Theory of high resolution TEM

Lecture 15

Outline

Introductory level theory

- Weak-phase object approximation
- Contrast transfer function
- Envelope functions

Some advanced concepts

- Delocalization
- Using pass bands
- Focal series reconstruction
- Variable C_s Imaging

HRTEM

general idea

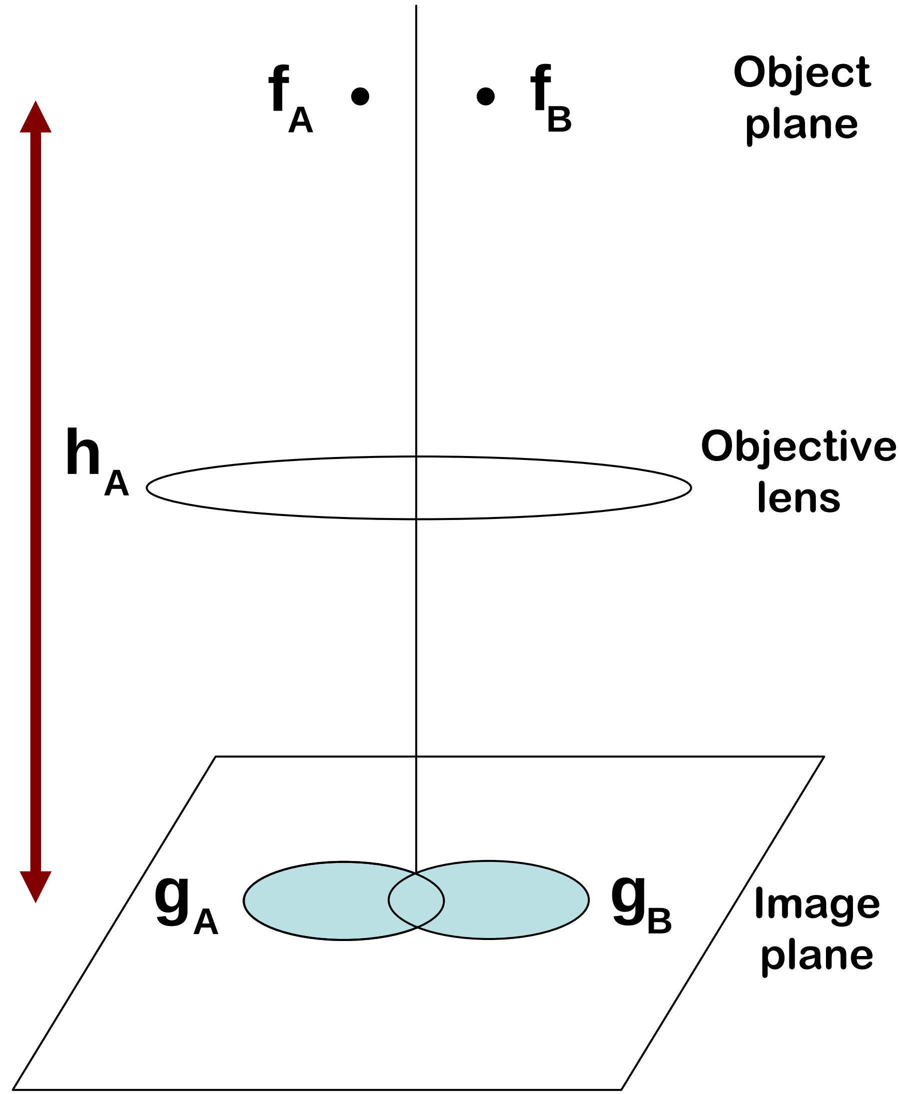
How do we express this mathematically?

$$g(\vec{r}) = \int f(\vec{r}') \otimes h(\vec{r} - \vec{r}')d\vec{r}'$$

- **The ⊗ is a mathematical symbol indicating 'convolution'***
- **$h(\vec{r})$ is thus a 'blurring function'**

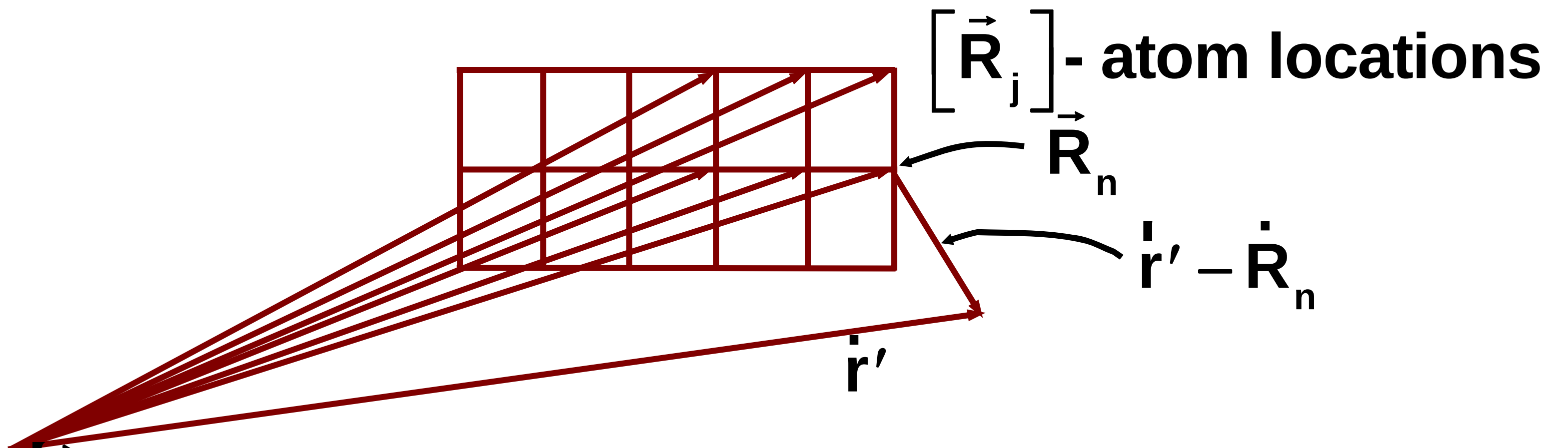
Or: aberrations, etc. limit spatial frequencies in image

⇒ Reciprocal space



* http://mathworld.wolfram.com/Convolution.html

Scattering from a lattice



$$\Psi_{scattered}\left(\vec{K},\vec{r}\right)=$$

$$\frac{-m}{2\pi h^2}\,\frac{\exp\left[2\pi i\left(\vec{k}_d\cdot\vec{r}\right)\right]}{\left|\vec{r}\right|}\int\sum V_{at}\left(\vec{r}'-\vec{R}_j\right)\exp\left[-2\pi i\left(\vec{K}\cdot\vec{r}'\right)\right]d^3\vec{r}'$$

So scattered wave from an array of N atoms:

$$\Psi_{scatt}\left(\vec{K}\right)=\sum_j^N f_{el}\left(\vec{R}_j\right)\exp\left[-2\pi i\left(\vec{K}\cdot\vec{R}_j\right)\right]$$

Remember: ψ is thus the Fourier Transform of the scattering potential

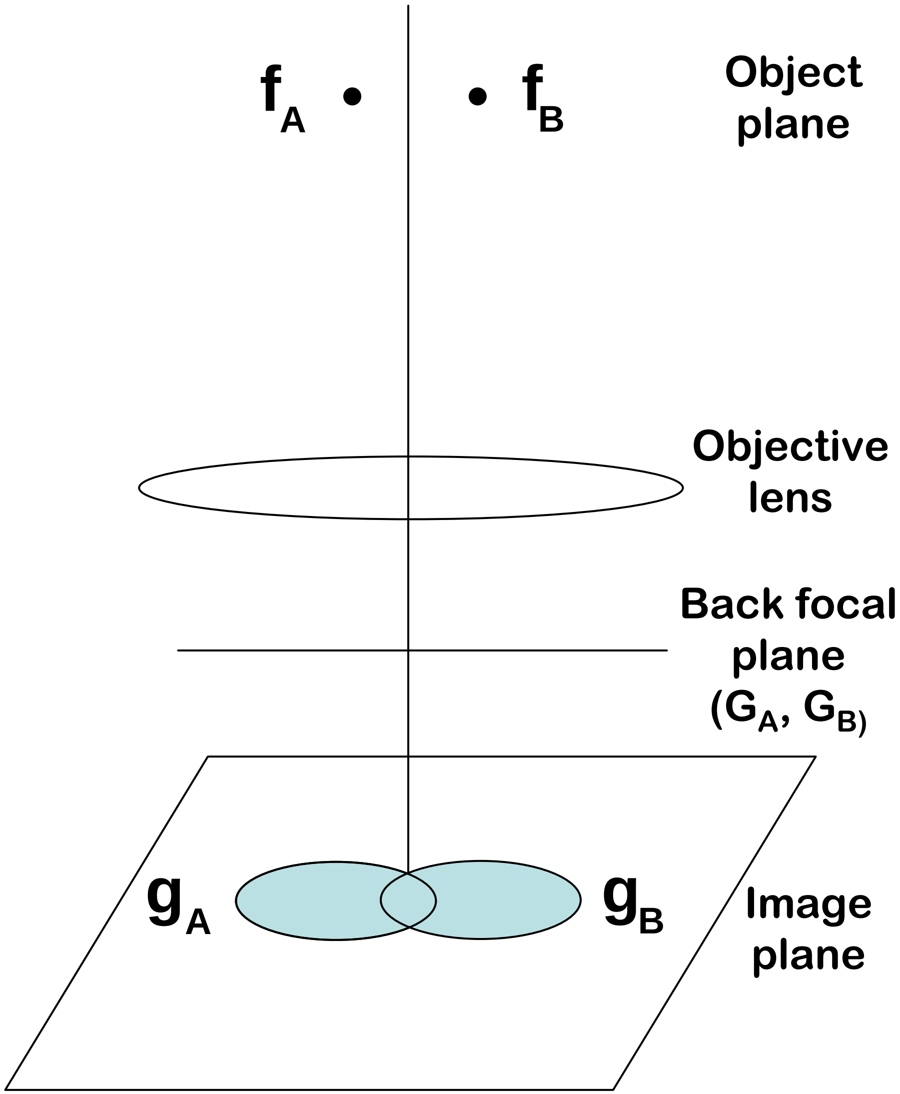
HRTEM

general idea

So, can express $g(\vec{r})$ generally as:

$$g(\vec{r}) = \sum_{\vec{u}} G(\vec{u}) \exp\left[2\pi i(\vec{u} \cdot \vec{r})\right]$$

- $\vec{u}$ are reciprocal lattice vectors
- $G(\vec{u})$ is scattering potential at each site
- Thus:
  - $g(\vec{r})$ is FT of $G(\vec{u})$



HRTEM

general idea

Similarly:

- F(u) is FT of f(r)
- H(u) is FT of h(r)

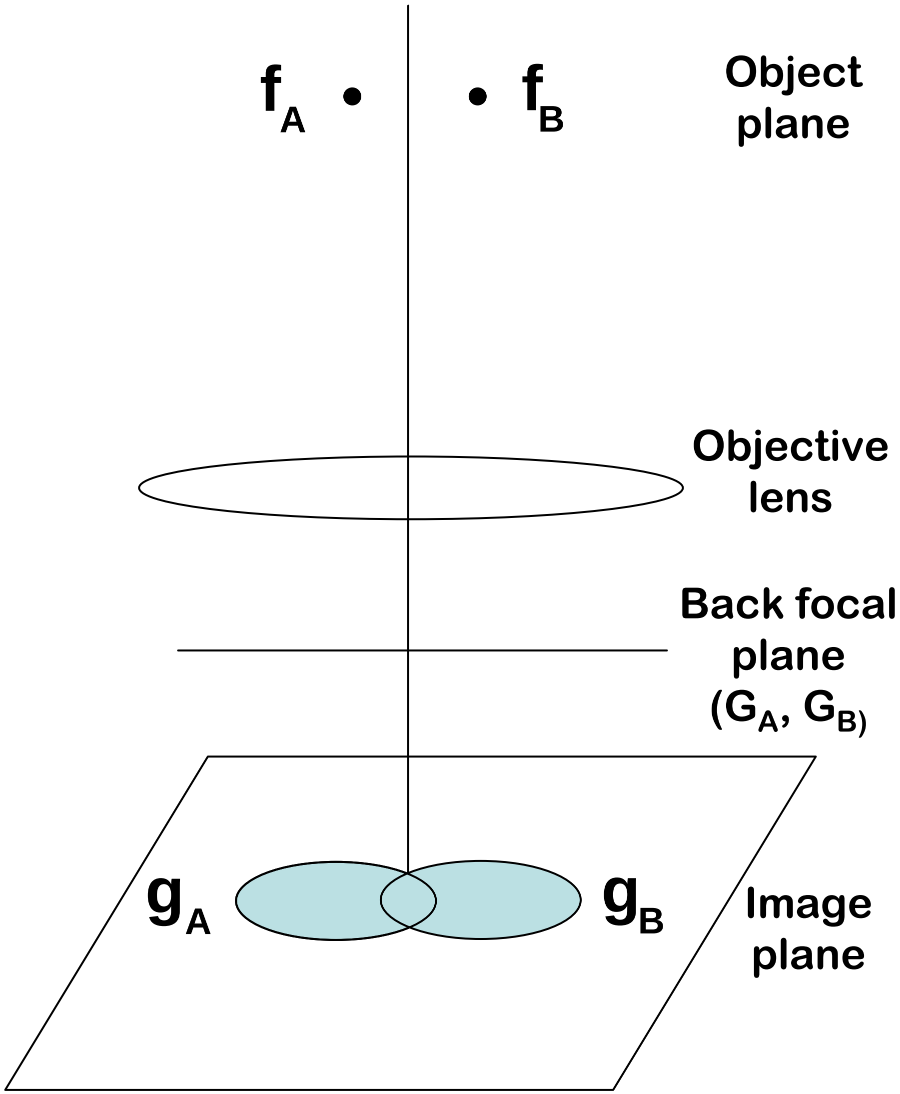
Key relation:

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

Convolution between functions in real space

equals

Multiplication of functions in reciprocal space



“Ideal” Specimen

General expression for specimen:

$$f(x,y) = A(x,y)\exp\left[-i\phi_t(x,y)\right]$$

Normalize to A(x,y) = 1

$$f(x,y) = \exp\left[-i\phi_t(x,y)\right]$$

Phase change depends only on mean inner potential through sample thickness

$$d\phi = \sigma\int_0^t V(x,y,z)\,dz = \sigma V_t(x,y)$$

Note: σ related to, but not same as cross-sections from earlier

Specimen transfer function

'weak phase object'

Can now have 'specimen transfer function'

- What's the wave look like as it exits sample - 'exit wave'
- This is the 'signal' we want in the end
- Include effect of absorption - $\mu(x,y)$

$$f(x,y) = \exp\left[-i\sigma V_t(x,y) - \mu(x,y)\right]$$

- Called a 'phase object'

"Weak phase object approximation" (WPOA)

- Assume sample very thin - $V_t(x,y) << 1$, neglect $\mu(x,y)$, expand above and neglect higher order terms:

$$f(x,y) = 1 - i\sigma V_t(x,y)$$

This is the final "model" of the sample

HRTEM

general idea

How do we express this mathematically?

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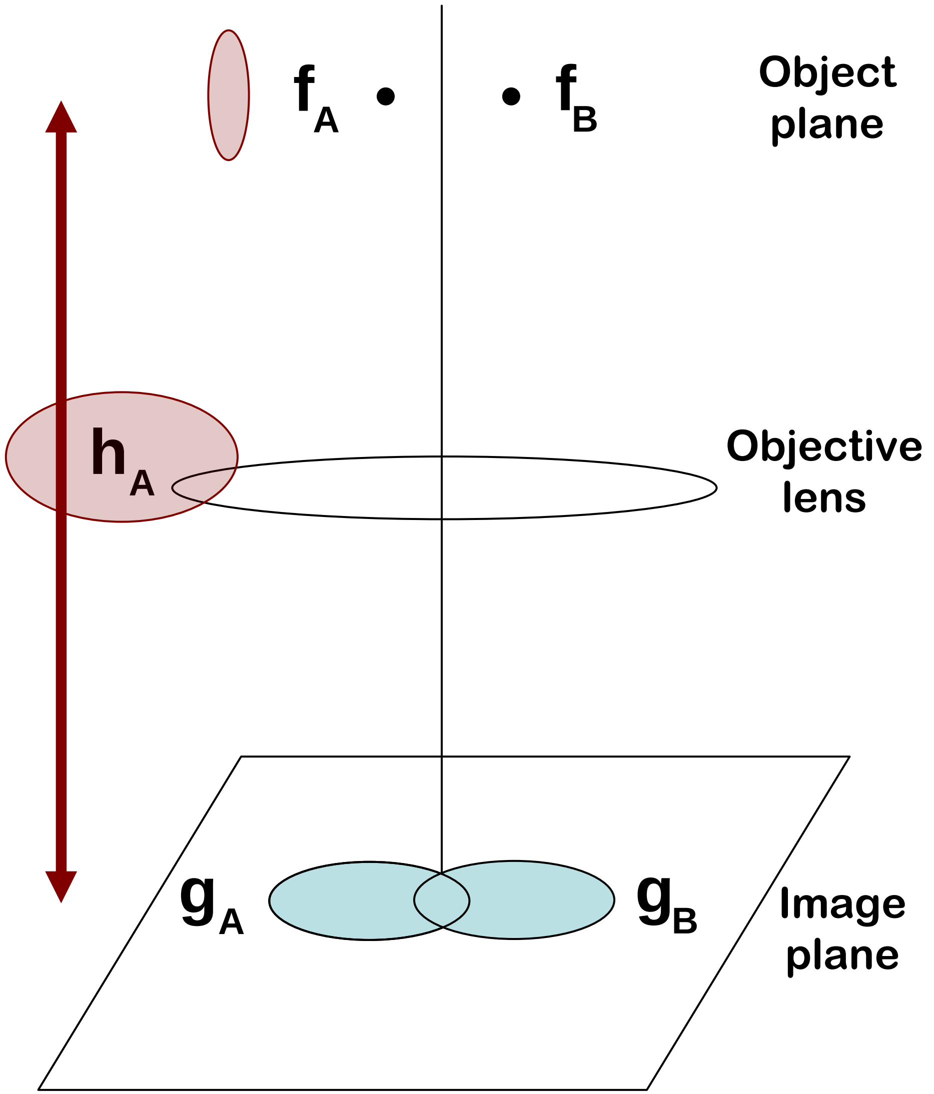

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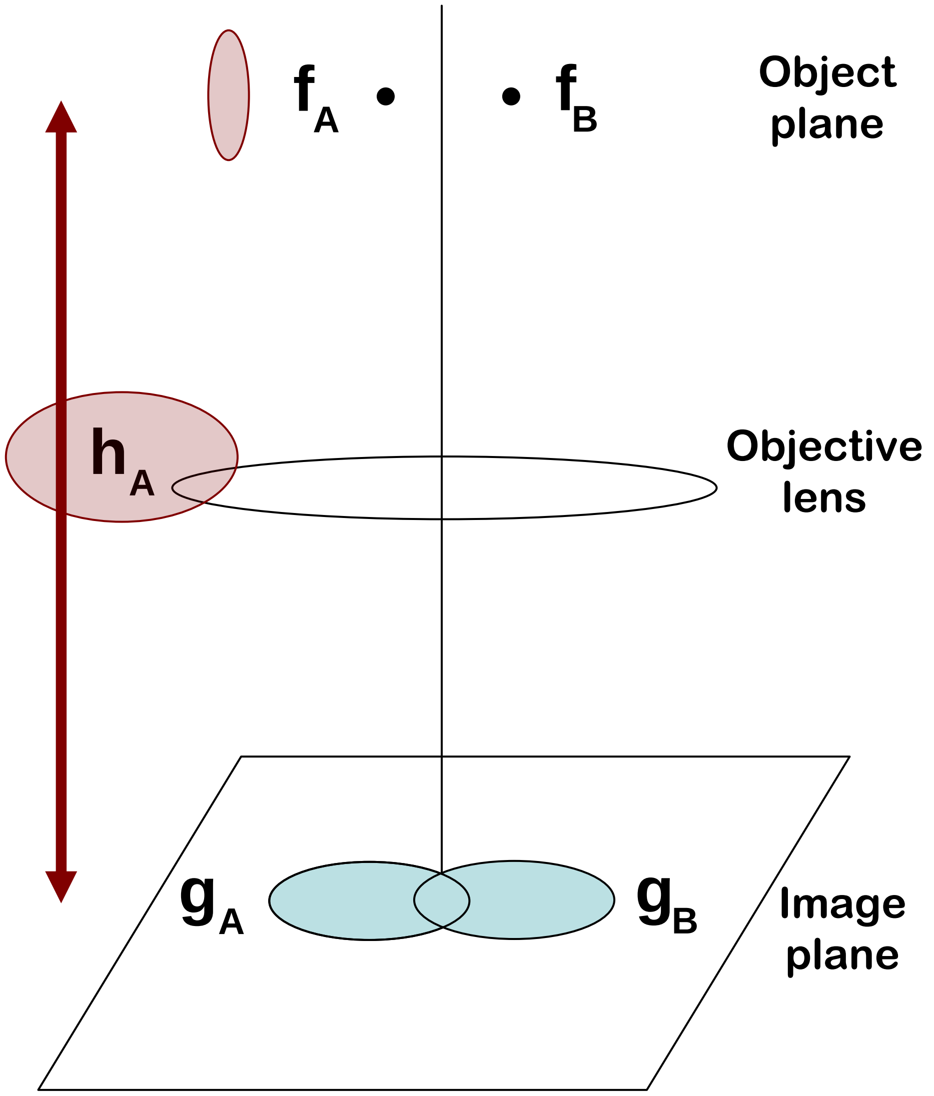
⇒ *Reciprocal space*



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WPOA & the Blurring Function

Electron exit wave is now modified by blurring function

$$\Psi(x,y) = \left[1 - i\sigma V_t(x,y)\right] \otimes h(x,y)$$

Represent h(x,y) as general wave:

$$h(x,y) = \cos(x,y) + i\sin(x,y)$$

$$\Psi(x,y) = \left[1 - i\sigma V_t(x,y)\right] \otimes \sin(x,y) + i\cos(x,y)$$

$$\Psi(x,y) = 1 + \sigma V_t(x,y) \otimes \sin(x,y) - i\cos(x,y)$$

Intensity:

$$I = \Psi\Psi^* = 1 + 2\sigma V_t(x,y) \otimes \sin(x,y)$$

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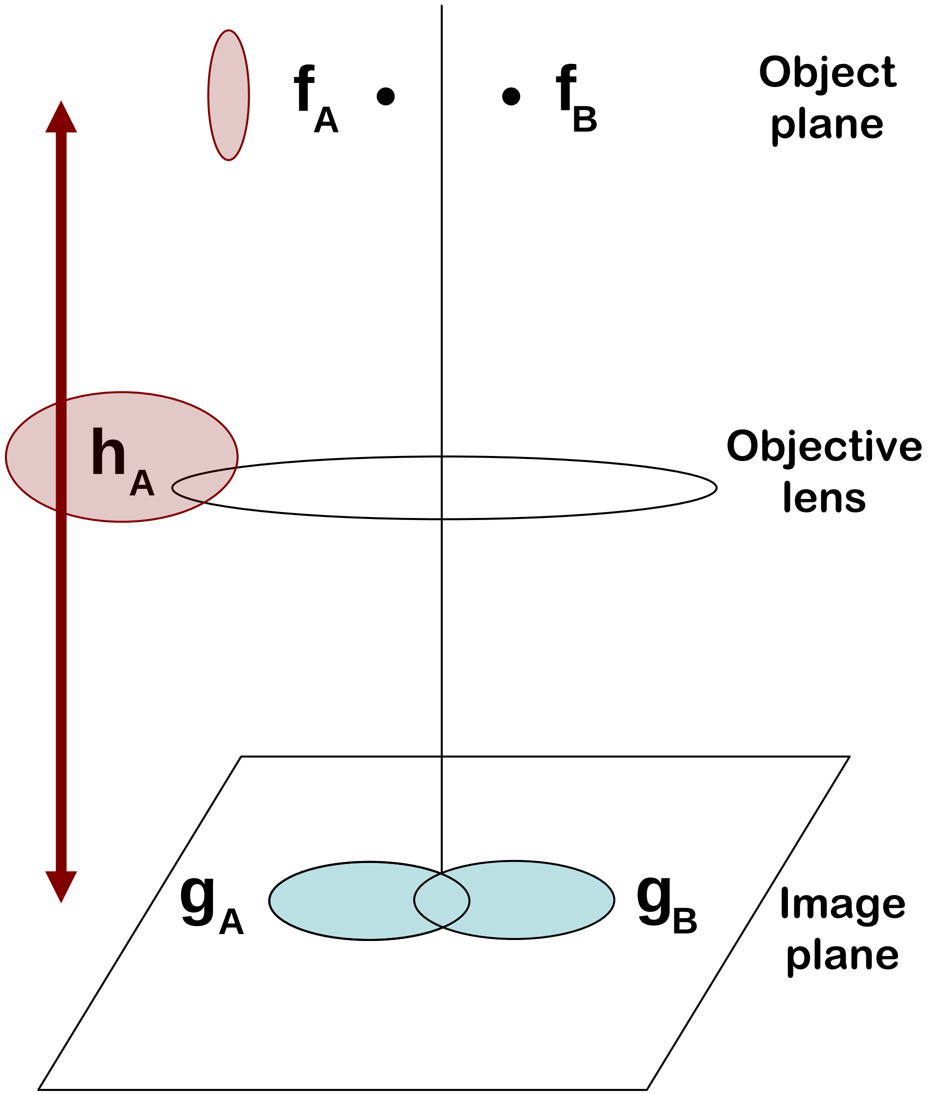

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Objective lens transfer function

What is internal to H(u)?

- Aperture function: A(u)
- Coherence function: E(u)
- Aberration function: B(u)

$$H(u) = A(u)E(u)B(u)$$

Let's dissect these terms …

Aperture function: A(u)

- Determined by size of objective aperture
- Objective aperture (or column liner if no OA used) limits spatial frequencies

Objective lens transfer function

Aberration function: B(u)

- Consider only spherical aberration & defocus
- Point in object becomes disc of diameter $\delta(\theta)$ in image:

$$\delta(\theta) = C_s\theta^3 + \Delta f\theta$$

- Integrate over all θ:

$$D(\theta) = \int_0^\theta \delta(\theta)\,d\theta = \frac{C_s\theta^4}{4} + \frac{\Delta f\theta^2}{2}$$

- Replace θ w/ λu (Braggs law, small angles $\Leftrightarrow$ $2\theta = \lambda u$)

$$D(u) = C_s\frac{\lambda^4 u^4}{4} + \Delta f\frac{\lambda^2 u^2}{2}$$

Objective lens transfer function

Interested in phase only: $\chi(u)$

$$\chi(u) = \frac{2\pi}{\lambda} D(u)$$

$$= \frac{2\pi}{\lambda}\left[C_s \frac{\lambda^4 u^4}{4} + \Delta f \frac{\lambda^2 u^2}{2} \right]$$

$$\chi(u) = \frac{1}{2}\pi C_s \lambda^3 u^4 + \pi \Delta f \lambda u^2$$

Aberration function $\chi(u)$ is a complicated function of Cs and Δf

Equivalence between real and reciprocal space

So - why did we do all of this?

Well, recall that in real space:

$$I = \Psi\Psi^* = 1 + 2\sigma V_t(x,y) \otimes \sin(x,y)$$

We make an equivalence in reciprocal space:

$$H(u) = 2A(u)E(u)\sin\chi(u)$$

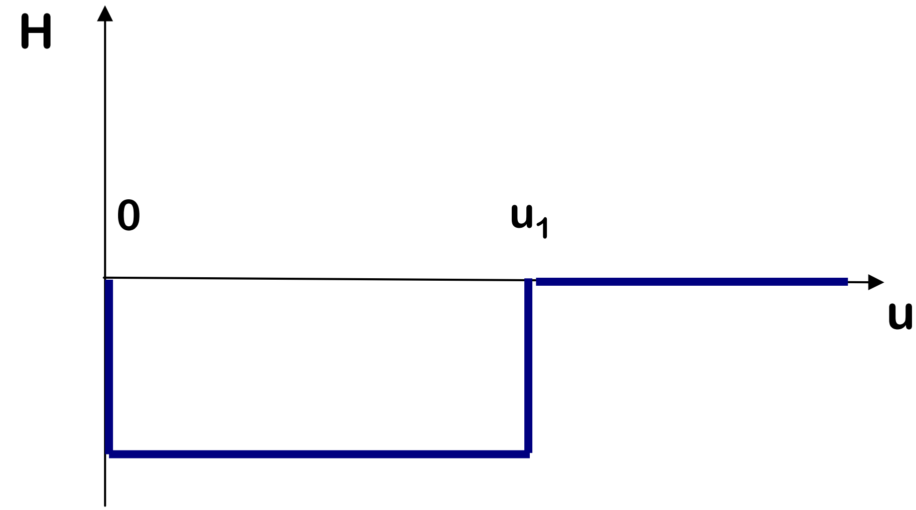
Which means that our image - G(u) - is:

$$G(u) = H(u)F(u) = \left[2A(u)E(u)\sin\chi(u)\right]F(u)$$

H(u) is thus a spatial frequency filter

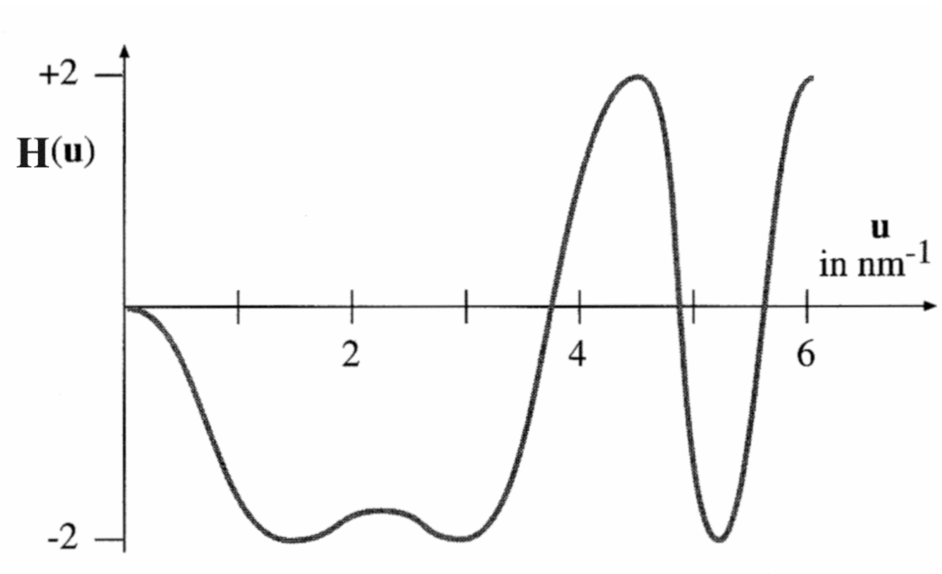
Contrast Transfer Function

Ideal transfer function passes all frequencies up to a given u



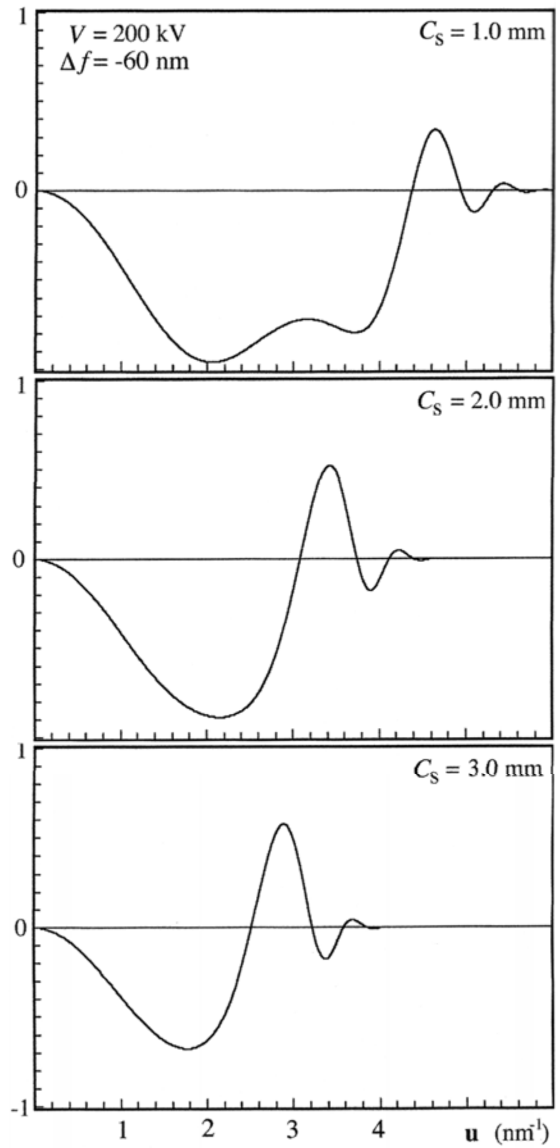
Real transfer functions modify frequencies

Example to right is close to ideal (Scherzer defocus)

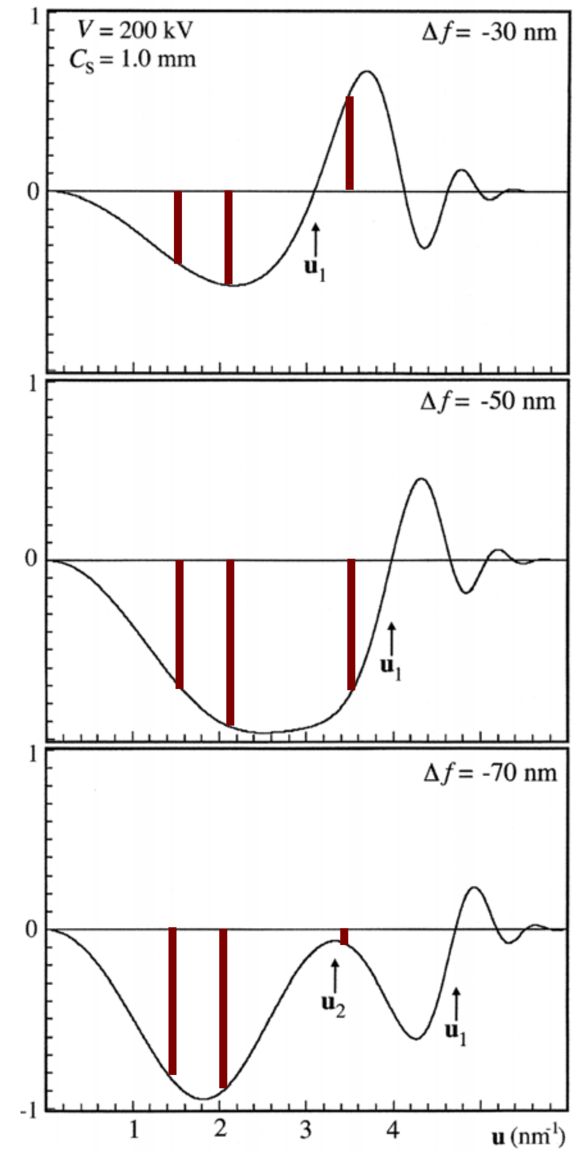


Contrast Transfer Function

Vary Cs



Vary defocus



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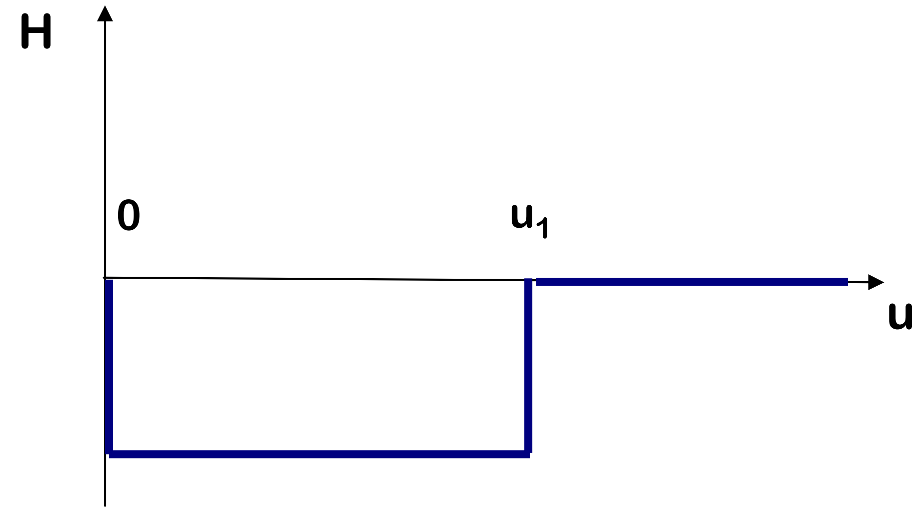

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