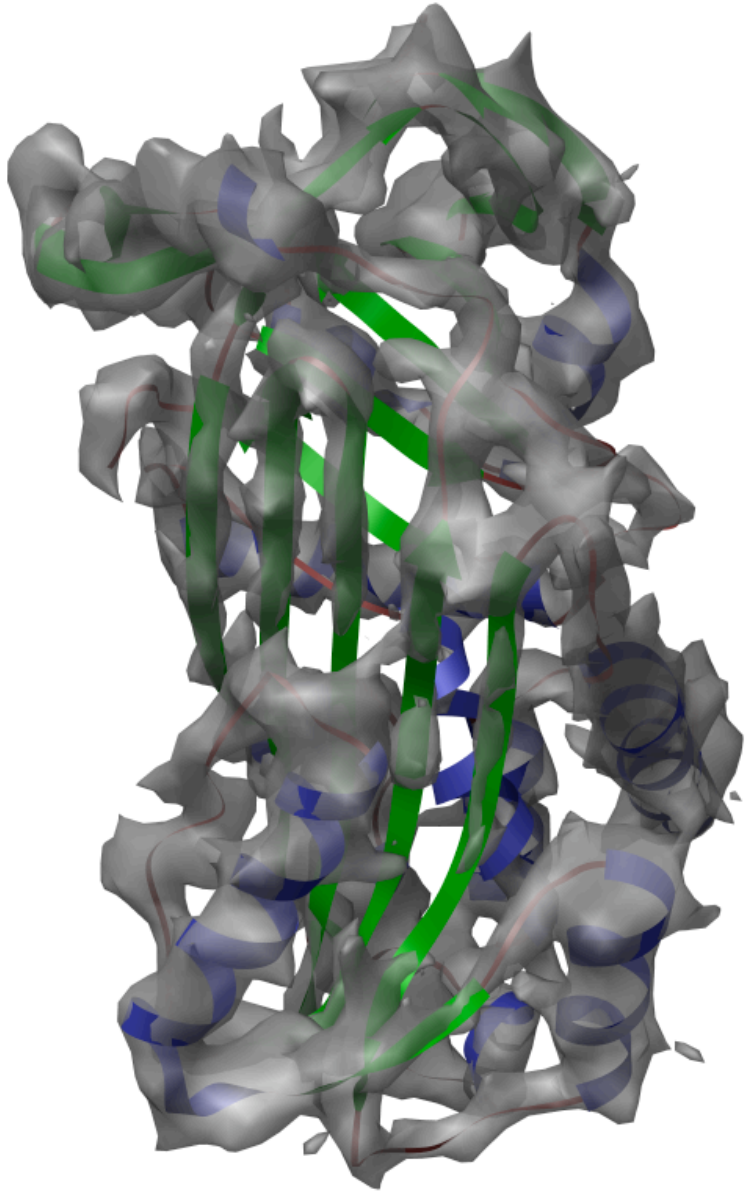
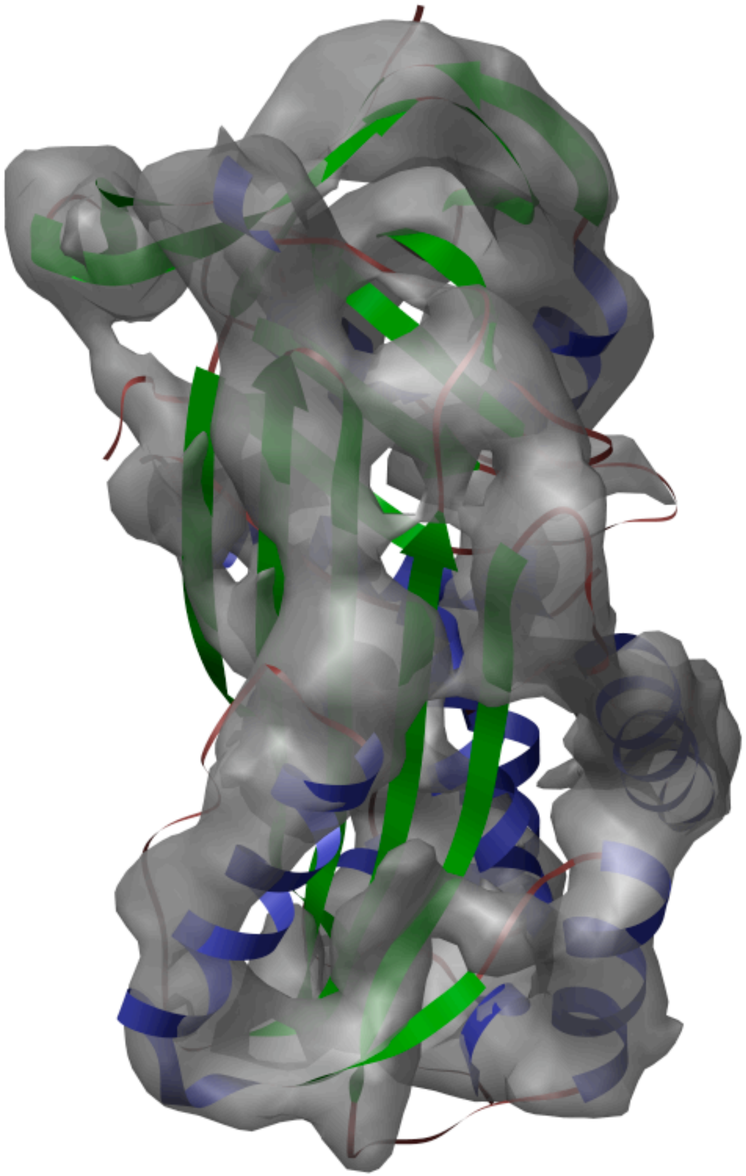
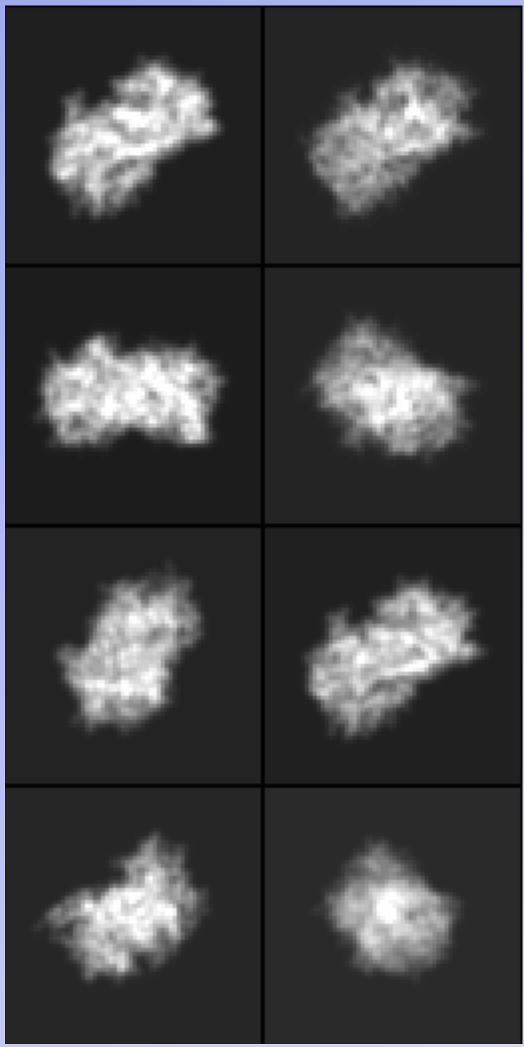


Phase Flipped (mult defocus)

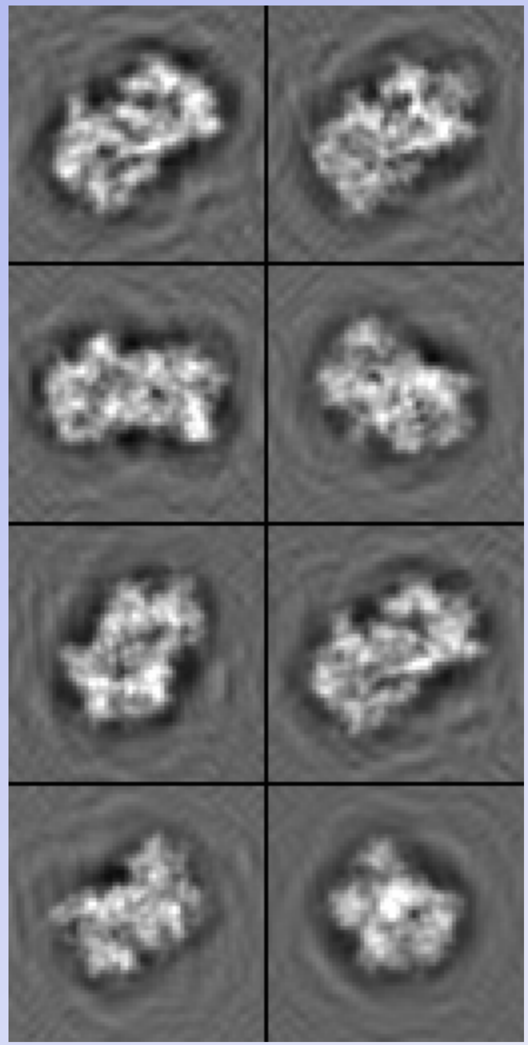


4CAA in 2D

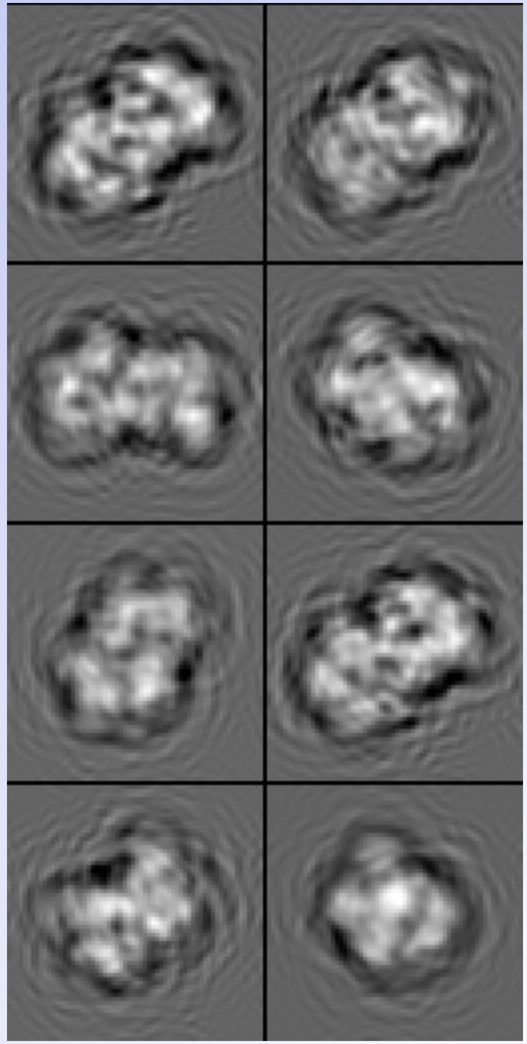
No CTF



CTF Amp



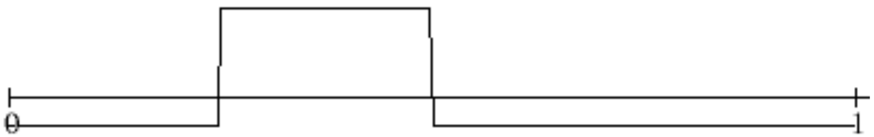
Amp & Pha



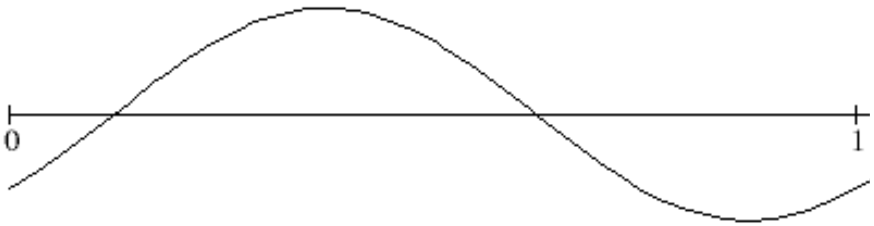
Fourier Transforms (FFT)

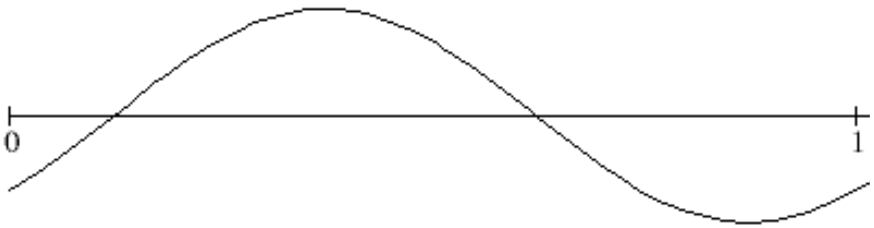
ANY function f(x) can be represented exactly as a sum of sin() functions with specific amplitudes and phases.

Fourier Representation

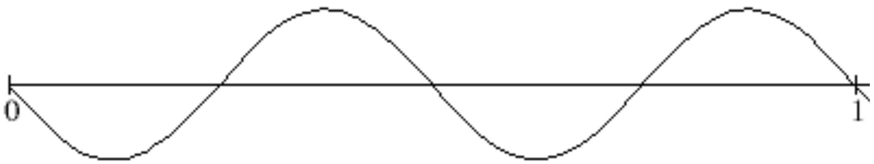


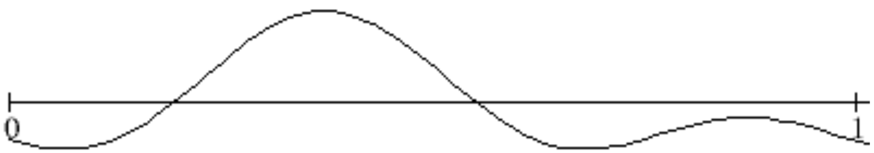
Fourier Representation



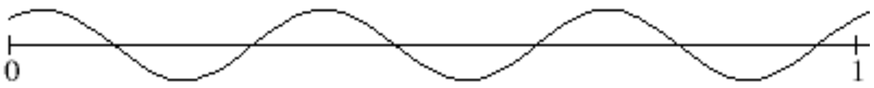


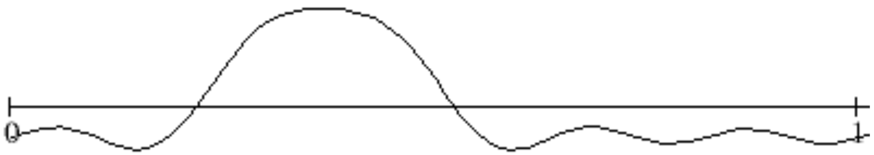
Fourier Representation



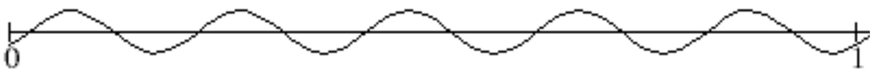


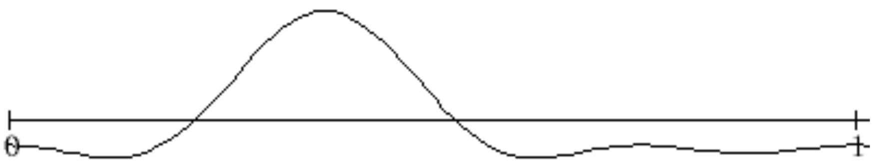
Fourier Representation



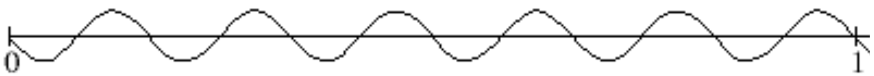


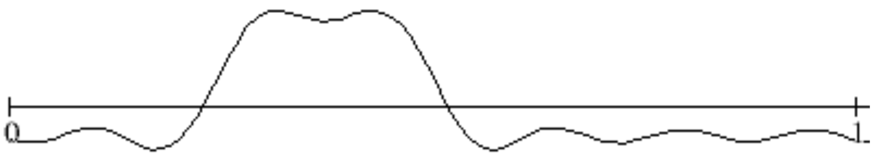
Fourier Representation



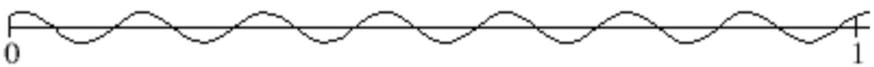


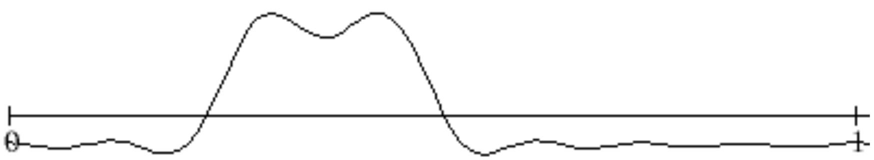
Fourier Representation





Fourier Representation





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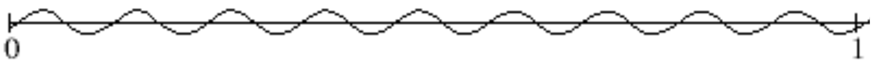

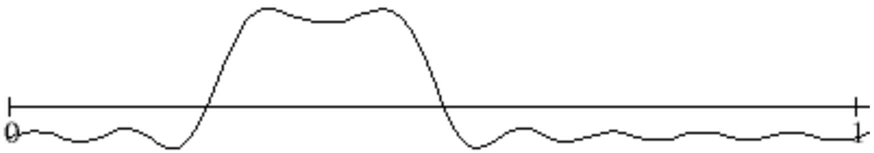

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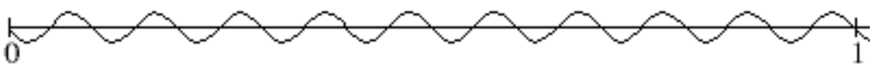
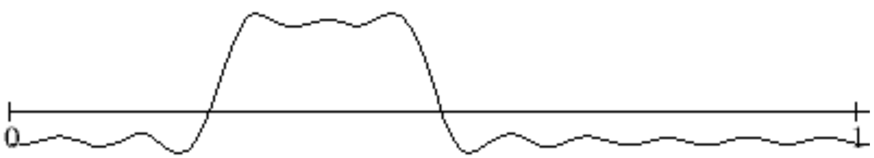
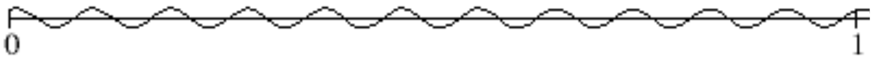
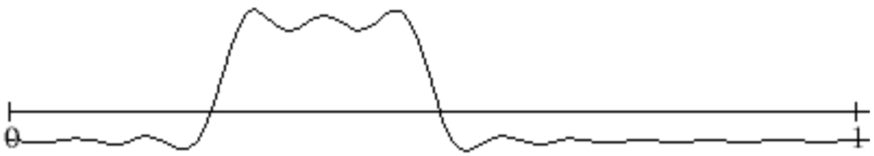


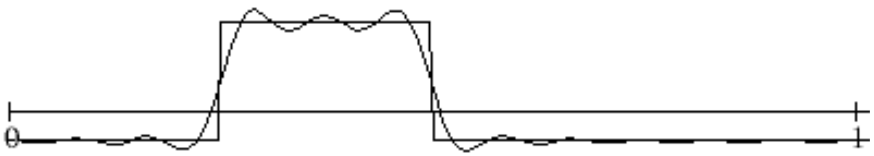


Fourier Representation

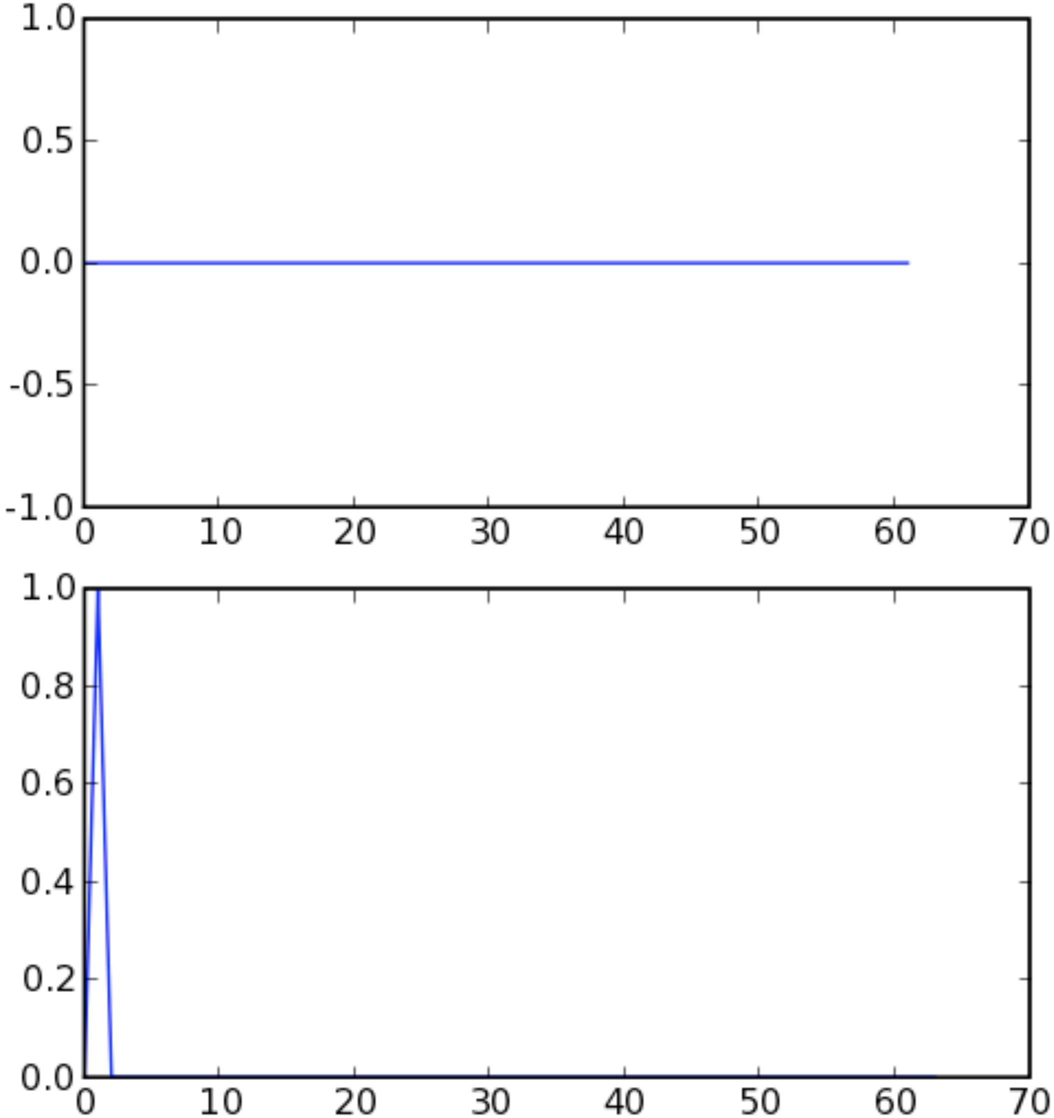




Fourier Representation



FFT



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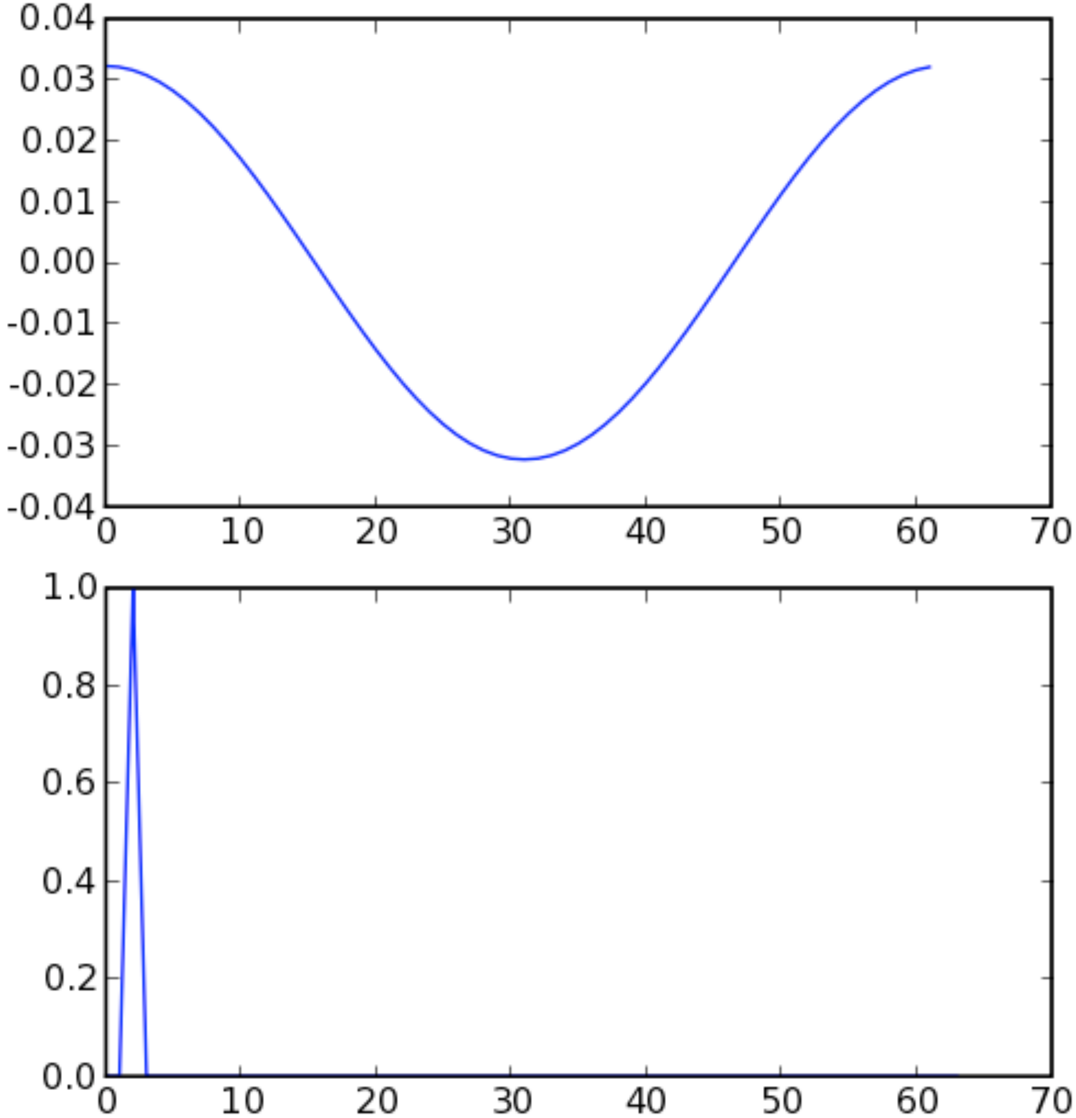
FFT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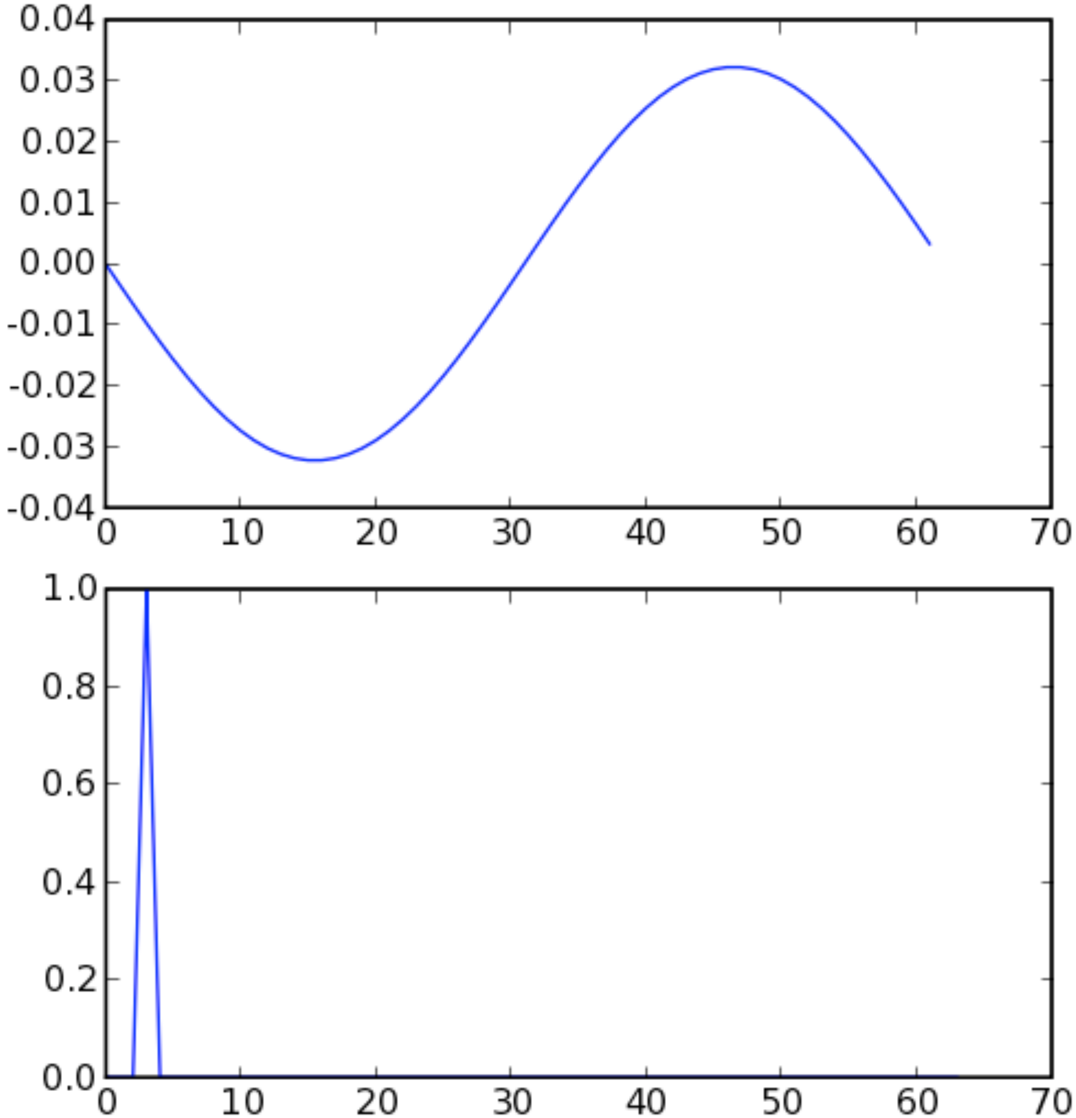

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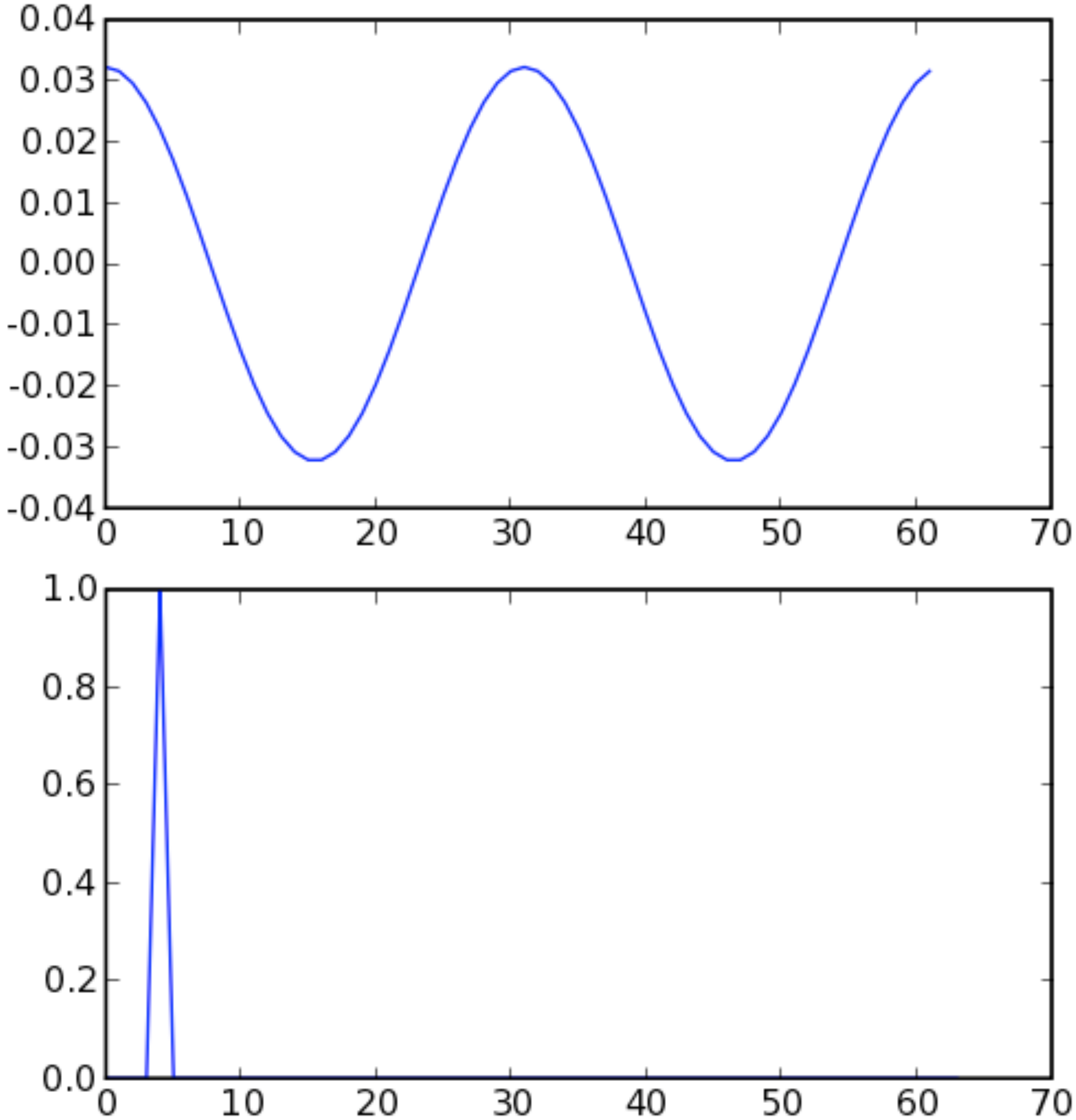

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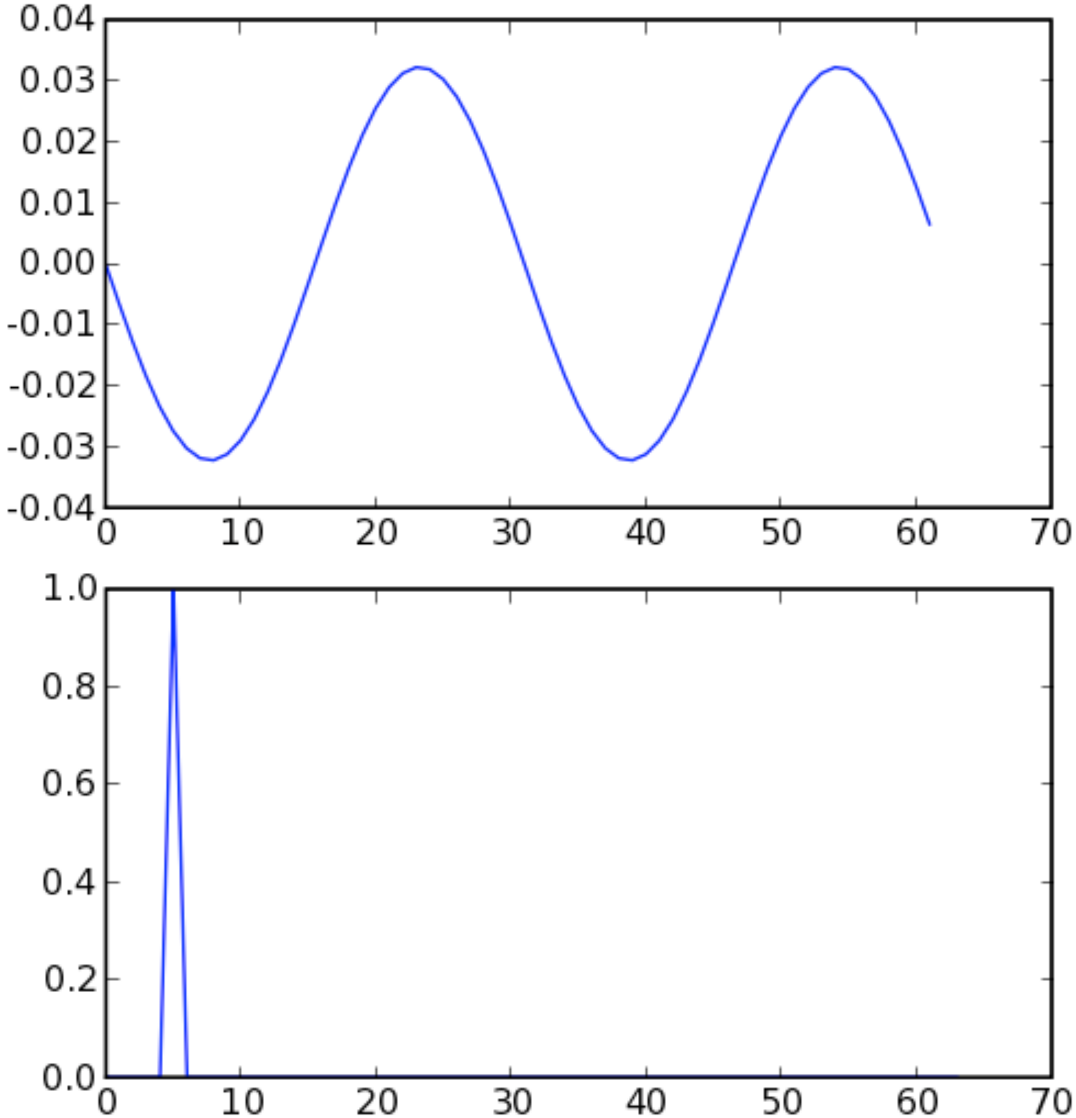
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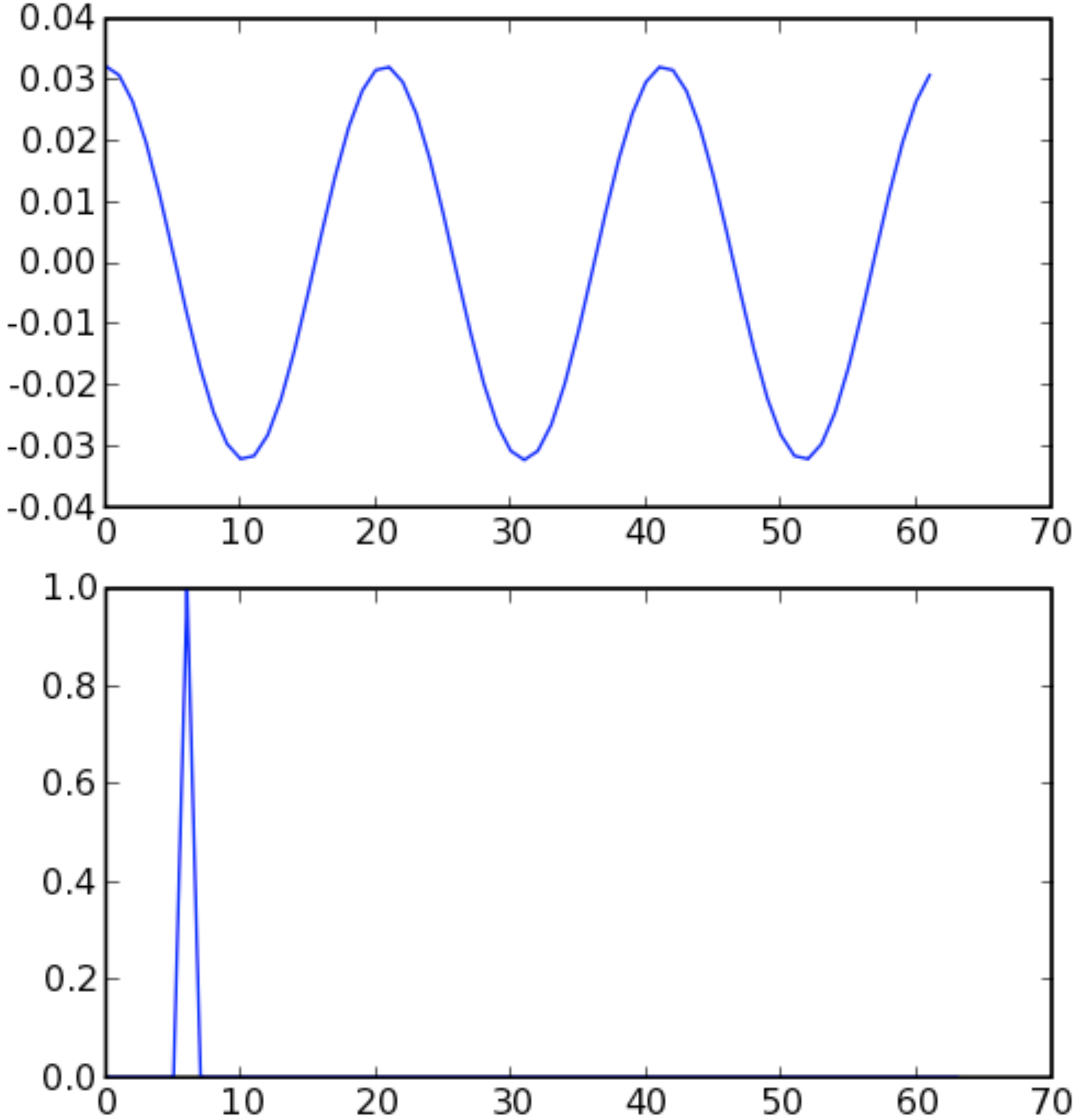

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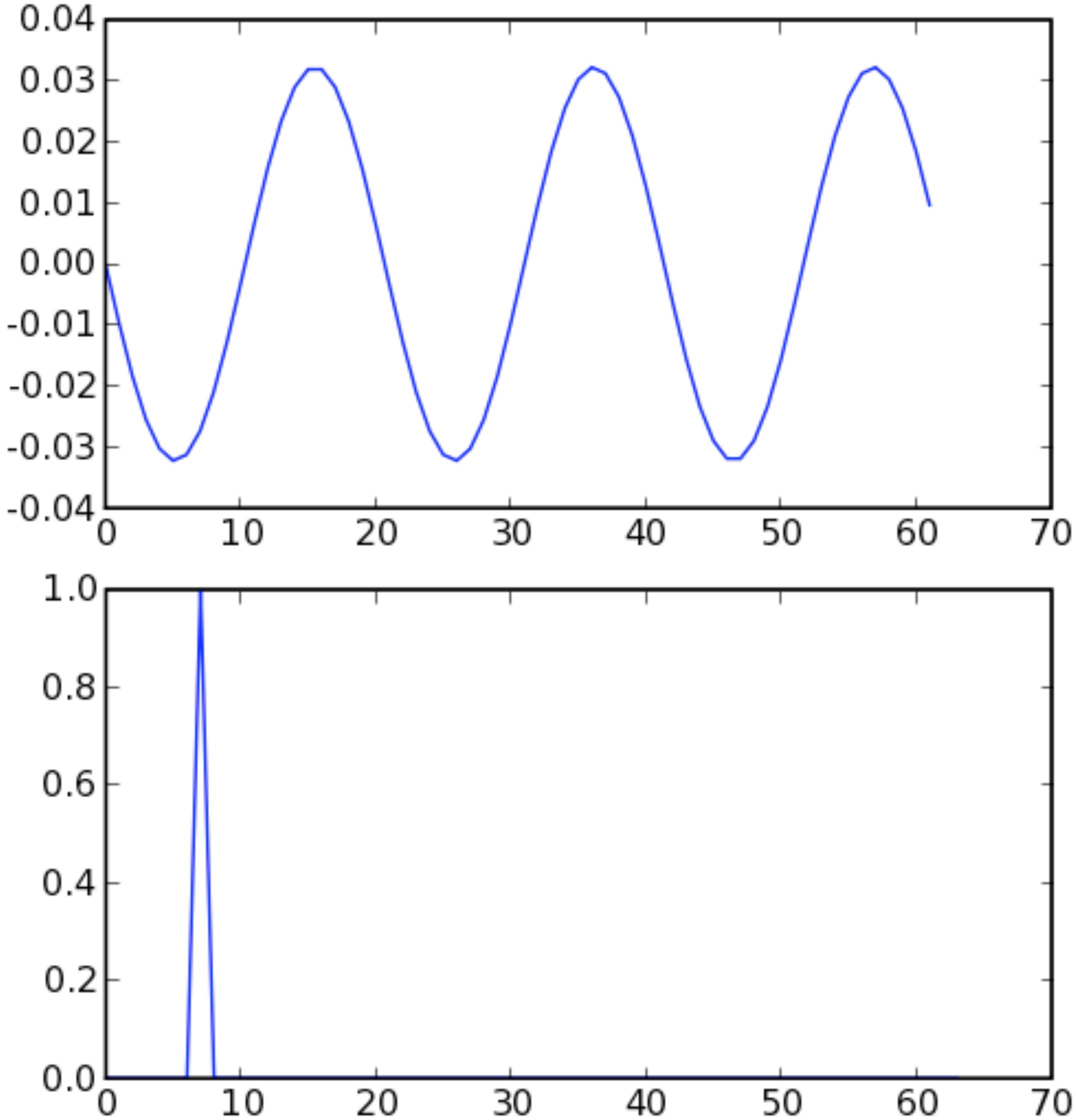
FFT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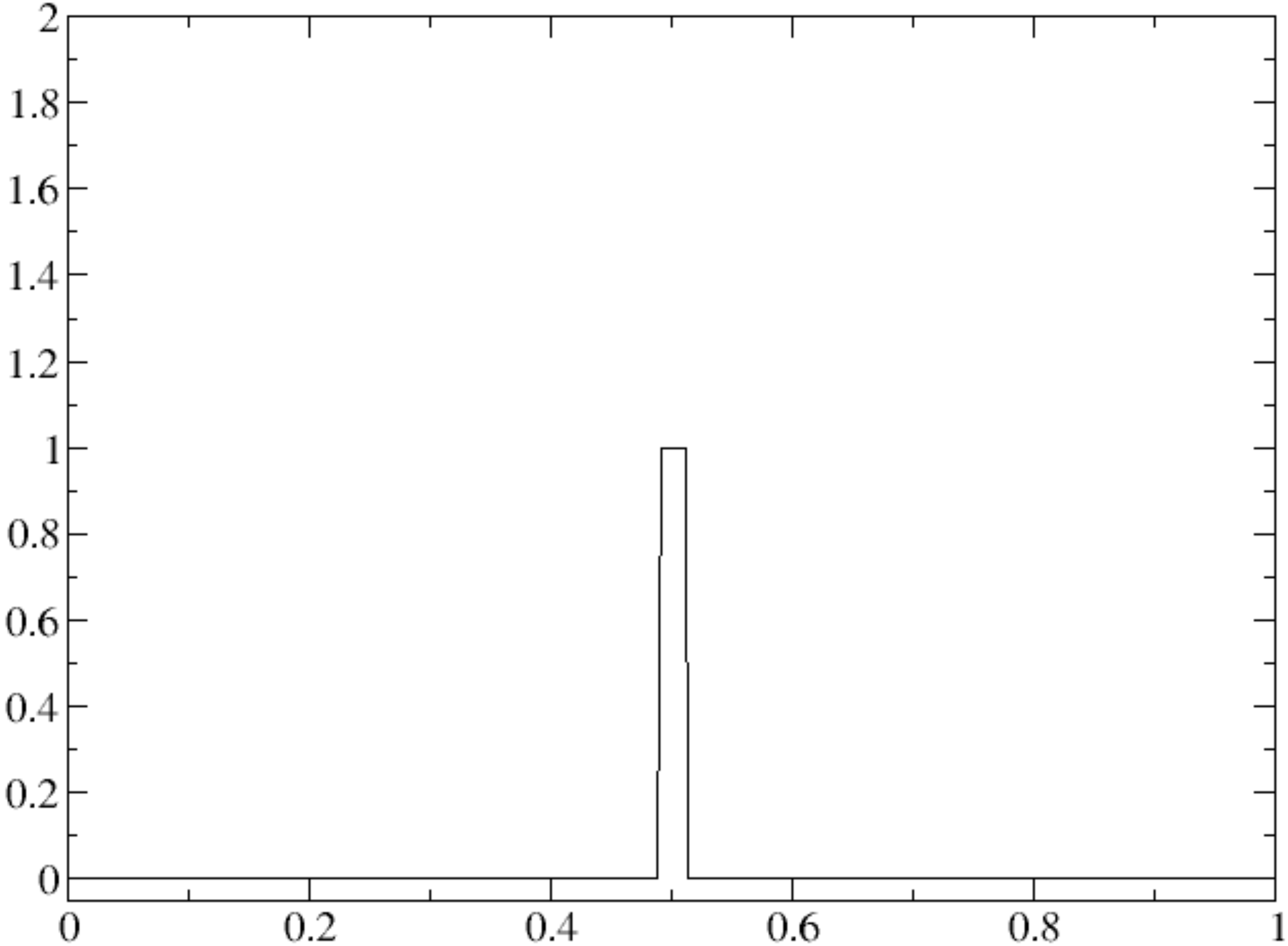
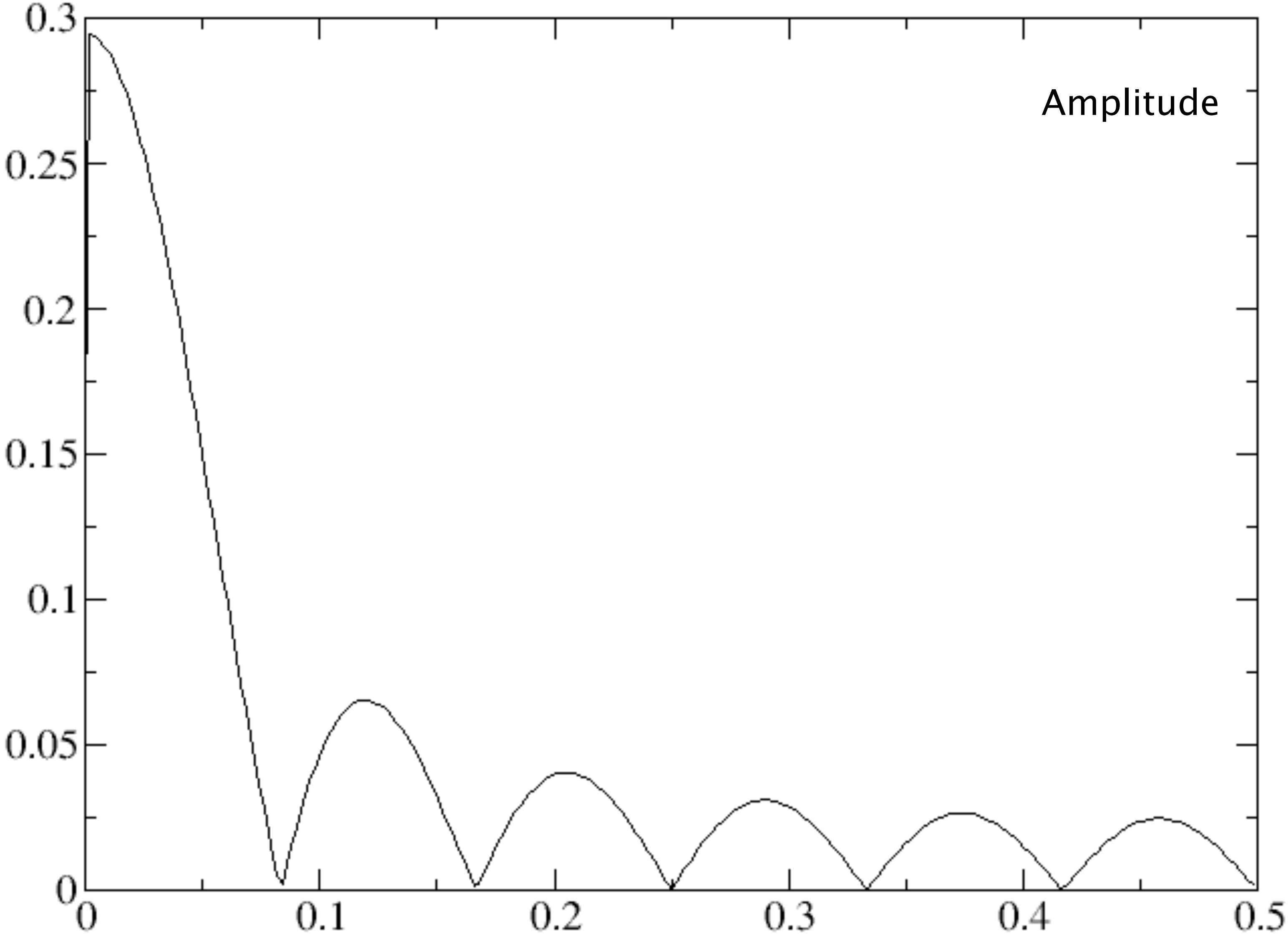
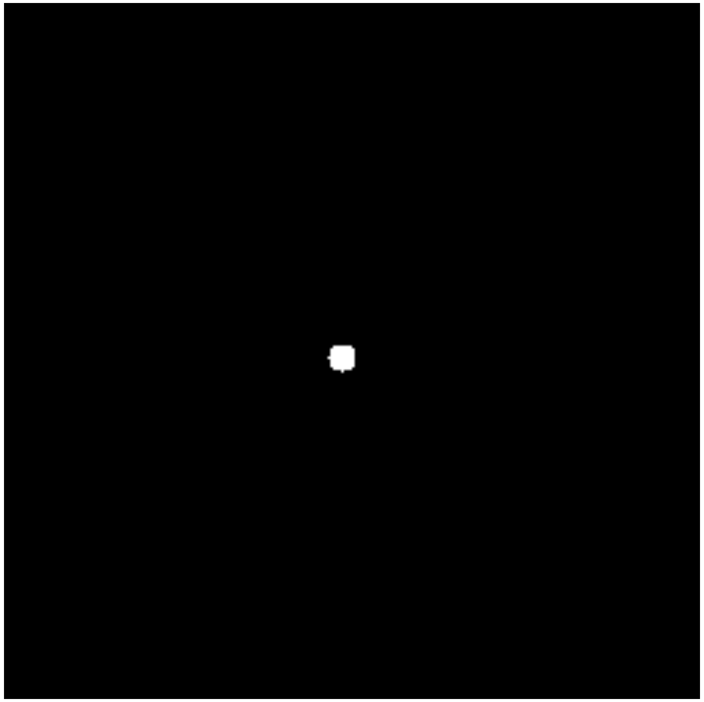
FFT of a Square Pulse



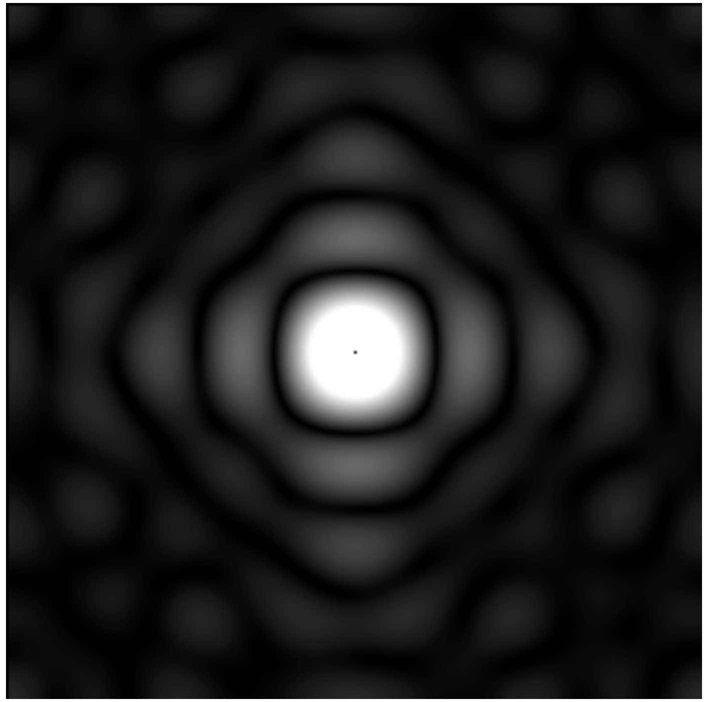
FFT of a Square Pulse



FFT Image demo

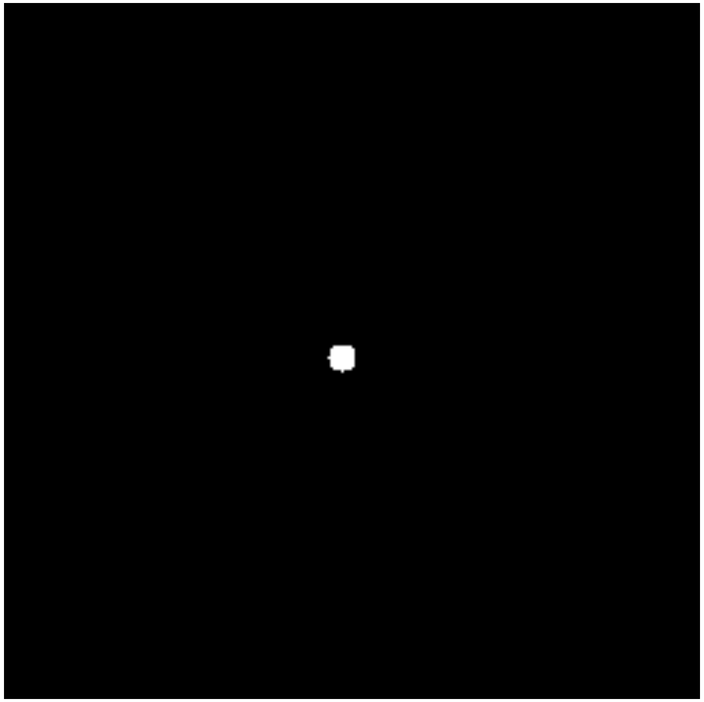


Real

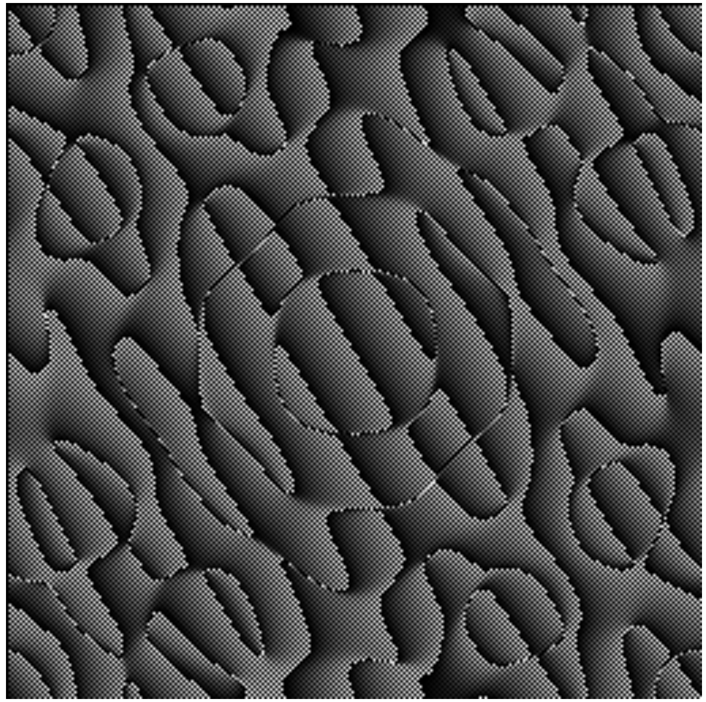


FFT Amplitude

FFT Image demo

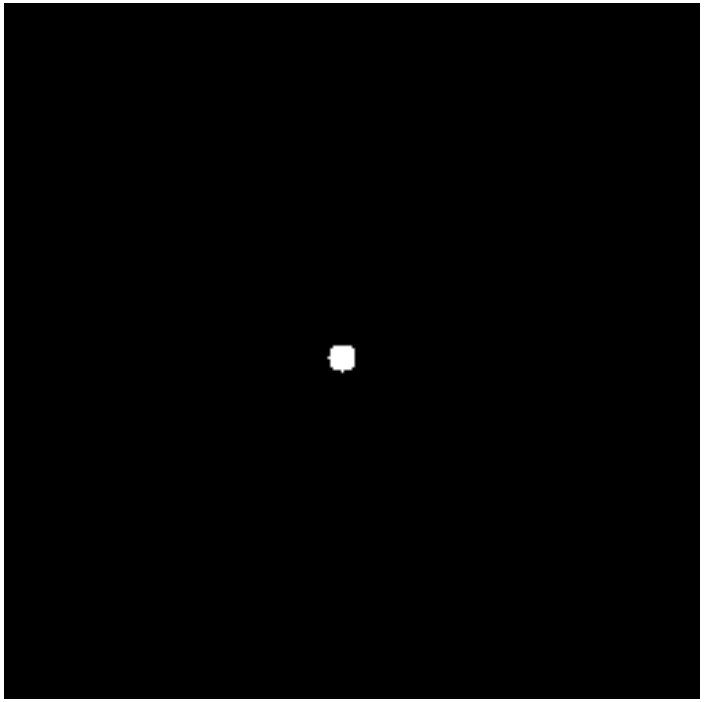


Real

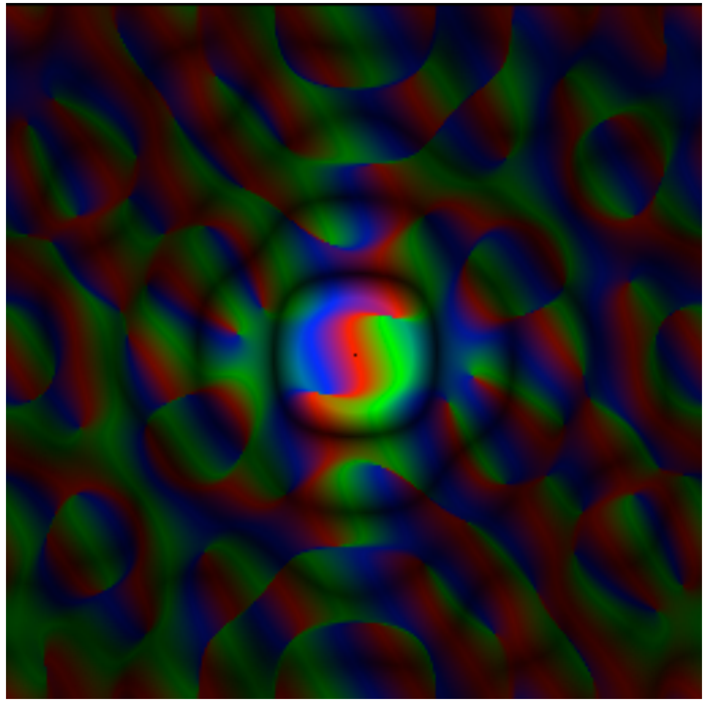


FFT Phase

FFT Image demo

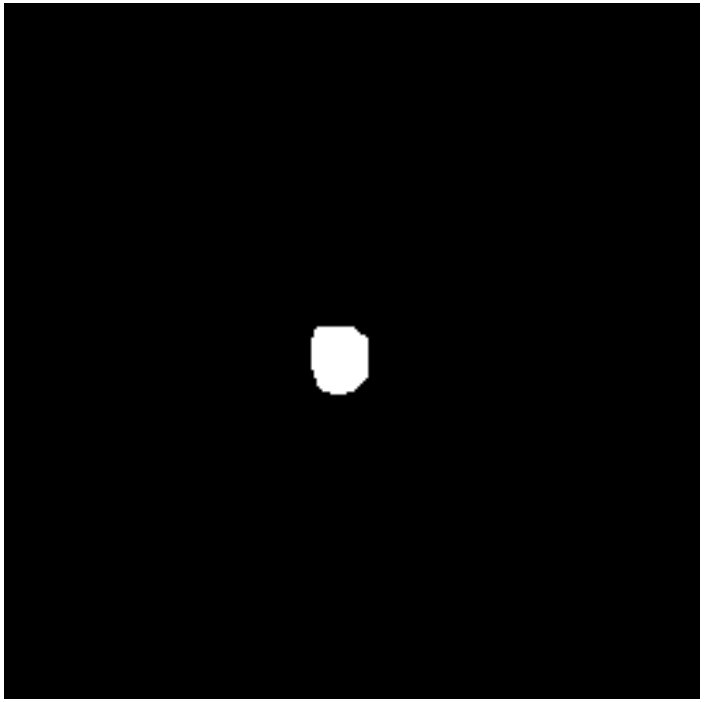


Real



Full FFT
(Phase in Color)

FFT Image demo



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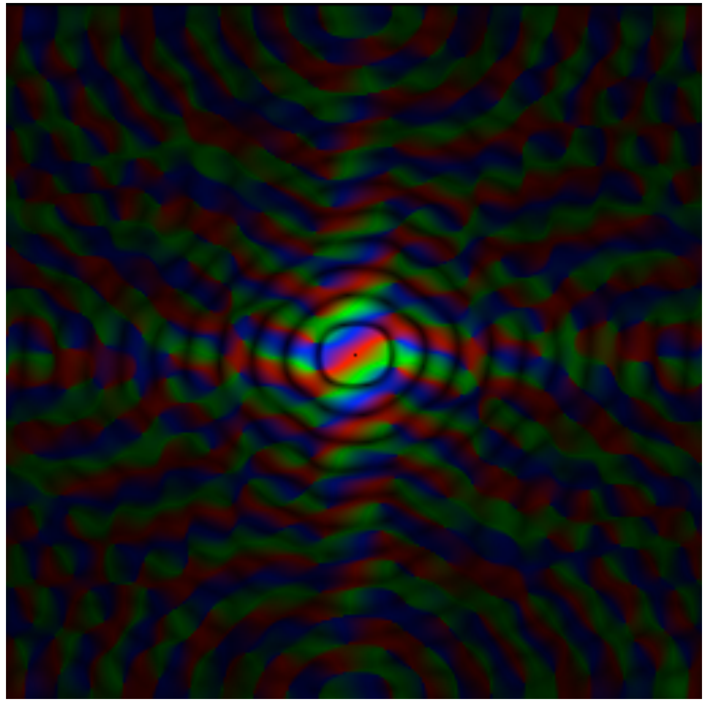
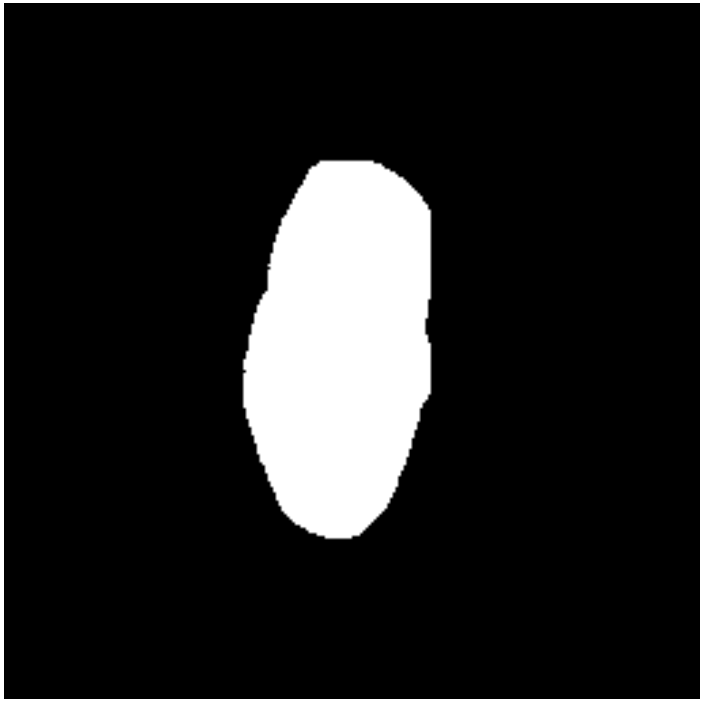


Full FFT
(Phase in Color)

FFT Image demo



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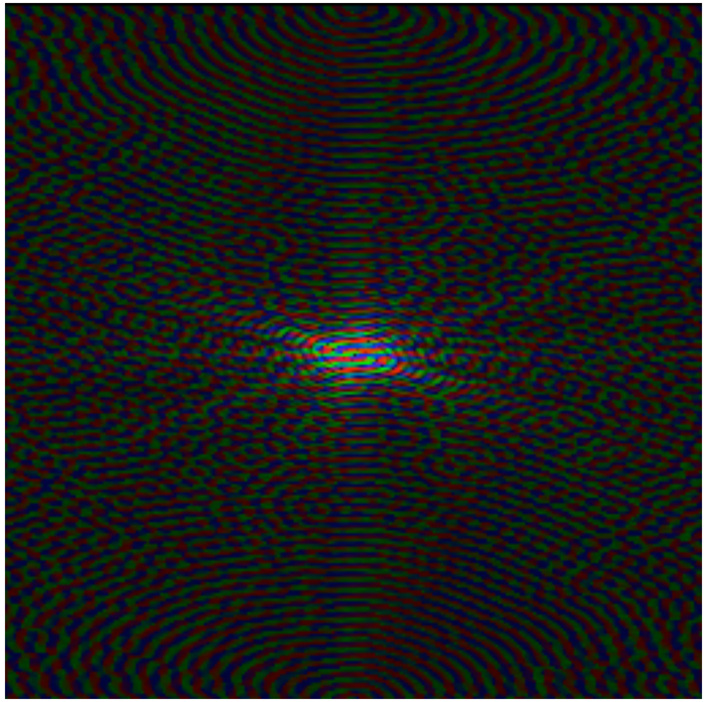
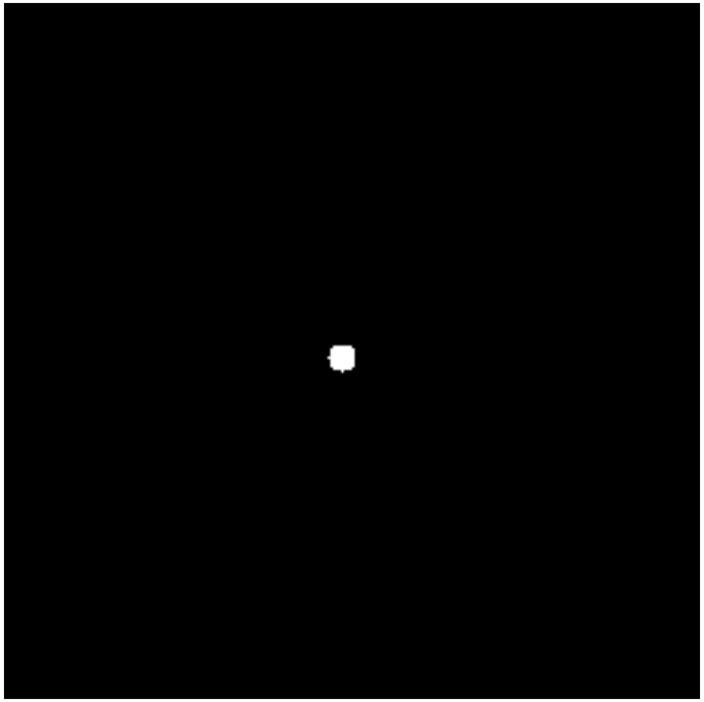


Full FFT
(Phase in Color)

FFT Image demo



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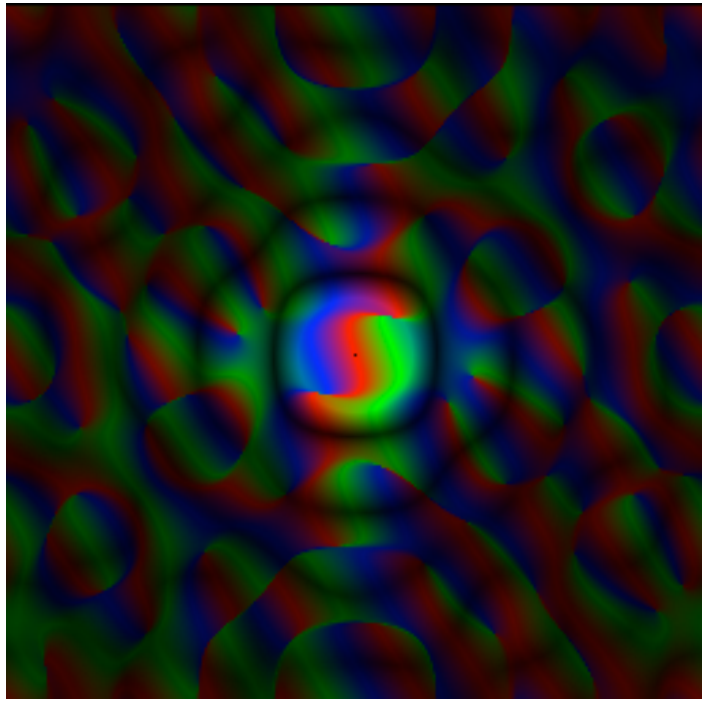
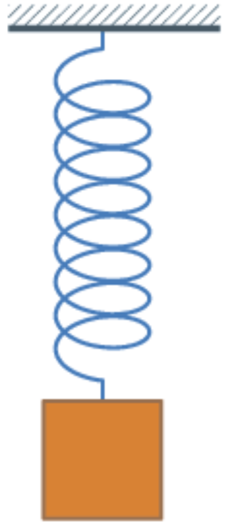


Full FFT
(Phase in Color)

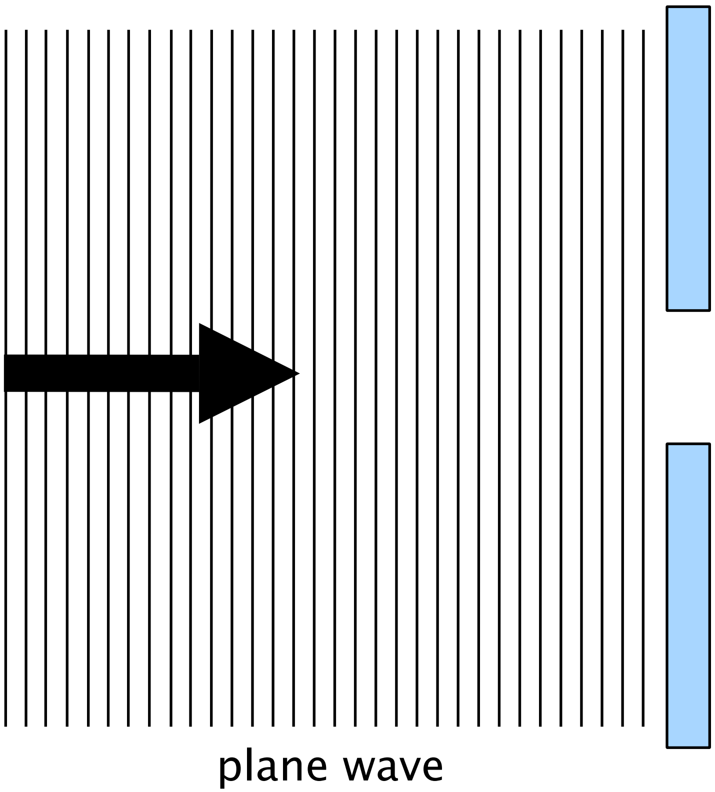
Resonance

- LC circuit (radio tuner)
- Musical instrument
- Harmonic oscillator



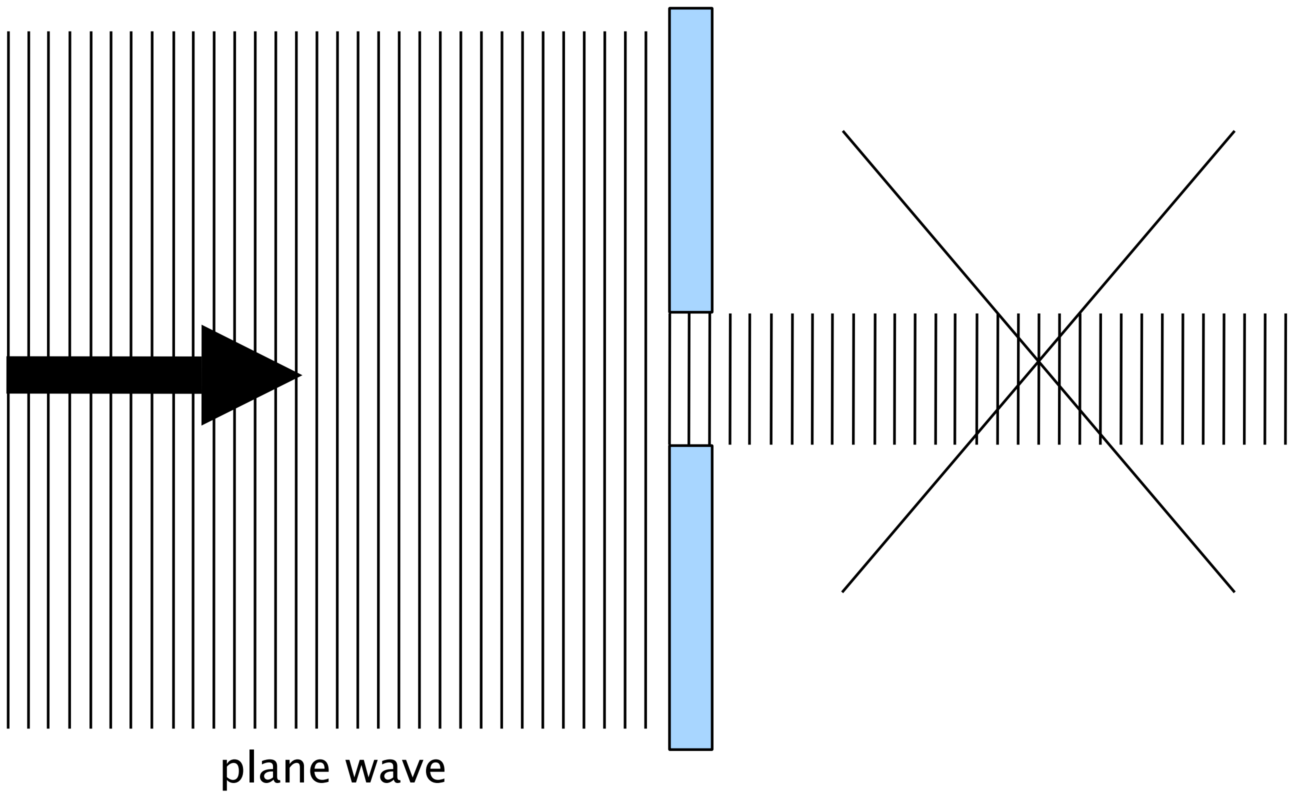
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



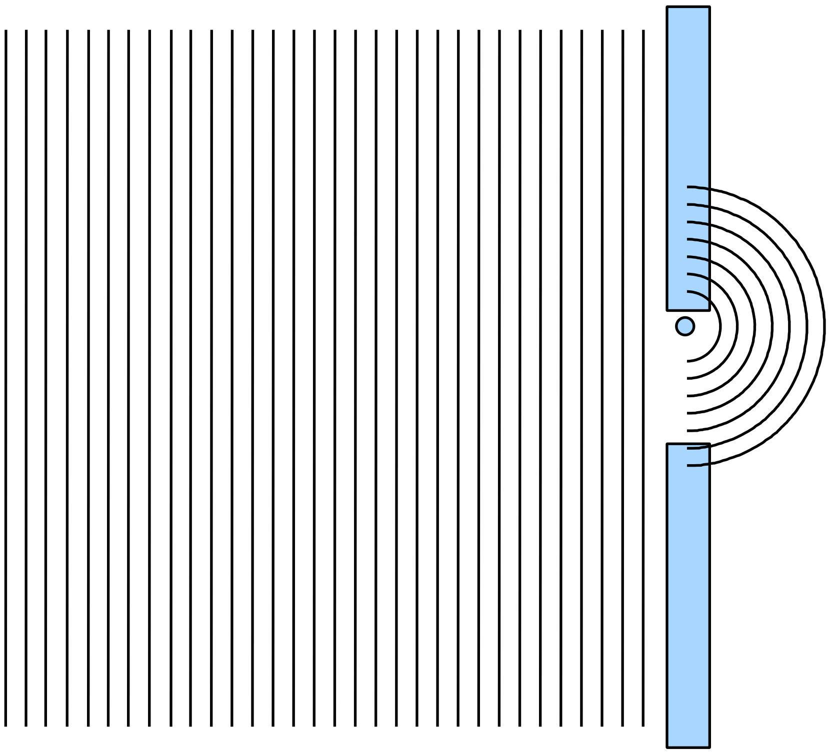
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



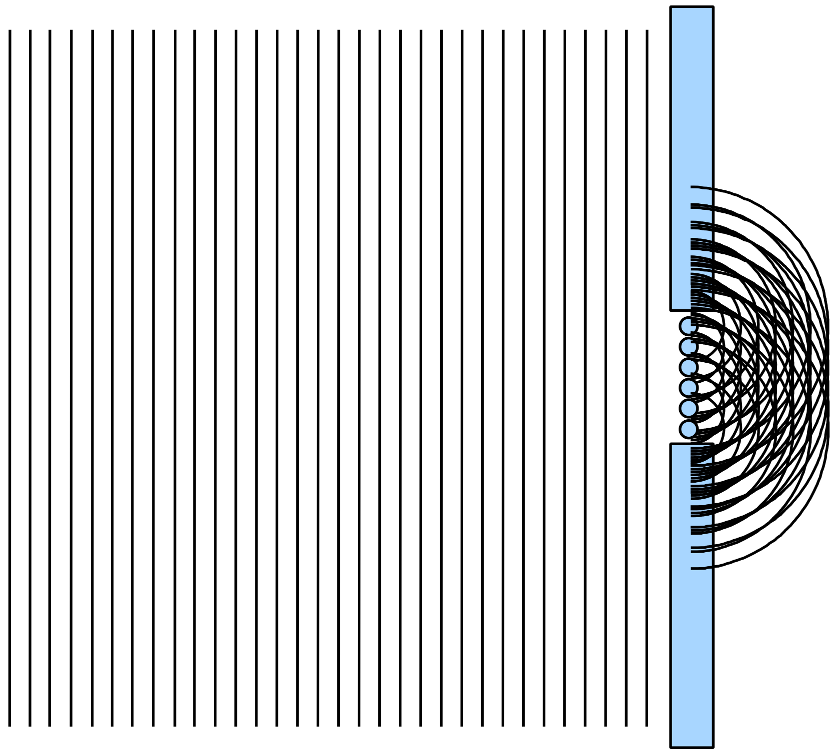
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



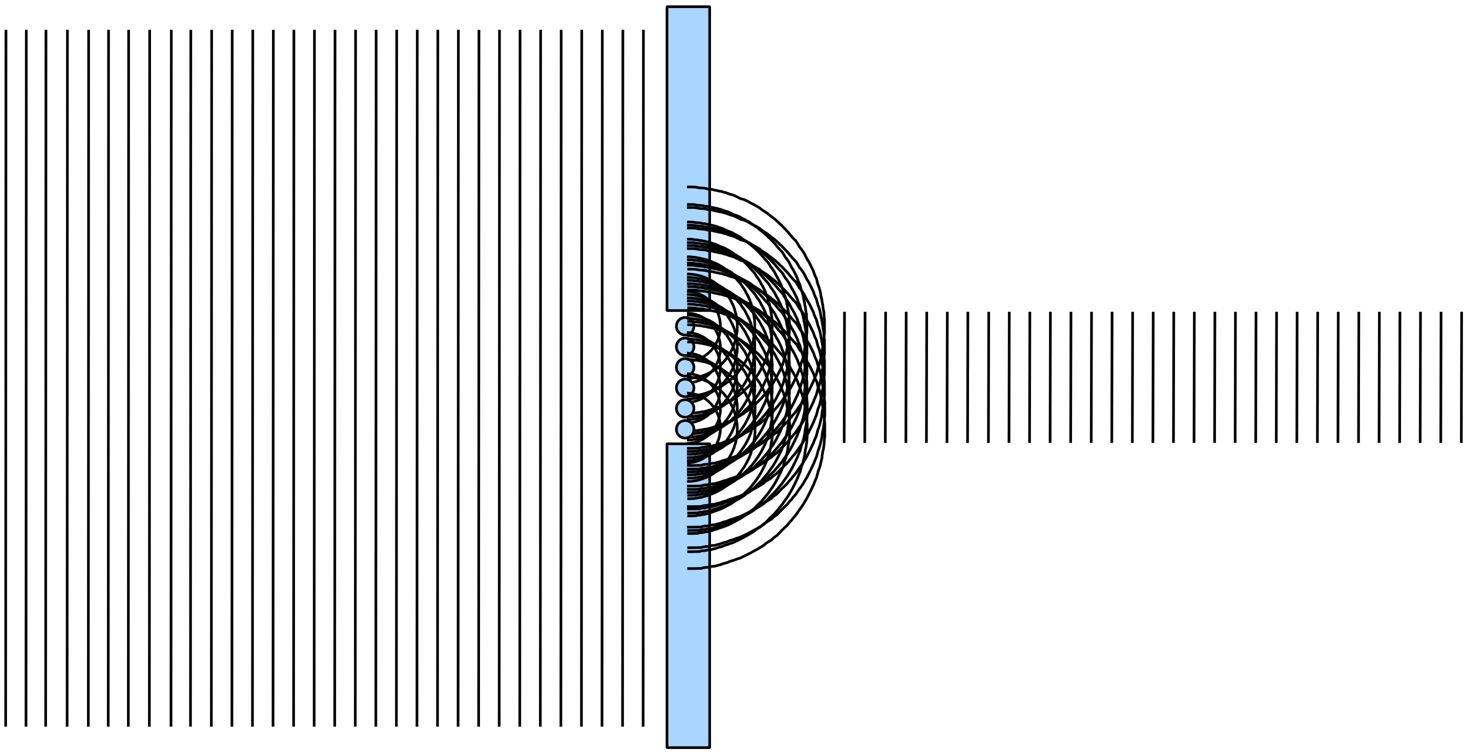
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



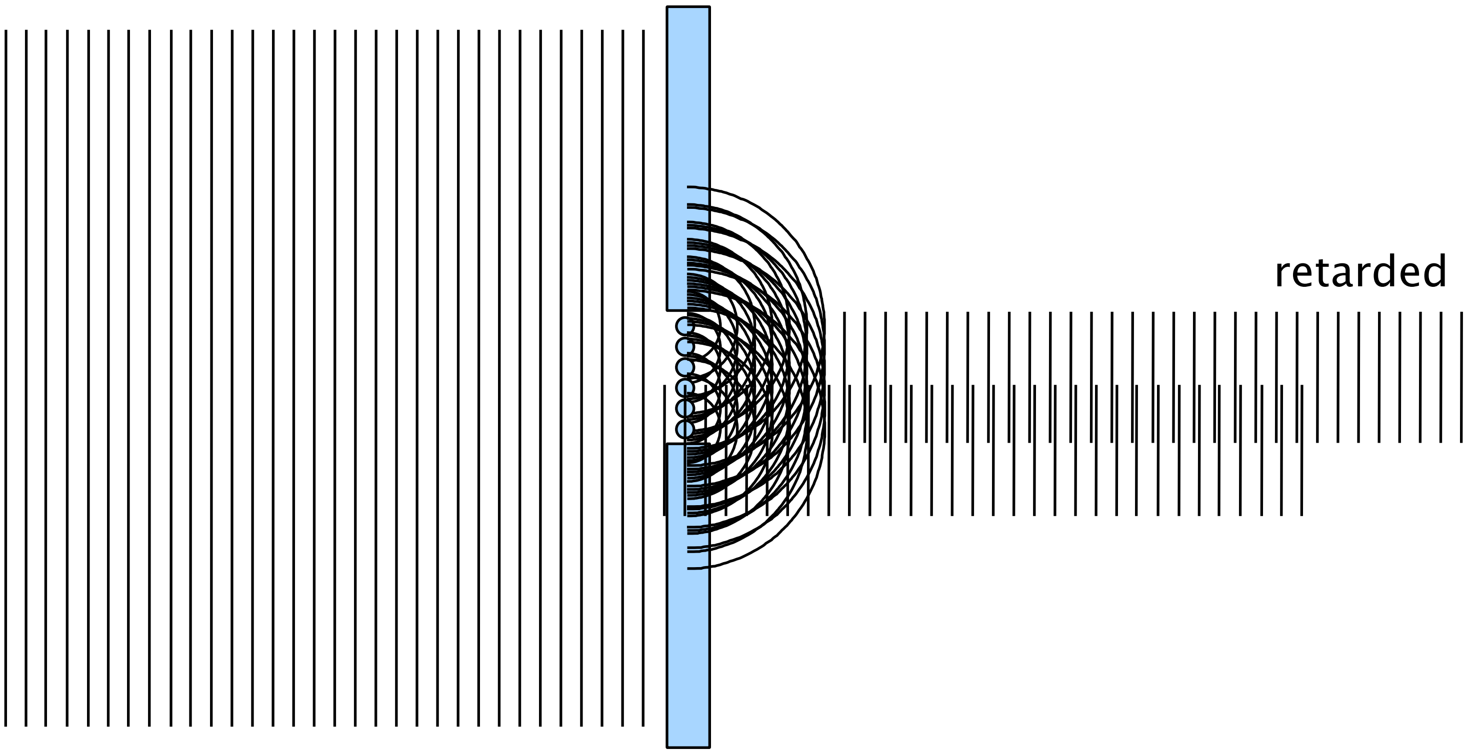
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



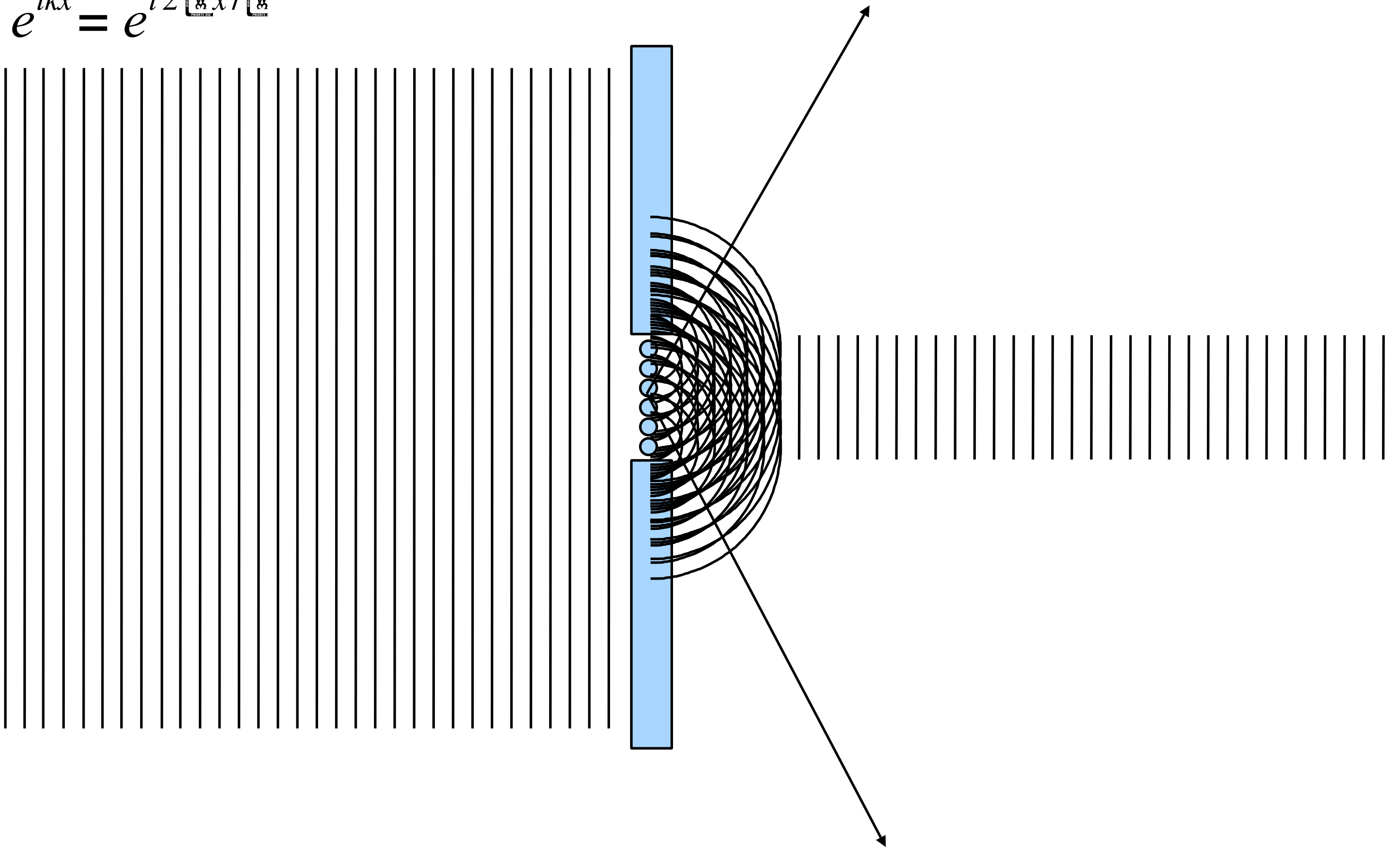
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



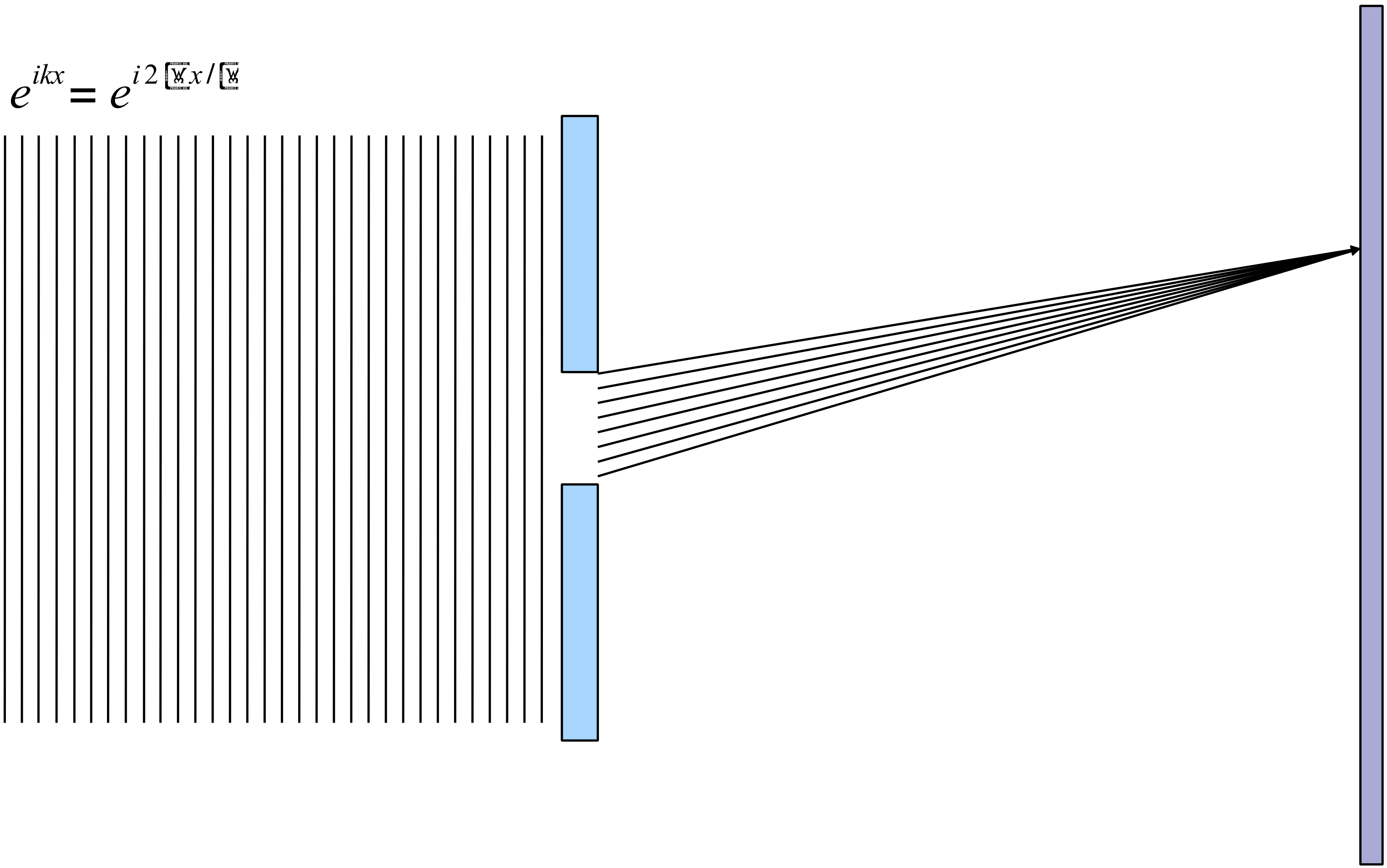
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



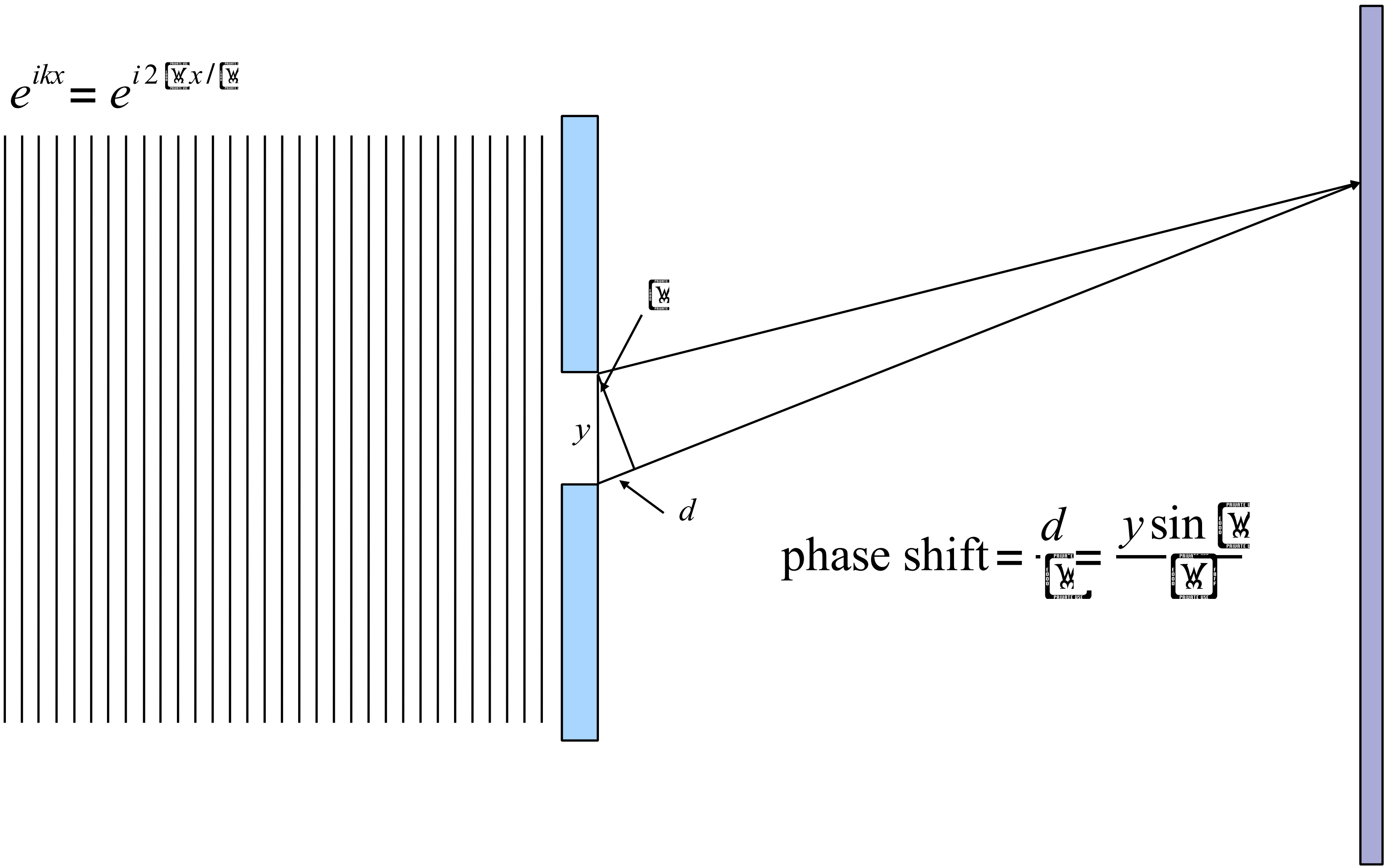
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



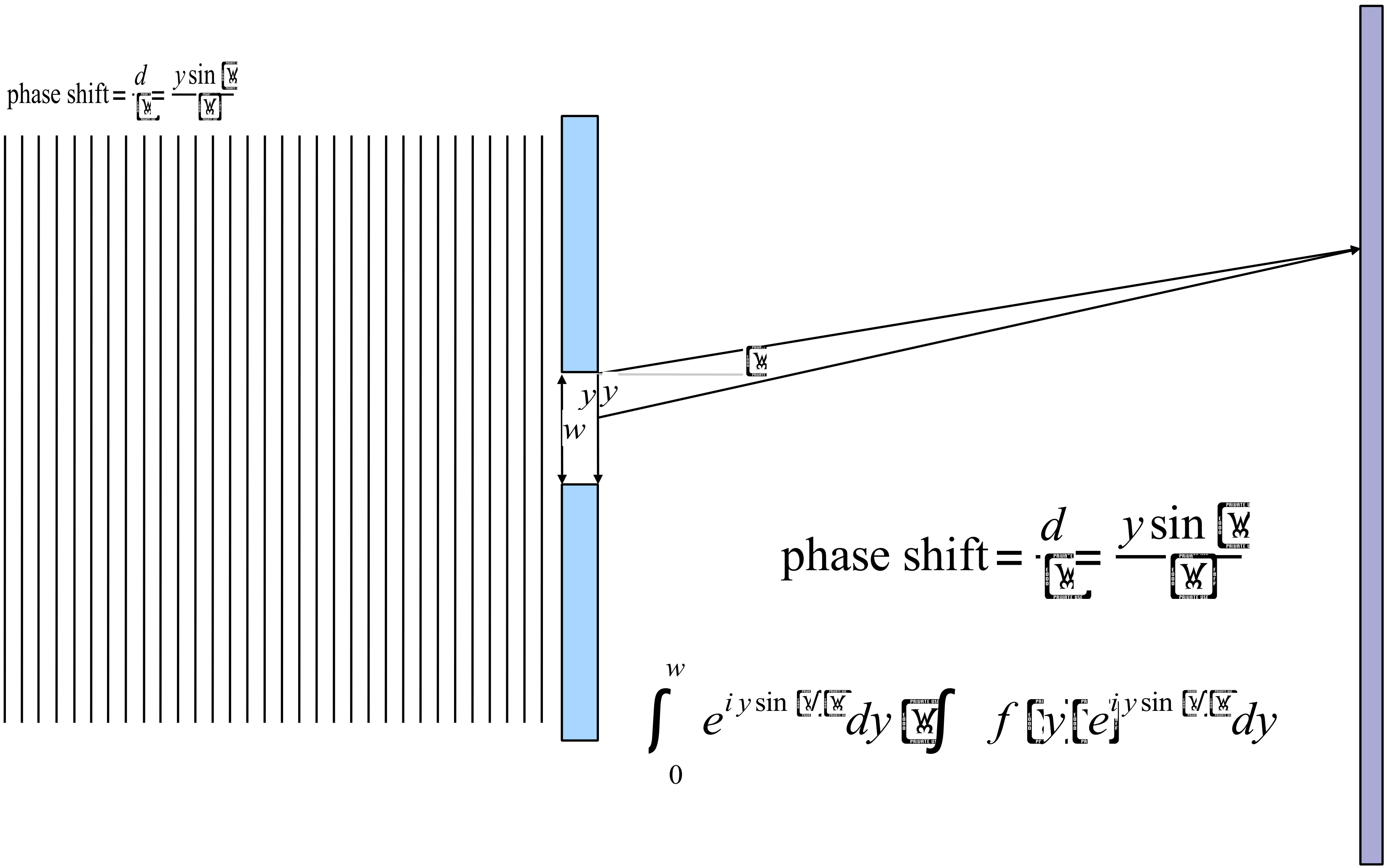
Single Slit Experiment

$$e^{ikx} = e^{i2\pi x/\lambda}$$



$$\text{phase shift} = \frac{d}{\lambda} = \frac{y \sin\theta}{\lambda}$$

Single Slit Experiment



$$\text{phase shift} = \cdot\frac{d}{\square} = \frac{y\sin\square}{\square}$$

$$\text{phase shift} = \cdot\frac{d}{\square} = \frac{y\sin\square}{\square}$$

$$\int_0^w e^{i\,y\sin\square/\square}\,dy \;\square\; \int f(y)\, e^{i\,y\sin\square/\square}\,dy$$

Test Image

Image Filtration
Gaussian Lowpass

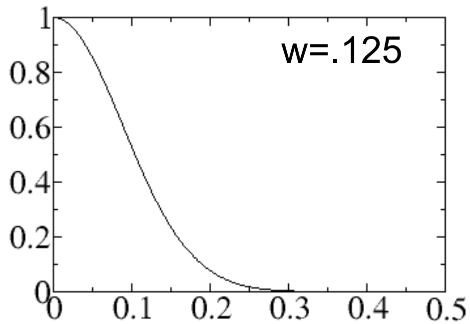


Image Filtration
Sharp Lowpass

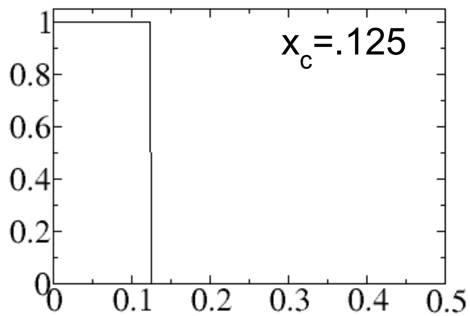


Image Filtration
Sharp Lowpass

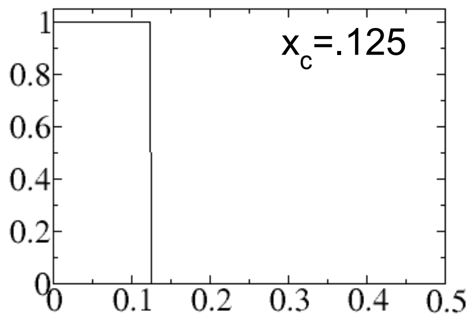


Image Filtration
Butterworth Lowpass

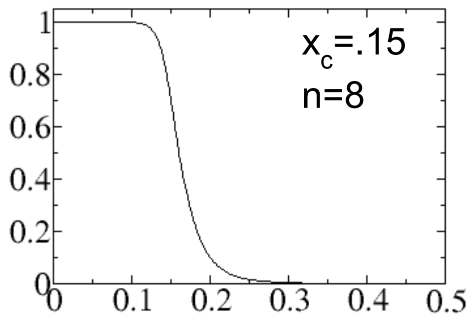
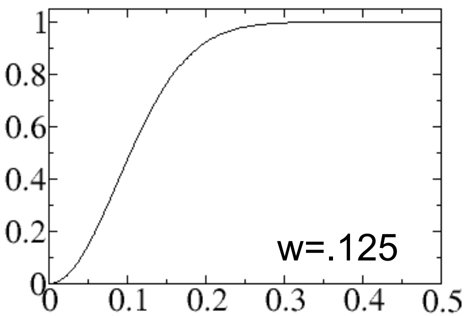
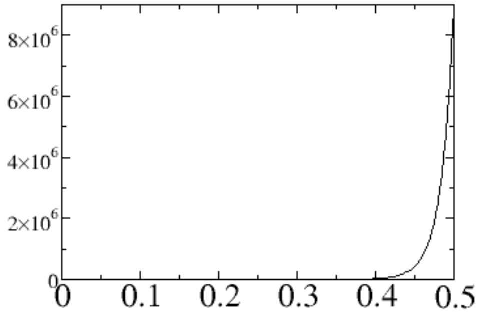


Image Filtration
Gaussian Highpass

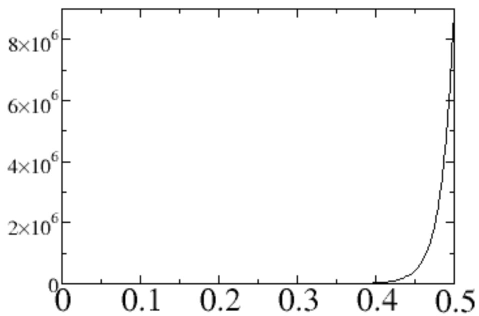


Deconvolution

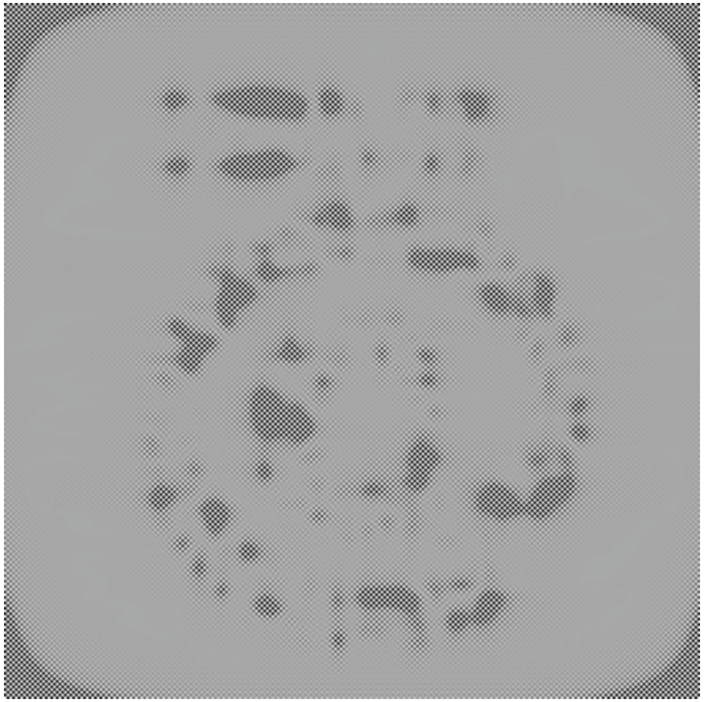
Deconvolution



Deconvolution



From Discrete valued image



CTF Correction

Measured Image

Ideal Particle

Random Noise

$$\overline{M}(s,\theta) = \overline{F}(s,\theta)C(s)E(s) + \overline{N}(s,\theta)$$

$$C(s) = \sqrt{1-Q^2}\,\sin\gamma + Q\cos\gamma$$

$$\gamma = -\pi\left(\frac{1}{2}C_S\lambda^3 s^4 - \Delta Z\lambda s^2\right)$$

$$E(s) = e^{-Bs^2}$$

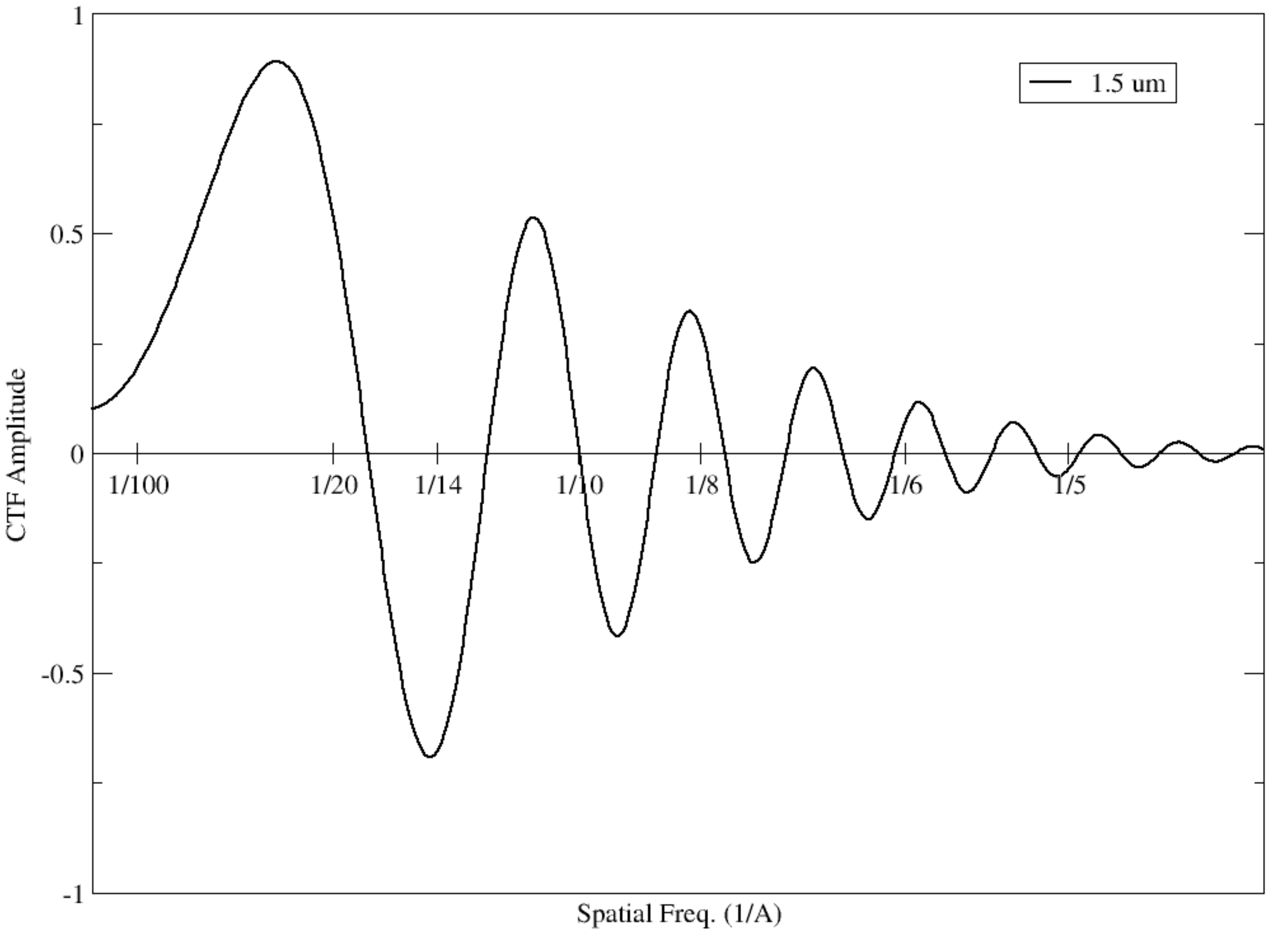
CTF Correction

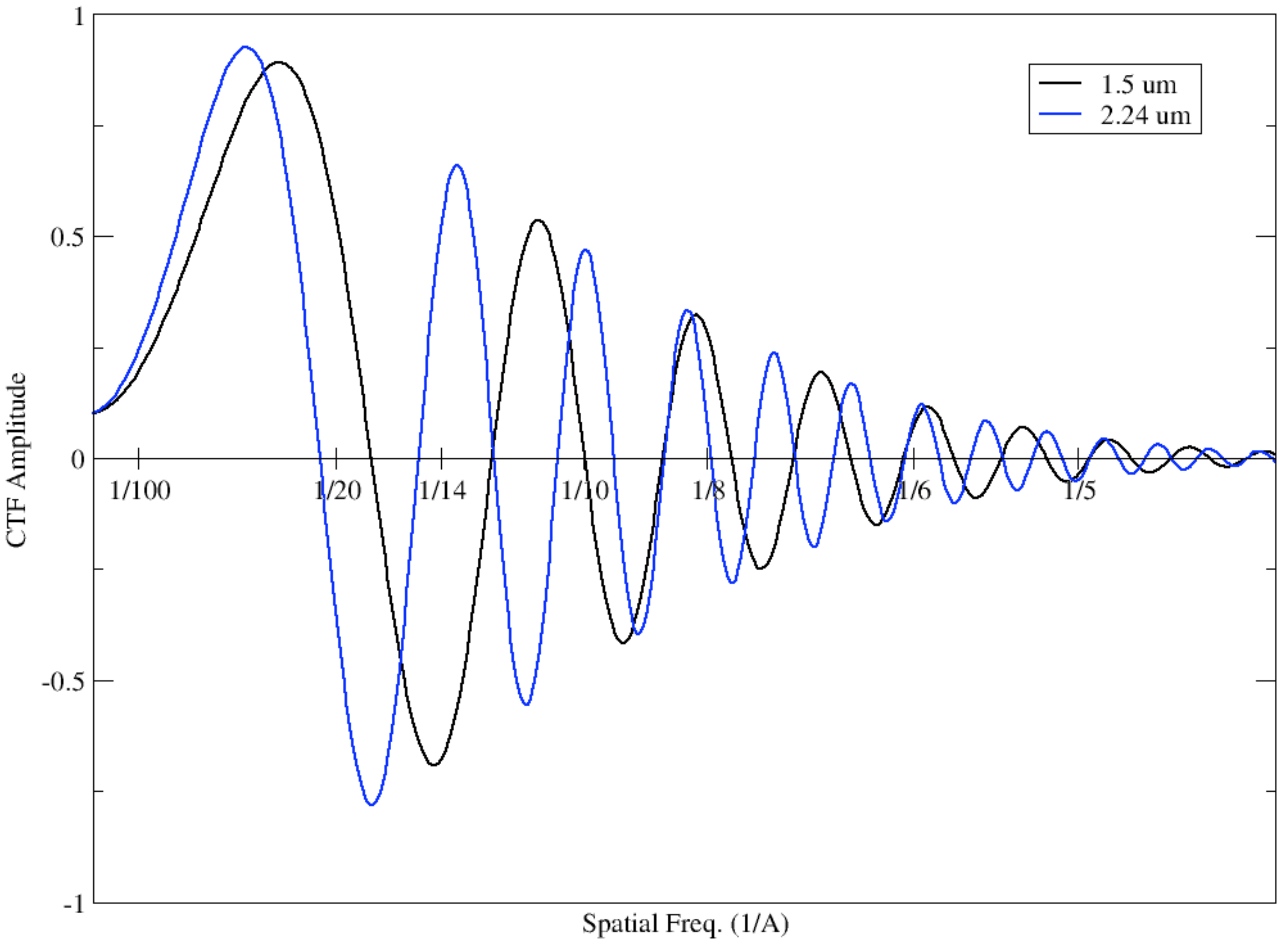
$$\overline{M}(s,\theta) = \overline{F}(s,\theta)C(s)E(s) + \overline{N}(s,\theta)$$

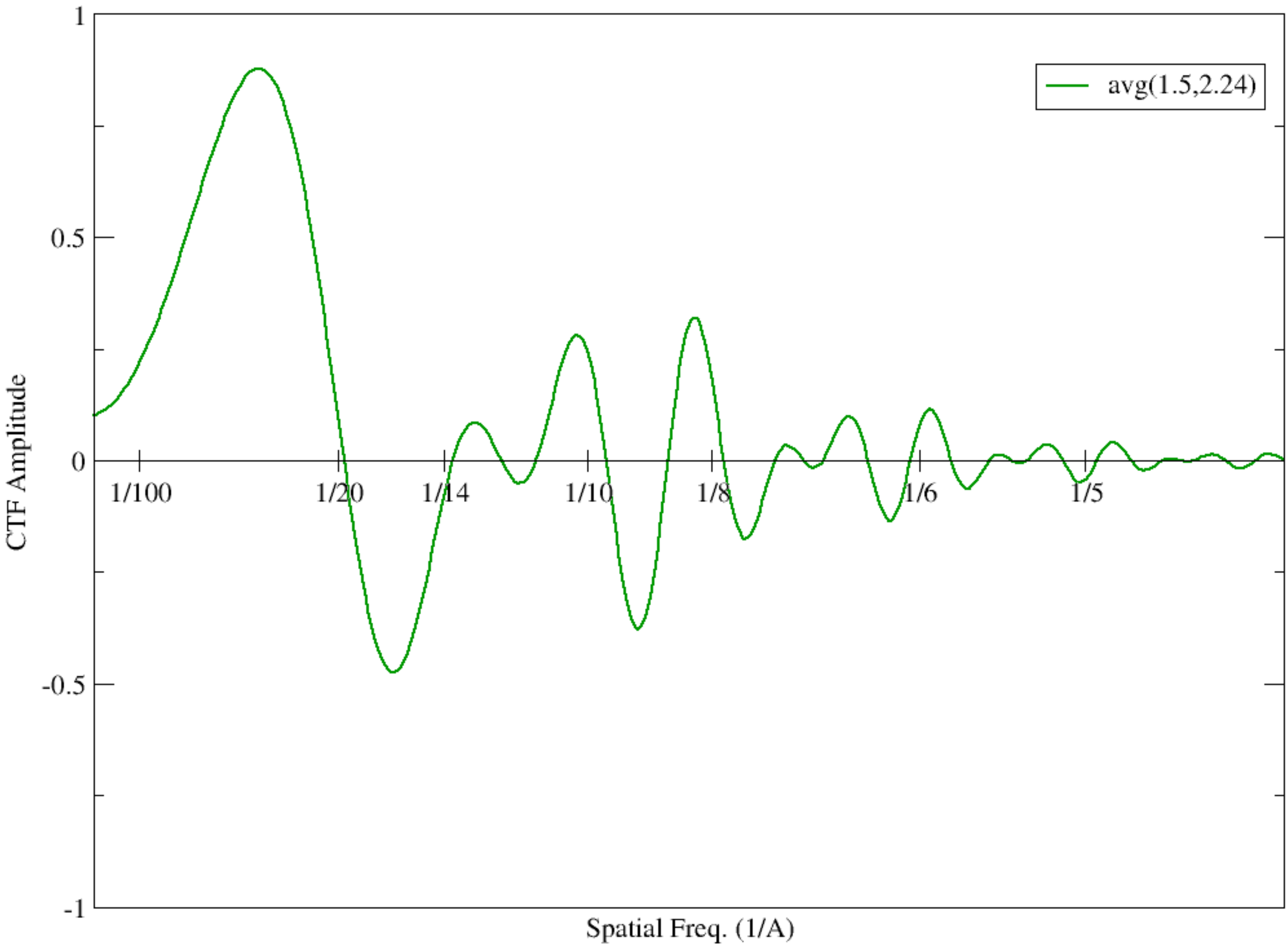
$$C(s) = \sqrt{1-Q^2}\sin\gamma + Q\cos\gamma$$

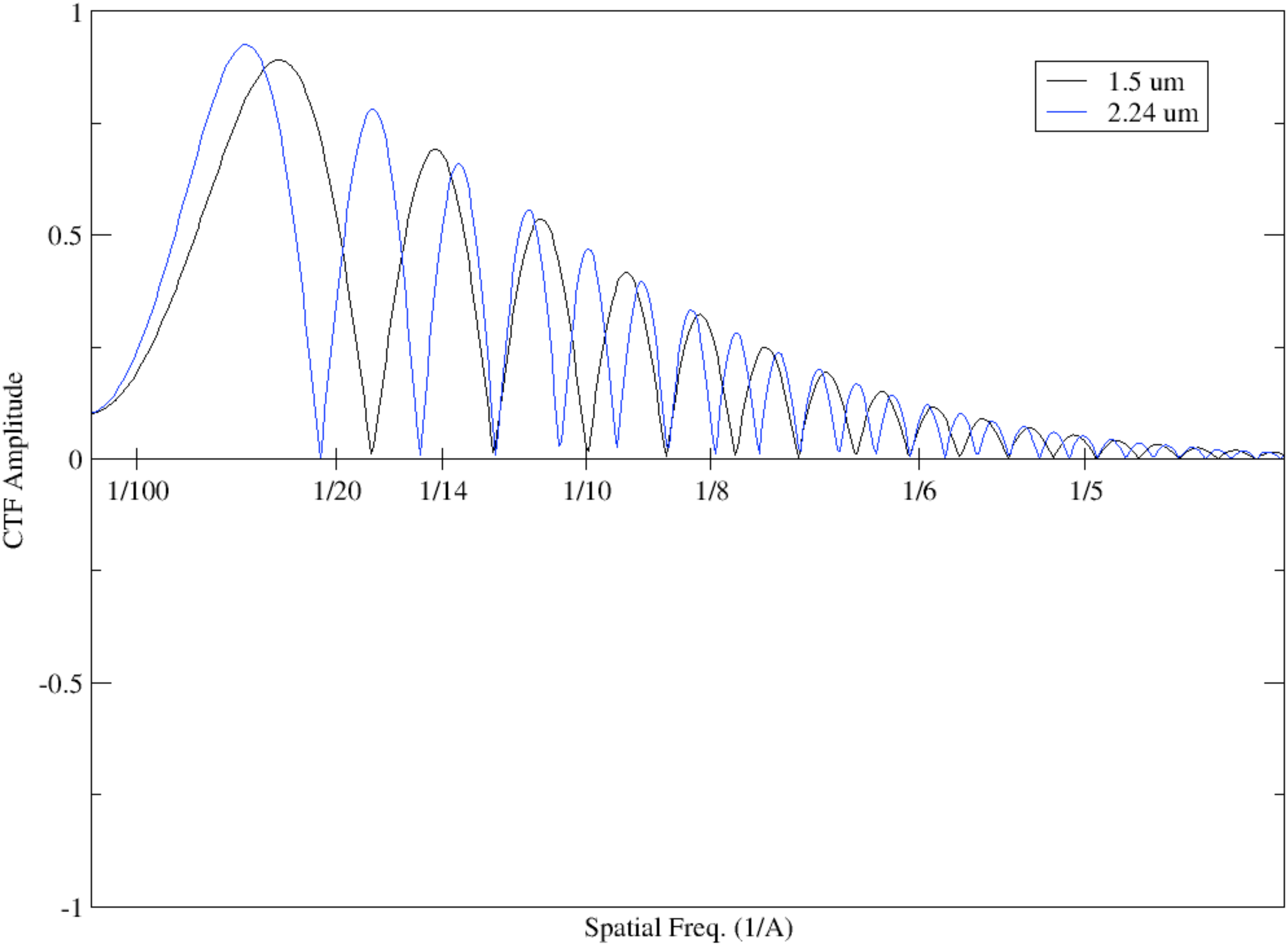
$$\gamma = -\pi\left(\frac{1}{2}C_S\lambda^3 s^4 - \Delta Z\lambda s^2\right)$$

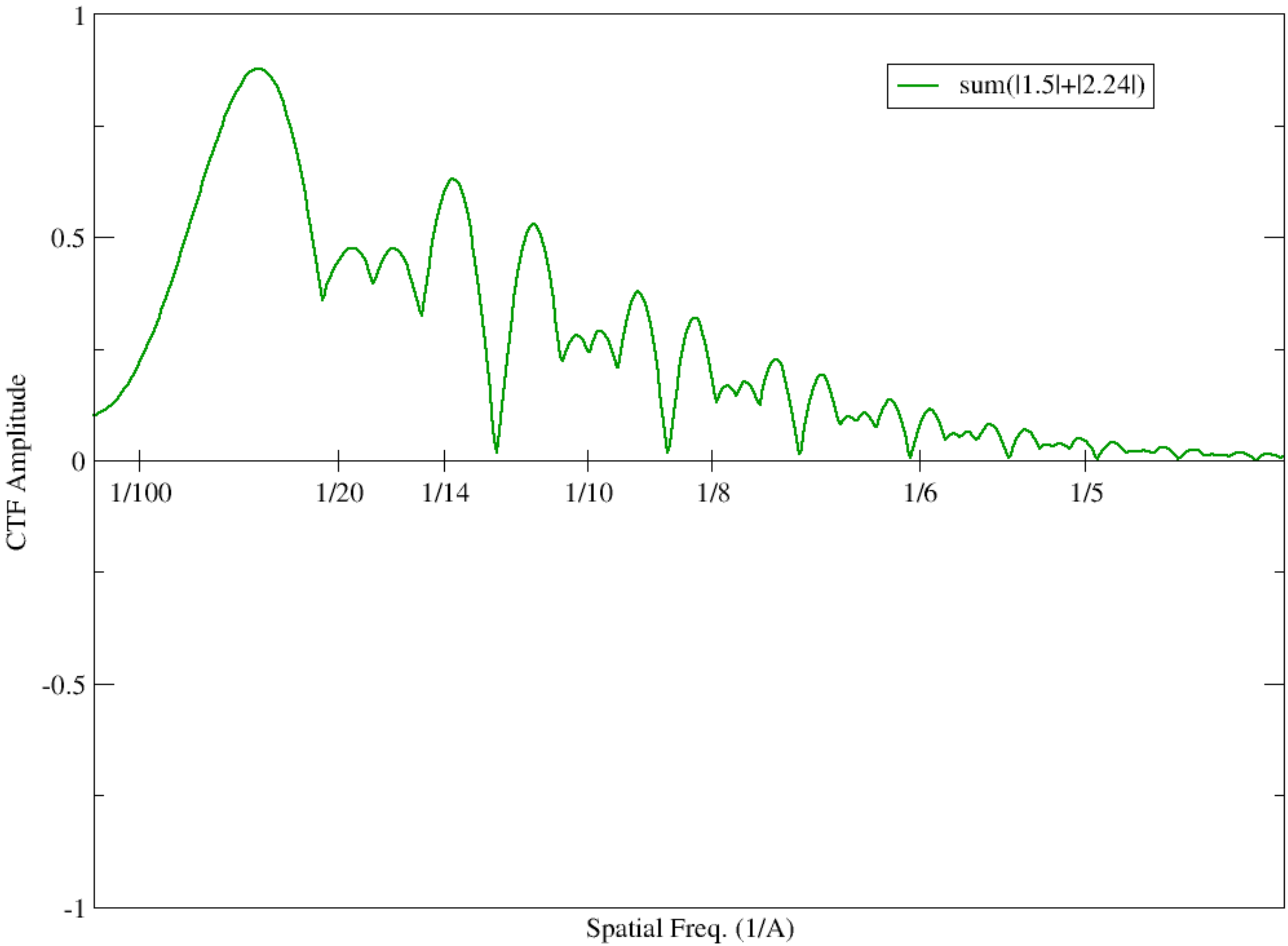
$$E(s) = e^{-Bs^2}$$

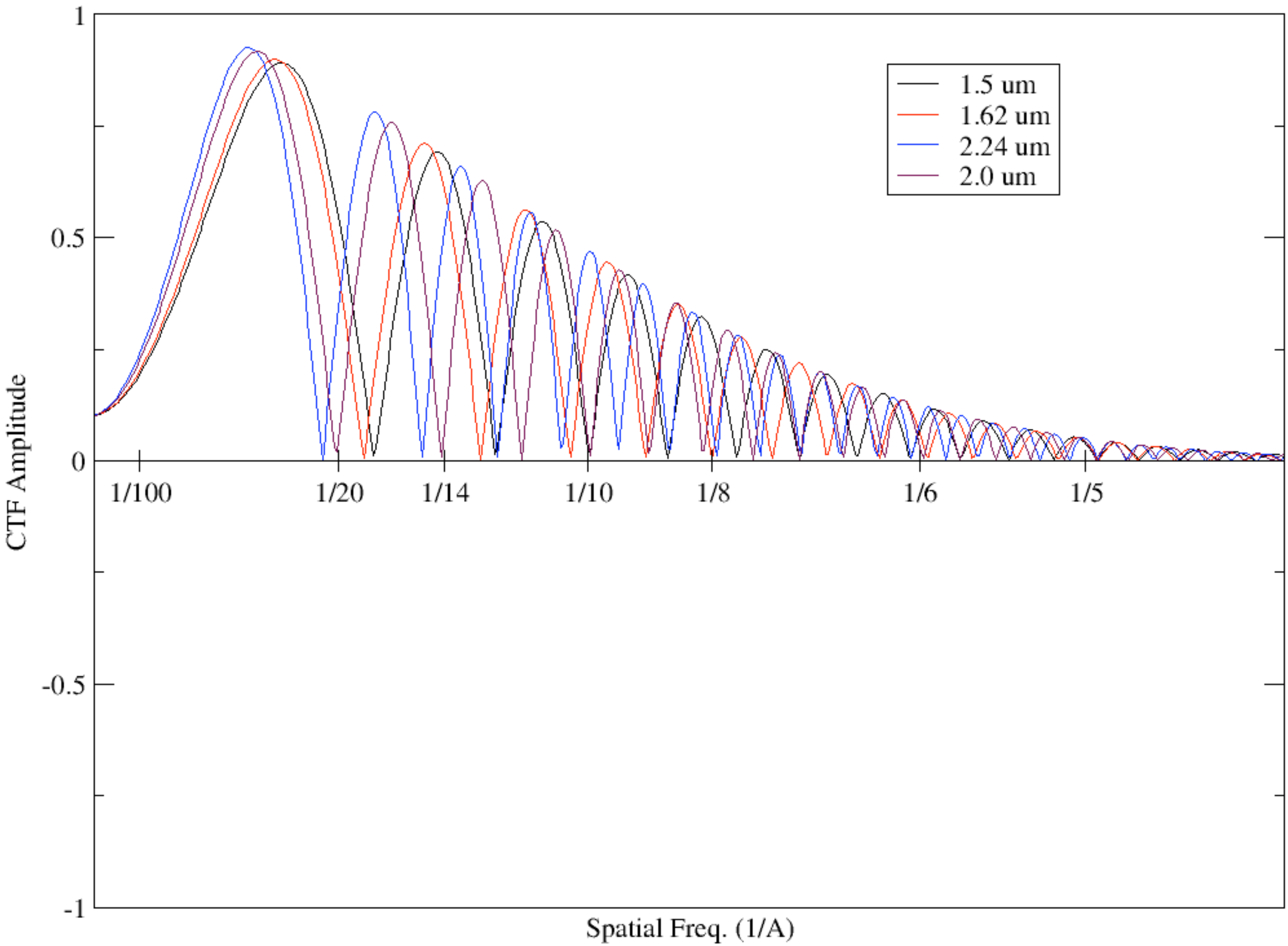

1.5 um
CTF Amplitude
1
0.5
0
-0.5
-1
1/100
1/20
1/14
1/10
1/8
1/6
1/5
Spatial Freq. (1/A)

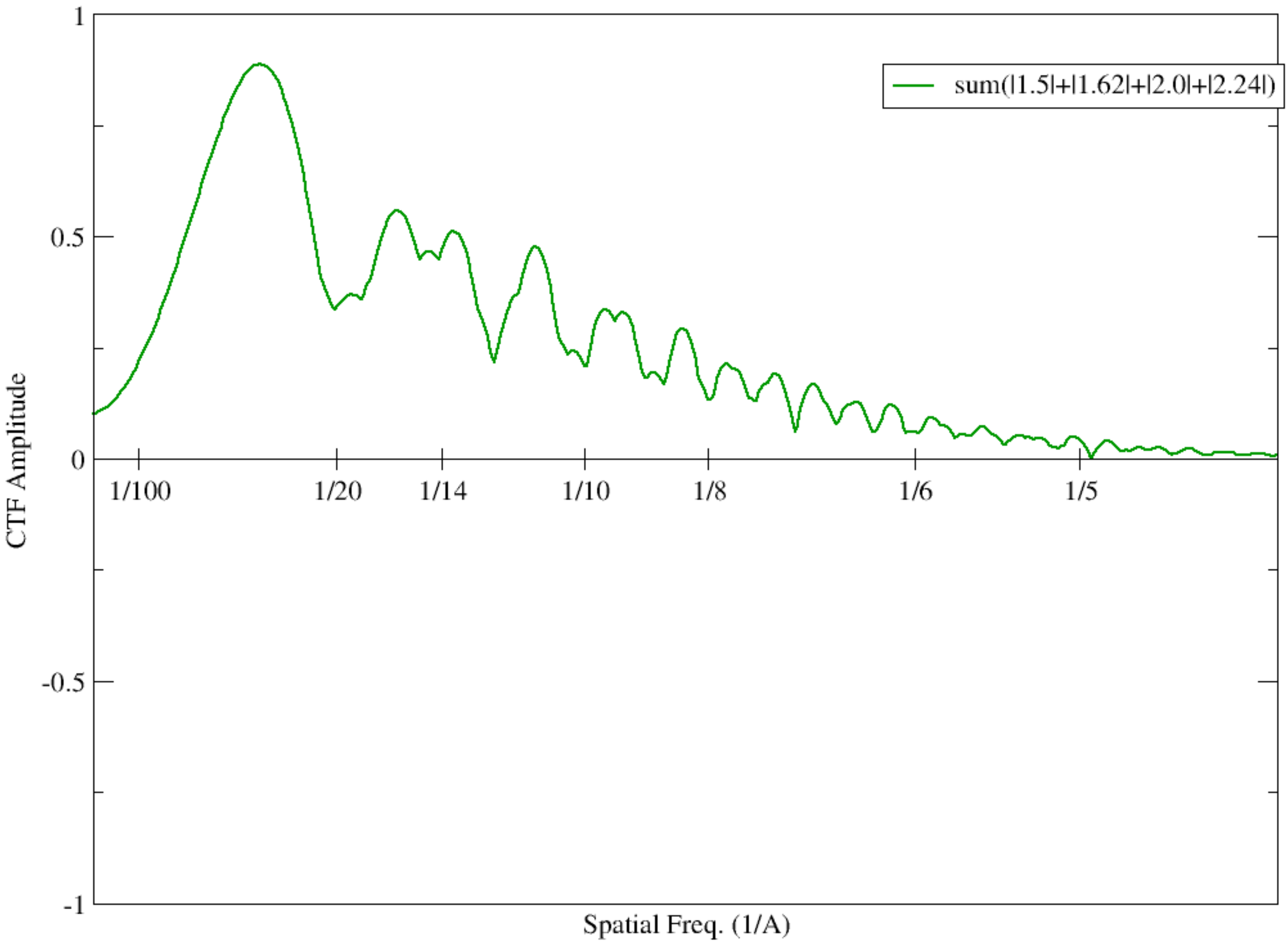

1.5 um
2.24 um
1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
Spatial Freq. (1/A)


avg(1.5,2.24)
1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
Spatial Freq. (1/A)


1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
Spatial Freq. (1/A)
1.5 um
2.24 um


sum(|1.5|+|2.24|)
1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
Spatial Freq. (1/A)


1.5 um
1.62 um
2.24 um
2.0 um
1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
Spatial Freq. (1/A)



sum(|1.5|+|1.62|+|2.0|+|2.24|)
1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
Spatial Freq. (1/A)

CTF Correction

$$\overline{M}(s,\theta) = \overline{F}(s,\theta)C(s)E(s) + \overline{N}(s,\theta)$$

$$C(s) = \sqrt{1-Q^2}\sin\gamma + Q\cos\gamma$$

$$\gamma = -\pi\left(\frac{1}{2}C_S\lambda^3 s^4 - \Delta Z\lambda s^2\right)$$

$$E(s) = e^{-Bs^2}$$

$$N(s)^2 = n_1 e^{n_2 s + n_3 s^2 + n_4\sqrt{s}}$$

$$M(s)^2 = F(s)^2 C(s)^2 E(s)^2 + N(s)^2$$

CTF Correction

Reconstruction

Weight

Measured image

$$\overline{T}(s,\theta) = \sum_i k_i \overline{M}_i(s,\theta)$$

$$k_i = ?$$

- Maximize SNR of $T(s,\theta)$
- Minimize RMSD between T and F

$$\sqrt{\sum_{x,y} (t(x,y) - f(x,y))^2}$$

CTF Correction

Wiener Filter | CTF Correction | SNR Weight

$$\overline{T}(s,\theta)=\frac{F^2(s)R(s)}{1+F^2(s)R(s)}\sum_i \frac{1}{C_i(s)E_i(s)}\frac{R_i(s)}{R(s)}\overline{M}_i(s,\theta)$$

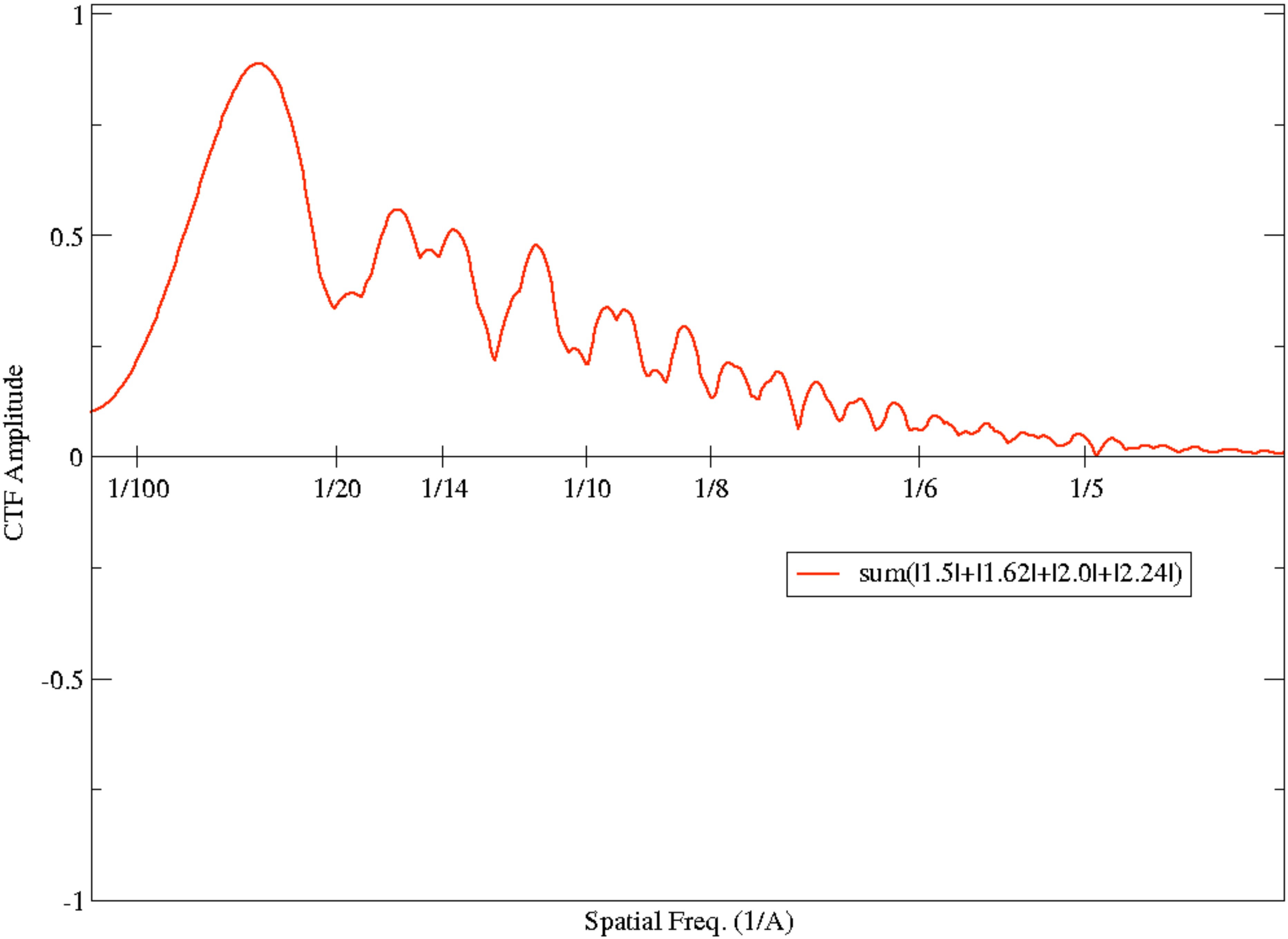
$$R_i(s)=\frac{C_i^2(s)E_i^2(s)}{N_i^2(s)} \qquad R(s)=\sum_i \frac{C_i^2(s)E_i^2(s)}{N_i^2(s)}$$

CTF Correction

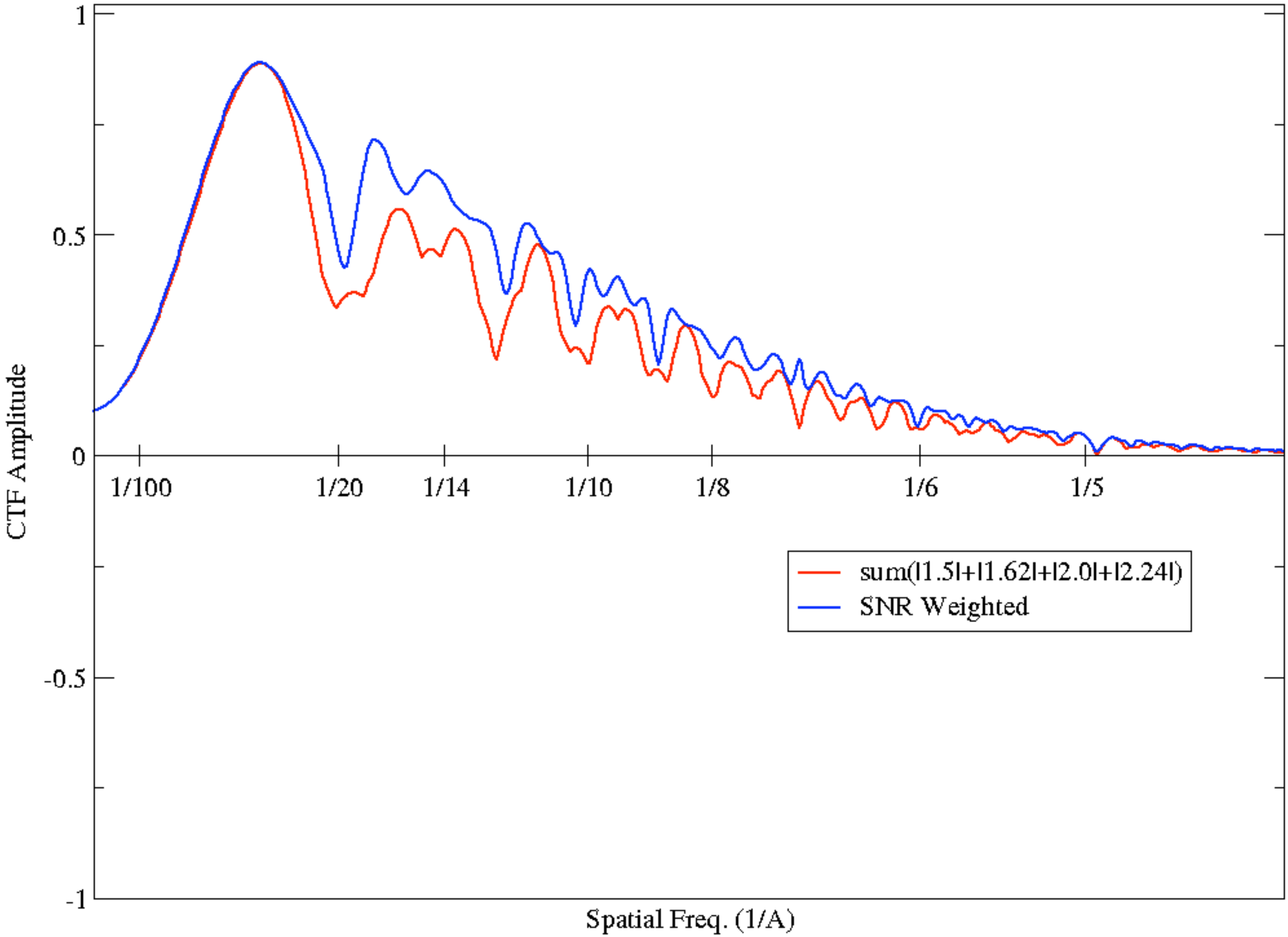
Wiener Filter		CTF Correction	SNR Weight

$$\overline{T}(s,\theta)=\frac{F^2(s)R(s)}{1+F^2(s)R(s)}\sum_i \frac{1}{C_i(s)E_i(s)}\frac{R_i(s)}{R(s)}\overline{M}_i(s,\theta)$$

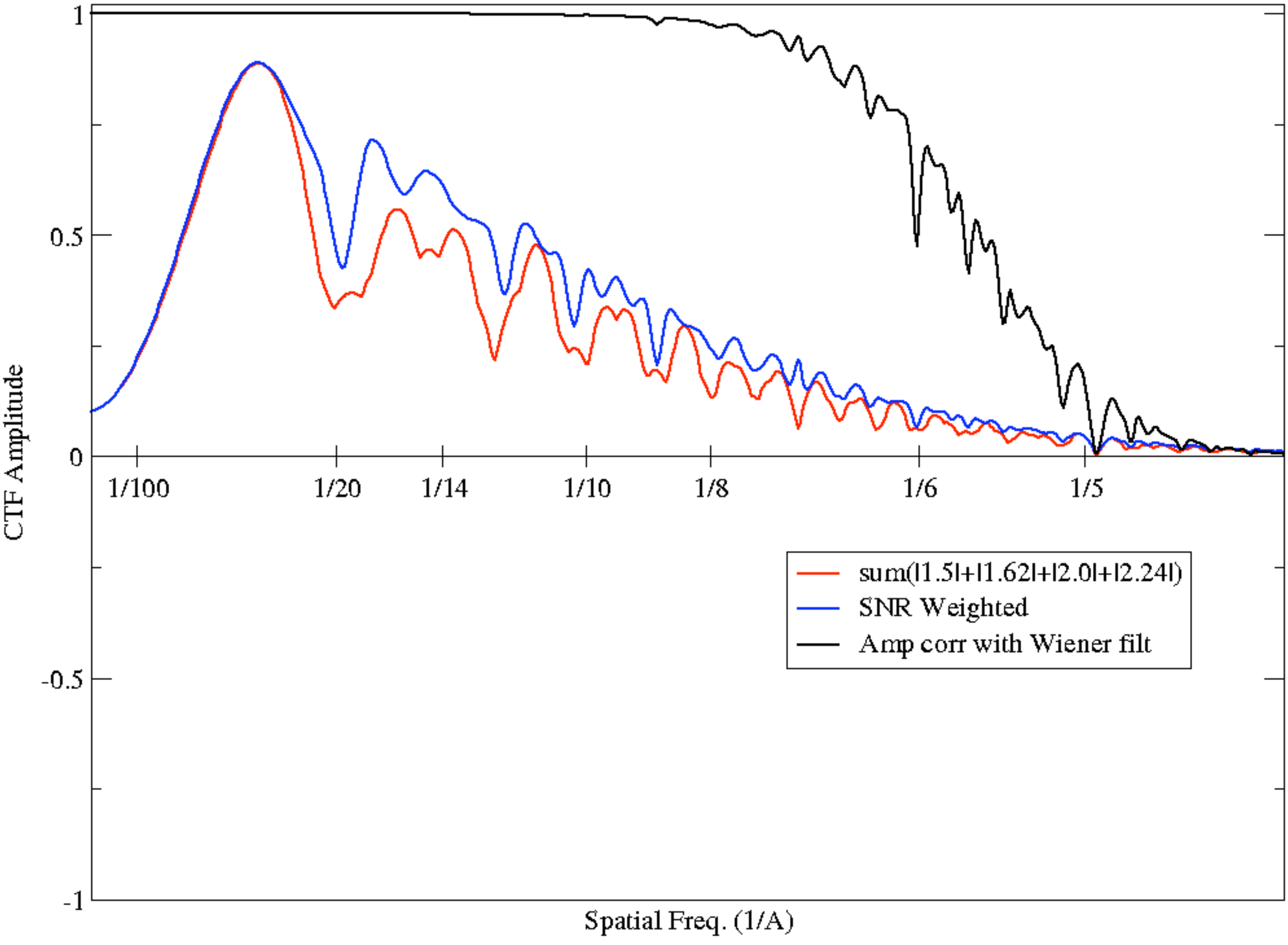
Note that this factor depends on ALL of the data and means you cannot 'precorrect' the data then do a reconstruction. You can phase-flip in preprocessing, but Wiener filtration and weighting depend on having all of the data at once.



1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
sum(|1.5|+|1.62|+|2.0|+|2.24|)
Spatial Freq. (1/A)



1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
sum(|1.5|+|1.62|+|2.0|+|2.24|)
SNR Weighted
Spatial Freq. (1/A)



1
0.5
0
-0.5
-1
CTF Amplitude
1/100
1/20
1/14
1/10
1/8
1/6
1/5
Spatial Freq. (1/A)
sum(|1.5|+|1.62|+|2.0|+|2.24|)
SNR Weighted
Amp corr with Wiener filt

CTF Correction

$$\overline{M}(s,\theta) = \overline{F}(s,\theta)C(s)E(s) + \overline{N}(s,\theta)$$

$$C(s) = \sqrt{1-Q^2}\sin\gamma + Q\cos\gamma$$

$$\gamma = -\pi\left(\frac{1}{2}C_S\lambda^3 s^4 - \Delta Z\lambda s^2\right)$$

$$E(s) = e^{-Bs^2}$$

$$N(s)^2 = n_1 e^{n_2 s + n_3 s^2 + n_4\sqrt{s}}$$

$$M(s)^2 = F(s)^2 C(s)^2 E(s)^2 + N(s)^2$$

8 Parameters

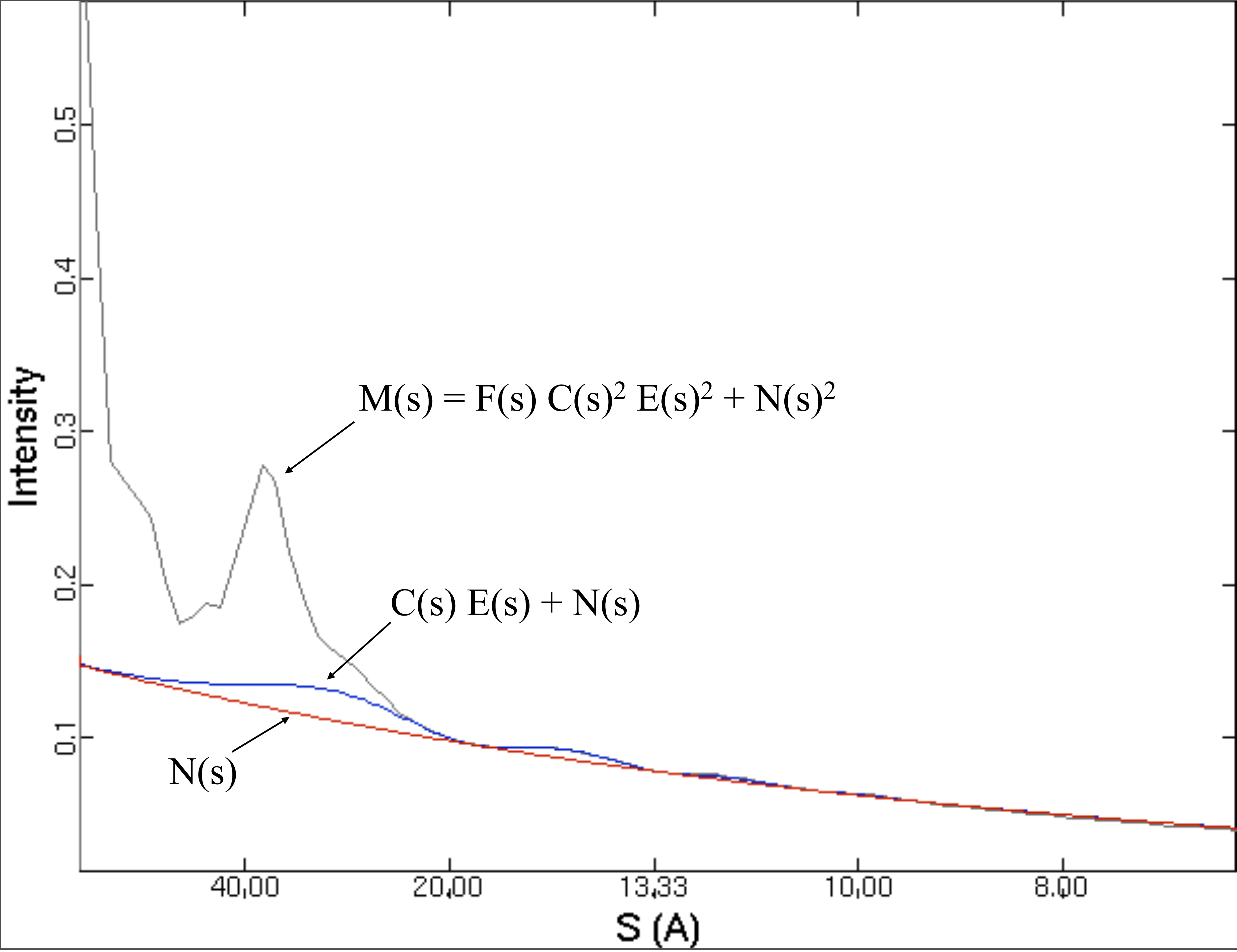
ΔZ - Defocus

Q - Amplitude Contrast

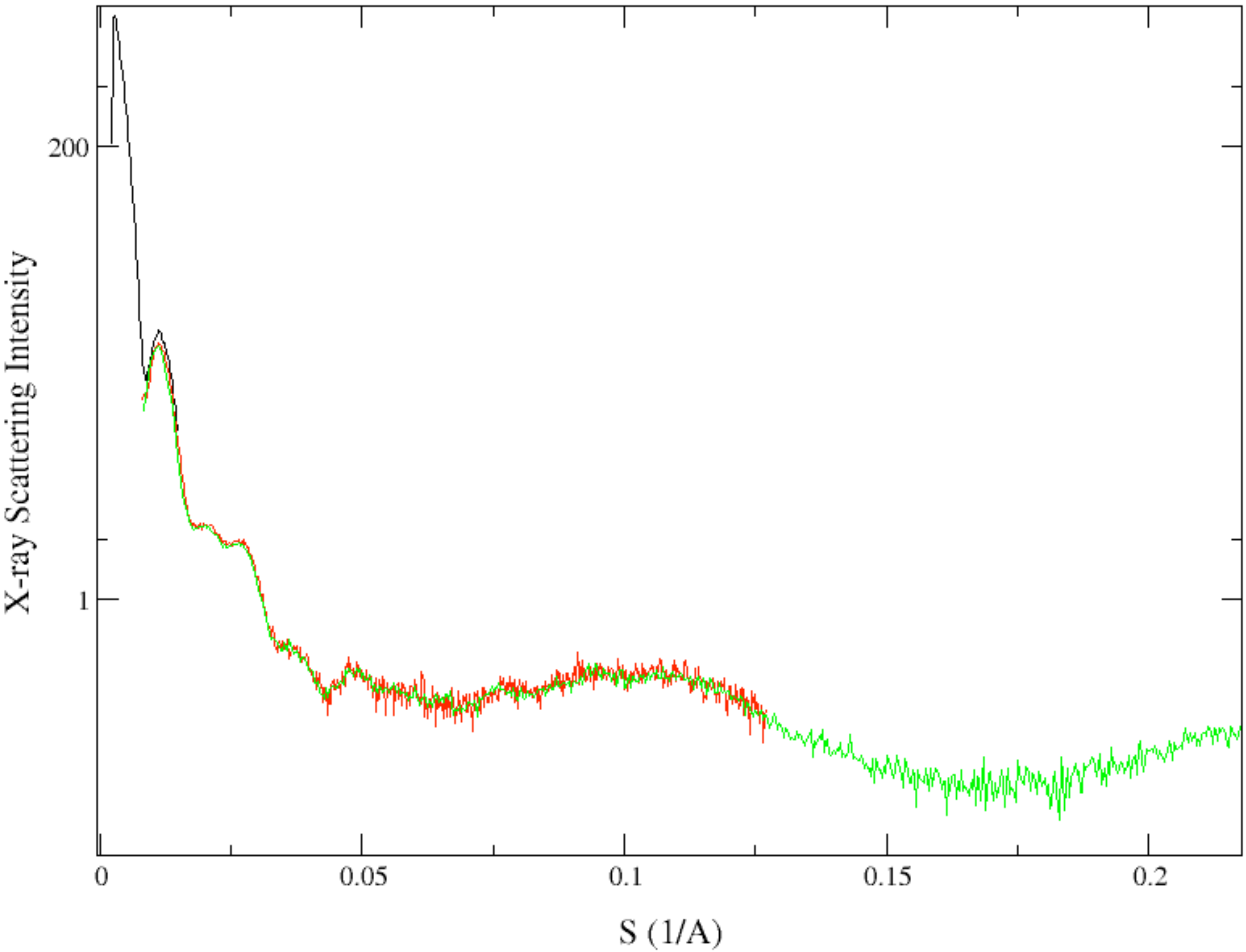
B - Gaussian Envelope Width

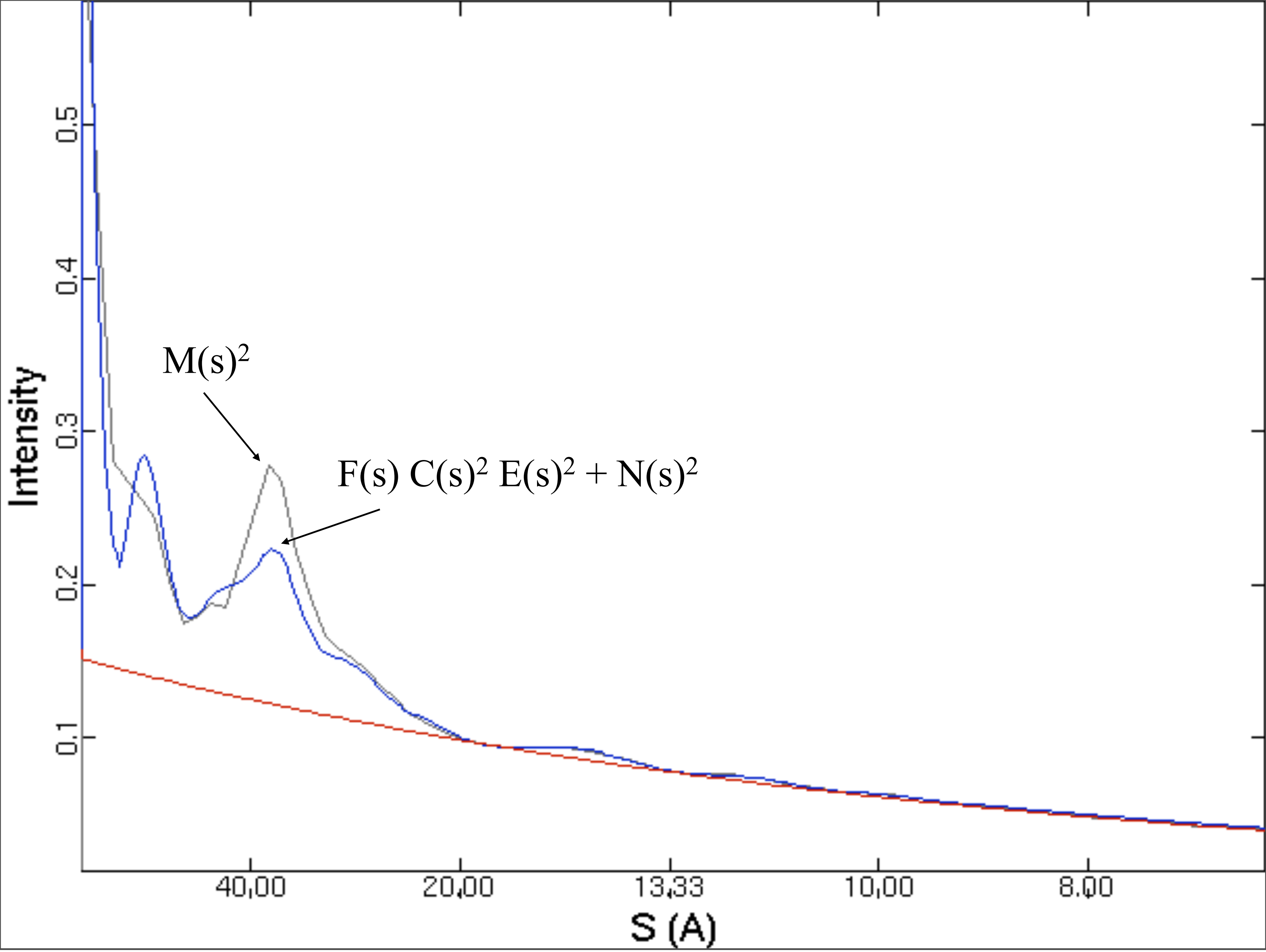
k - Signal Amplitude

$n_{1\text{-}4}$ - Noise Parameters



0.5
0.4
0.3
0.2
0.1
Intensity
M(s) = F(s) C(s)2 E(s)2 + N(s)2
C(s) E(s) + N(s)
N(s)
40,00
20,00
13,33
10,00
8,00
S (A)


200
1
X-ray Scattering Intensity
0
0.05
0.1
0.15
0.2
S (1/A)


M(s)2
F(s) C(s)2 E(s)2 + N(s)2
Intensity
0.5
0.4
0.3
0.2
0.1
40,00
20,00
13,33
10,00
8,00
S (A)