



# **A Global View of Diffraction and Surface Scatter Phenomena**

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# Abstract

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Radiometry is a neglected stepchild in the physics curriculum at most universities, and electrical engineers learn even less about radiometry as there is not even a quantity analogous to *radiance* in classical electrical engineering fields. The fact that electrical engineers have been writing most of our optics textbooks for the last few decades has thus done little to advance the understanding of radiometric nomenclature and principles. The recent revelation that *diffracted radiance* is the fundamental quantity predicted by scalar diffraction theory, and is shift-invariant in direction cosine space, has led to the development of a generalized linear systems formulation of non-paraxial scalar diffraction phenomena. Thus simple Fourier techniques can now be used to predict a variety of wide-angle diffraction phenomena. These include: (1) the redistribution of radiant energy from evanescent diffracted waves into propagating ones, (2) the angular broadening (and apparent shifting) of wide-angle diffracted orders, and (3) diffraction efficiencies predicted with an accuracy usually thought to require rigorous electromagnetic theory. In addition, a unified surface scatter theory has been shown to be more accurate than the classical Beckmann-Kirchhoff theory in predicting non-intuitive scatter effects at large incident and scattered angles, without the smooth-surface limitation of the Rayleigh-Rice scattering theory. This new understanding of non-paraxial diffraction phenomena is becoming increasingly important in the design and analysis of optical systems, particularly those dealing with nano-structures or the increasingly popular field of nano-photonics.

# Understanding Natural Phenomena requires Simple Mathematical Models

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The true nature of most physical phenomena becomes evident when simple elegant theories and mathematical models conform with experimental observations.

## Planetary Motion

### Geocentric Universe

A complex theory, with epicycles upon epicycles, was required to describe observed retro-grade planetary motion when the earth was thought to be the center of the universe.

### Heliocentric Universe

The concept of a heliocentric universe, with the planets revolving around the sun, allowed a simple and elegant theory of planetary motion governed by Kepler's Law's.

## Photoelectric Effect

### Electromagnetic Theory

Electromagnetic theory failed to explain the emission of electrons from metal surfaces under the action of radiant energy.

### Quantum Theory

Quantum Theory elegantly accounts for the photoelectric threshold frequencies and work functions associated with the photoelectric effect.

# Simple Transformations can often make the Nature of Physical Phenomena Evident

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**Simple transformations can often make the math easy—and provide insight—without changing the physics.**

## **Examples:**

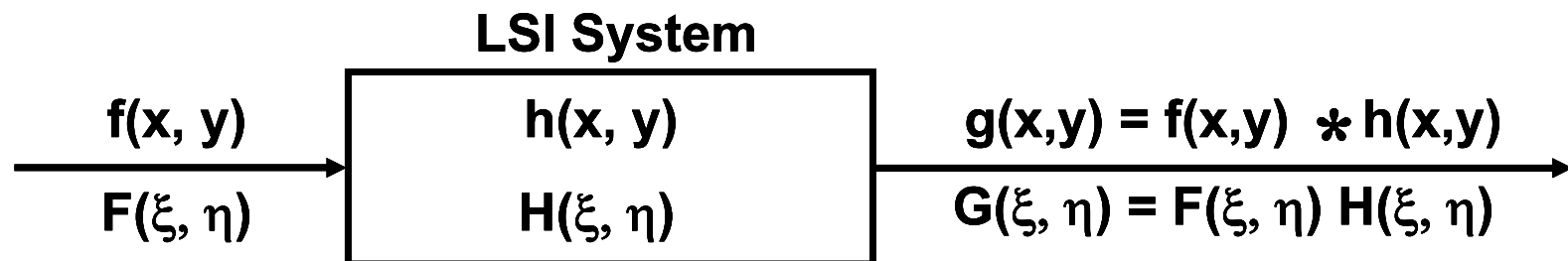
**Transforming from Cartesian to spherical coordinates greatly simplifies solving Schrodinger's equation for the hydrogen atom.**

**Transforming to cylindrical polar coordinates simplifies the description of transverse propagating modes in optical fibers**

**High-energy physicists always transform into the center-of-mass coordinate system when performing atomic collision, or radioactive decay calculations. They then apply the laws of conservation of linear and angular momentum, and finally transform back and express the results in the laboratory coordinate system.**

# Natural Phenomena Exhibiting Linear, Shift-invariant Behavior are Readily Understood

Even complicated natural phenomena can often be approximated, over a limited range of some relevant parameter, as a linear, shift-invariant process. It can then be characterized by a system transfer function, and be more readily understood.



$$H(\xi, \eta) = \frac{G(\xi, \eta)}{F(\xi, \eta)} \equiv \text{System Transfer Function} \quad (1)$$

Imaging systems with field-dependent aberrations are routinely characterized by their modulation transfer function (MTF) curves; albeit a separate one for each field angle.

# The Development of Scalar Diffraction Theory did not end with Sommerfeld in 1896

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- Grimaldi Discovers Diffraction (1665)
- Huygens' Wavefront Construction (1678)
- Young's Interference Experiment (1802)
- Huygens-Fresnel Principle (1818)
- Fresnel-Kirchhoff Formulation (1882)
- Rayleigh-Sommerfeld Theory (1896)

**Historical  
Development**

- Linear Systems Formulation of Diffraction (1960's)
- A Global View of Diffraction (Shack, 1972)
- Aberrations of Diffracted Wave Fields (Harvey, 1978)

**Not so  
Recent**

- Diffracted Radiance: A Fundamental Quantity . . . (1999)
- Non-paraxial Scalar . . . Sinusoidal Phase Gratings (2006)

**Very  
Recent**

# Outline

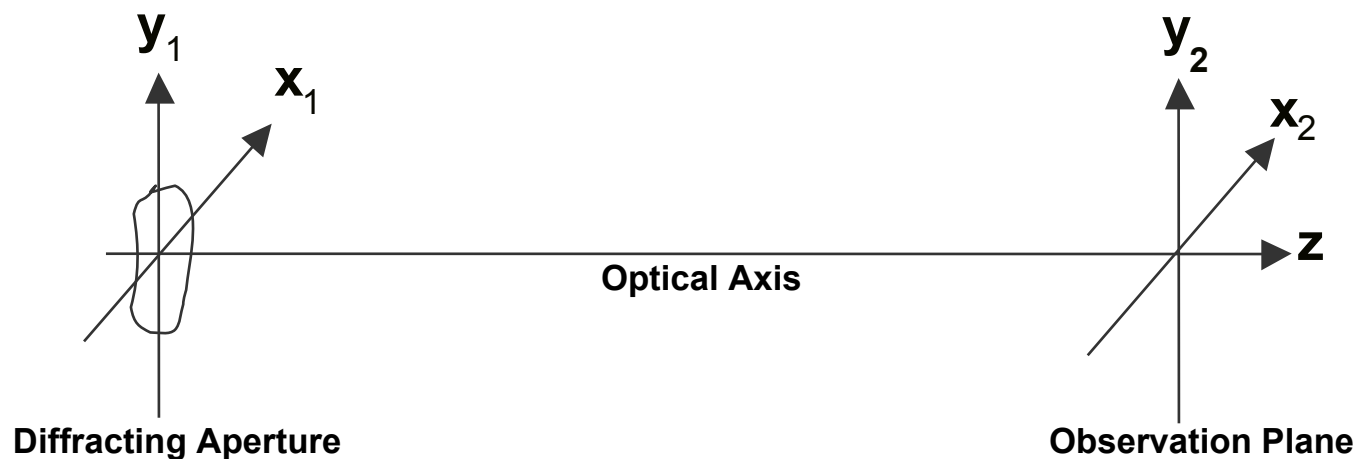
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- **Paraxial Limitation in Conventional Fourier Optics**
  - Fraunhofer Diffraction and the Paraxial Limitation
  - Diffraction Grating Behavior in Cartesian Space
- **A Global View of Diffraction (1973-1979)**
  - Aberrations of Diffracted Wave Fields
  - Non-paraxial Shift-invariance in Direction Cosine Space
- **Radiometry/Scalar Diffraction (1999)**
  - Diffracted Radiance: The Fundamental Quantity
  - Re-normalization in the Presence of Evanescent waves
- **Examples**
  - Non-paraxial Behavior of Sinusoidal Phase Gratings
  - Surface Scatter Behavior for Large Incident and Scattered Angles
- **Summary and Conclusions**

# Paraxial Limitation Inherent in Fraunhofer Diffraction\*

It is well known that the irradiance distribution on a plane in the far field (Fraunhofer region) of a diffracting aperture is given by the squared modulus of the Fourier transform of the complex amplitude distribution emerging from the diffracting aperture.<sup>1,2</sup>

$$E(x_2, y_2) = \frac{1}{\lambda^2 z^2} \left| \mathcal{F} \left\{ U_o^+(x_1, y_1) \right\}_{\xi = \frac{x_2}{\lambda z}, \eta = \frac{y_2}{\lambda z}} \right|^2 \quad (2)$$



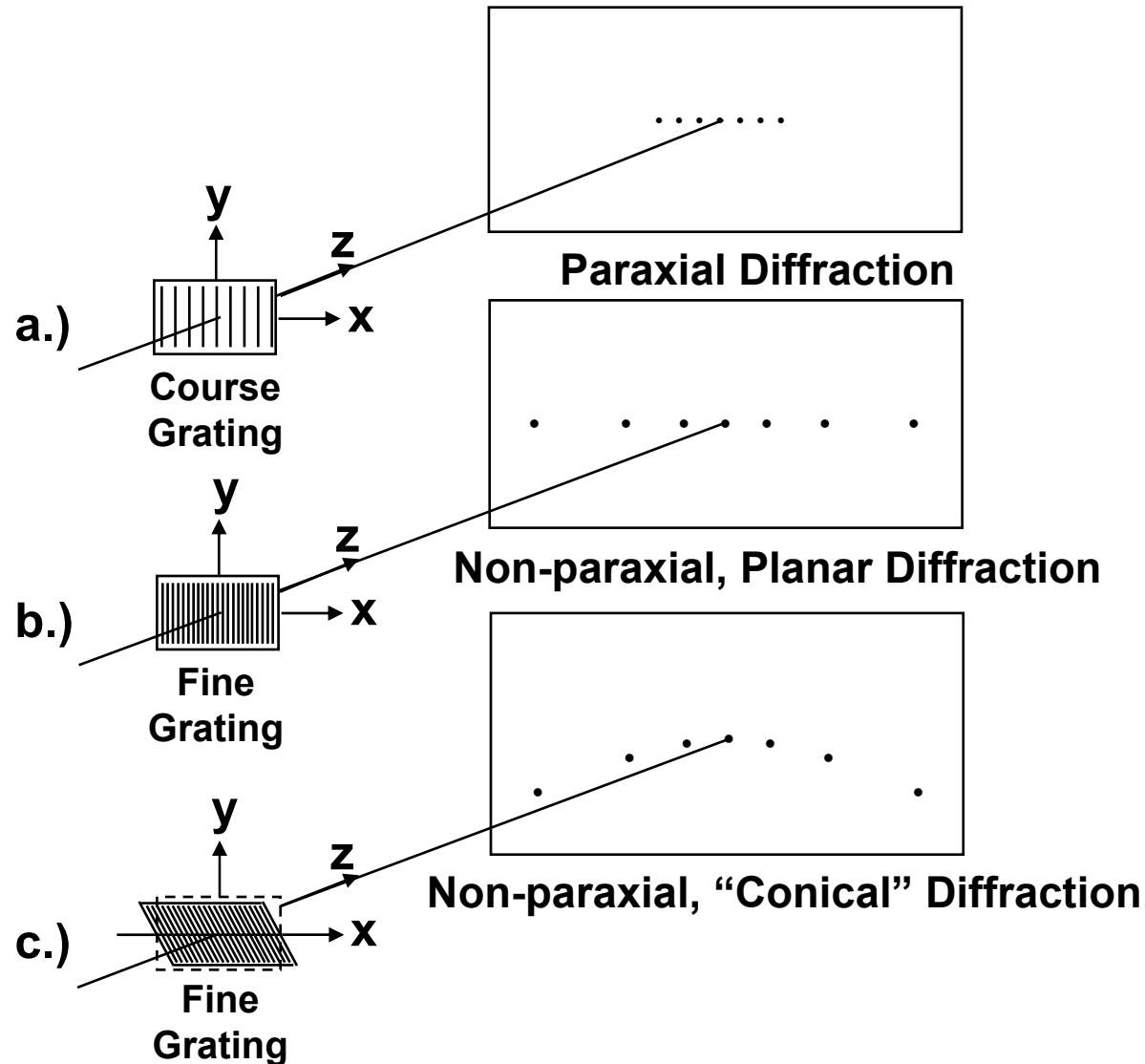
**The Fraunhofer Approximation, and even Fresnel Approximation, Implicitly Contain a Paraxial Limitation!**

- \* 1. J. W. Goodman, *Introduction to Fourier Optics*, McGraw-Hill, New York (1968).  
2. J. D. Gaskill, *Linear Systems, Fourier Transforms, and Optics*, John Wiley & Sons, New York, (1978).



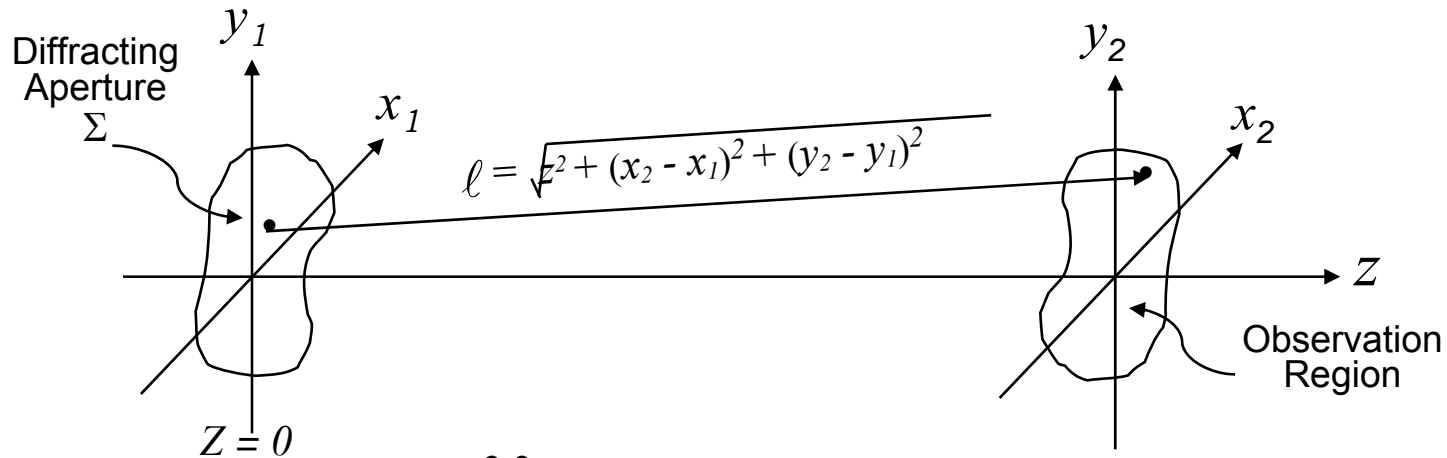
# However, not all Diffraction Phenomena of Interest are limited to the Paraxial Regime

Diffraction gratings are inherently wide-angle devices.



Only for very coarse gratings, exhibiting paraxial diffraction angles, does the simple Fourier treatment describe the diffraction pattern projected onto a plane screen (Cartesian coordinates).

# The Fresnel Approximation



$$U_2(x_2, y_2) = \frac{1}{i\lambda} \iint_{\Sigma} U_1^+(x_1, y_1) \frac{\exp(ik\ell)}{\ell} \cos(\vec{n} \cdot \vec{\ell}) dx_1 dy_1 \quad (3)$$

**Rayleigh-Sommerfeld Diffraction Formula for arbitrary illumination.**

If one makes a binomial expansion of the quantity  $\ell$  in the exponent and throws away all but the first two terms (which is valid if  $z^3 \gg \frac{\pi}{4\lambda} [(x_2 - x_1)^2 + (y_2 - y_1)^2]_{\max}^2$ ), then we obtain

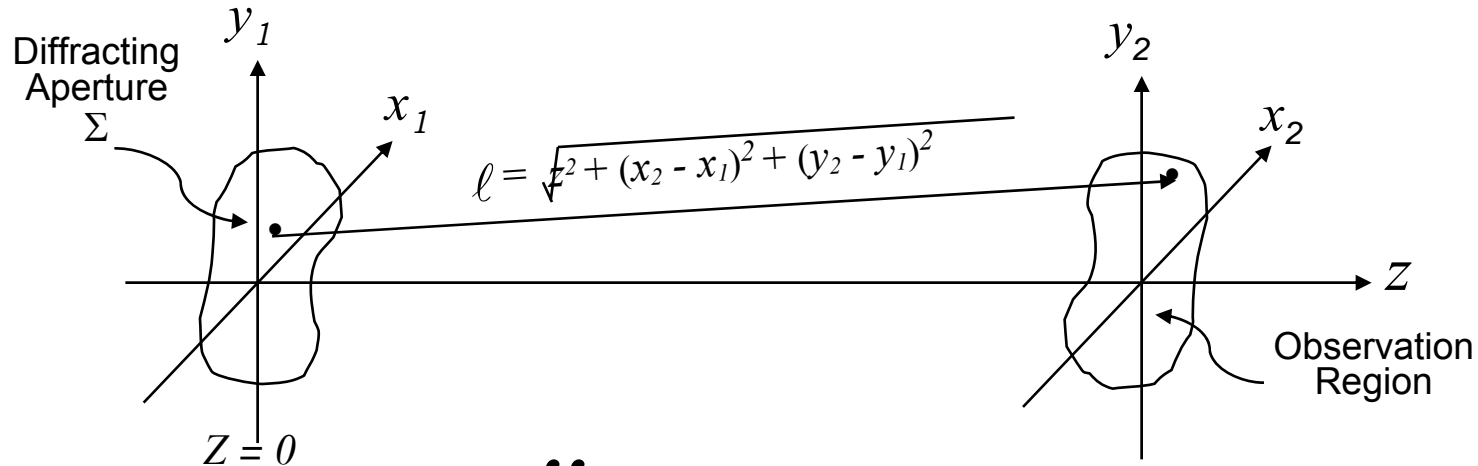
$$U_2(x_2, y_2) = \frac{\exp(ikz)}{i\lambda z} \exp\left[i\frac{k}{2z}(x_2^2 + y_2^2)\right] \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_1^+(x_1, y_1) \exp\left[i\frac{k}{2z}(x_1^2 + y_1^2)\right] \exp\left[-i\frac{2\pi}{\lambda z}(x_1 x_2 + y_1 y_2)\right] dx_1 dy_1$$

which we recognize as the following Fourier Transform integral.

$$U_2(x_2, y_2) = \frac{\exp(ikz)}{i\lambda z} \exp\left[i\frac{k}{2z}(x_2^2 + y_2^2)\right] \mathcal{F}\left\{U_1^+(x_1, y_1) \exp\left[i\frac{k}{2z}(x_1^2 + y_1^2)\right]\right\} \Bigg|_{\xi=\frac{x_2}{\lambda z}, \eta=\frac{y_2}{\lambda z}} \quad (4)$$

**Fresnel Diffraction Formula**

# The Fraunhofer Approximation



$$U_2(x_2, y_2) = \frac{1}{i\lambda} \iint_{\Sigma} U_1^+(x_1, y_1) \frac{\exp(ik\ell)}{\ell} \cos(\vec{n} \cdot \vec{\ell}) dx_1 dy_1$$

Rayleigh-Sommerfeld Diffraction Formula for arbitrary illumination.

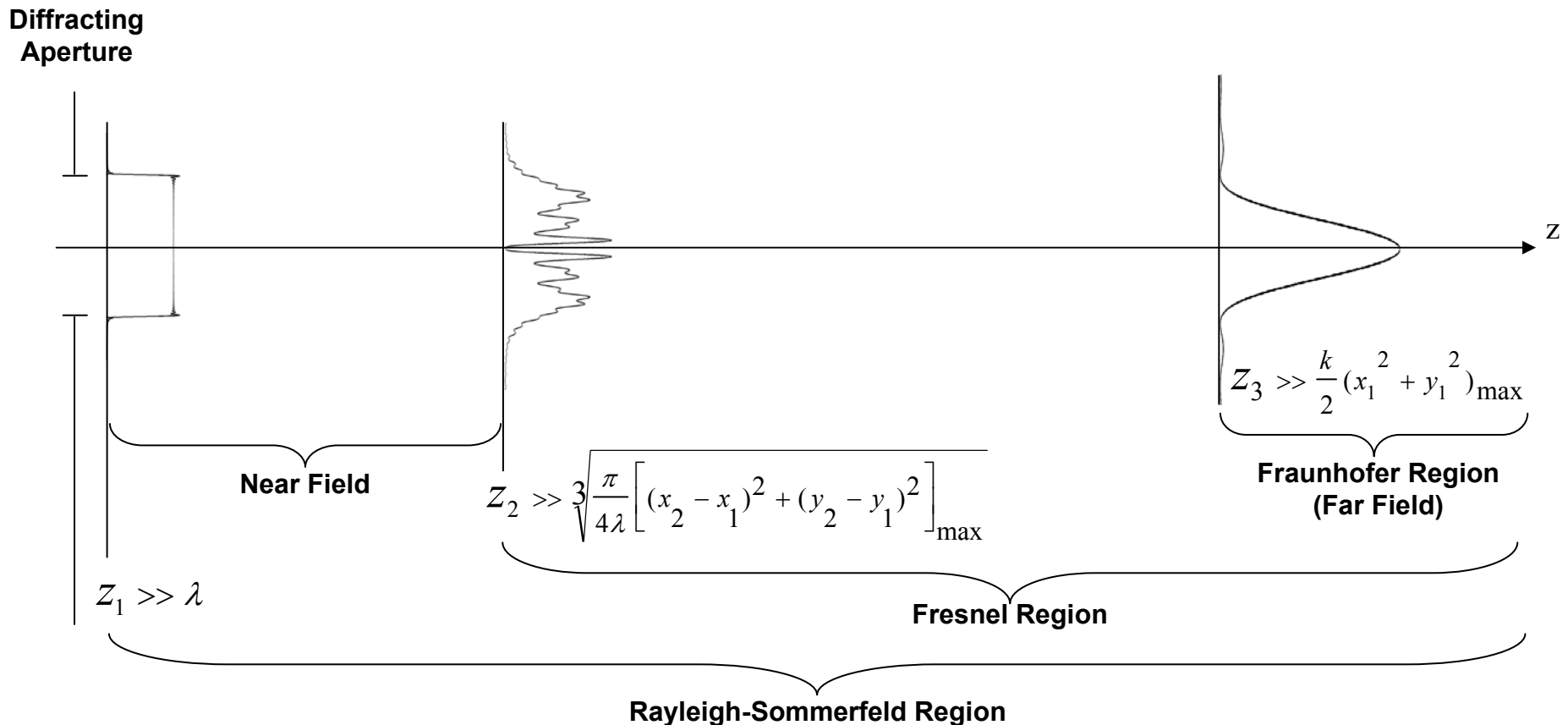
If the more stringent Fraunhofer criterion ( $z \gg k(x_1^2 + y_1^2)_{\max}$ ) is satisfied, then the quadratic phase factor in the argument of the Fourier Transform operation is approximately unity over the entire aperture, and the complex amplitude distribution on the observation plane can be found directly from the Fourier Transform of the complex amplitude distribution emerging from the diffracting aperture.

$$U_2(x_2, y_2) = \frac{\exp(ikz)}{i\lambda z} \exp\left[i \frac{k}{2z} (x_2^2 + y_2^2)\right] \mathcal{F}\{U_1^+(x_1, y_1)\} \Big|_{\xi=\frac{x_2}{\lambda z}, \eta=\frac{y_2}{\lambda z}}$$

(5)

Fraunhofer Diffraction Formula

# Fresnel and Fraunhofer Criteria\* (and Regions of Validity)



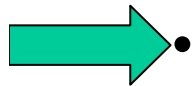
The Fraunhofer criterion imposes very severe restrictions upon the observation distance. For example, a circular diffracting aperture 4 cm (1.6 inches) in diameter and a wavelength  $\lambda = 0.5 \mu\text{m}$  requires that  $z \gg 2.5 \text{ km}$ . Or alternatively, for a 2.5 cm wide square aperture, the Fraunhofer diffraction integral is valid only if the observation distance  $z \gg 1.6 \text{ km}$ .

# Outline

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- Fraunhofer Diffraction and the Paraxial Limitation
- Diffraction Grating Behavior in Cartesian Space



- **A Global View of Diffraction (1973-1979)**

- Aberrations of Diffracted Wave Fields
- Non-paraxial Shift-invariance in Direction Cosine Space

- **Radiometry/Scalar Diffraction (1999)**

- Diffracted Radiance: The Fundamental Quantity
- Re-normalization in the Presence of Evanescent waves

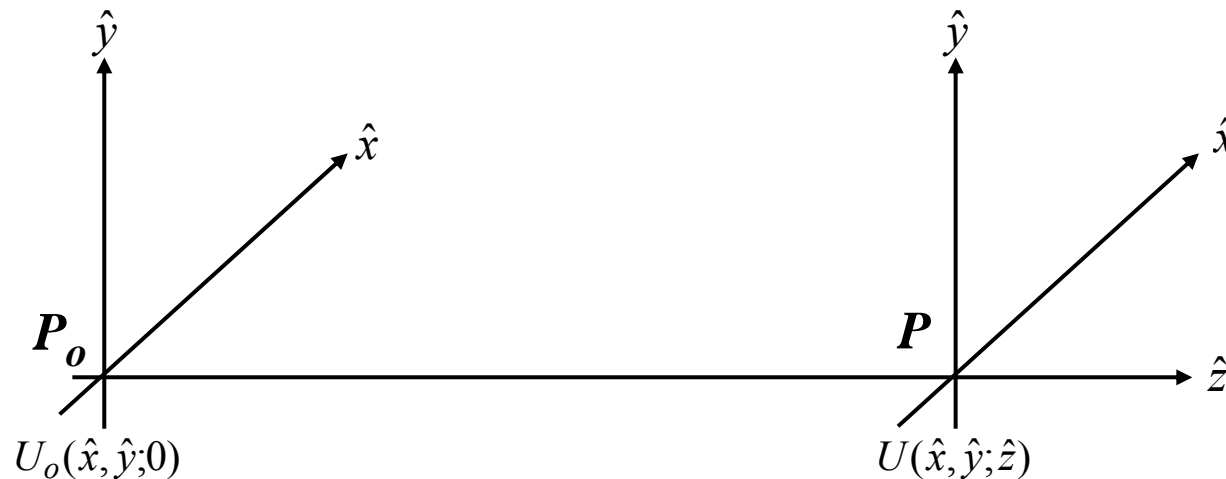
- **Examples**

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# Linear Systems Formulation of Near-field Scalar Diffraction Theory\*

A very simple and elegant derivation of the Rayleigh-Sommerfeld diffraction integral can be obtained by the direct application of Fourier transform theory. Let us first scale the spatial variables by the wavelength of light  $\hat{x} = x / \lambda$ ,  $\hat{y} = y / \lambda$ , and,  $\hat{z} = z / \lambda$ . The reciprocal variables in Fourier transform space are then the direction cosines of the propagation vectors of the resulting angular spectrum of plane waves.



We now *assume* that the Fourier transform of the complex amplitude distribution emerging from the diffracting aperture exists; and likewise for the complex amplitude distribution in the observation plane. We can thus write the following Fourier transform pairs.

$$A_o(\alpha, \beta; 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_o(\hat{x}, \hat{y}; 0) \exp[-i2\pi(\alpha\hat{x} + \beta\hat{y})] d\hat{x} d\hat{y} \quad (6) \quad \left| \quad A(\alpha, \beta; \hat{z}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(\hat{x}, \hat{y}; \hat{z}) \exp[-i2\pi(\alpha\hat{x} + \beta\hat{y})] d\hat{x} d\hat{y} \quad (8)$$

$$U_o(\hat{x}, \hat{y}; 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A_o(\alpha, \beta; 0) \exp[i2\pi(\alpha\hat{x} + \beta\hat{y})] d\alpha d\beta \quad (7) \quad \left| \quad U(\hat{x}, \hat{y}; \hat{z}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A(\alpha, \beta; \hat{z}) \exp[i2\pi(\alpha\hat{x} + \beta\hat{y})] d\alpha d\beta \quad (9)$$

\* The diffracted wave field as a superposition of plane waves.

# Transfer Function of Free Space

In the scaled coordinate system  $\hat{\nabla}^2 = \lambda^2 \nabla^2$ , and  $\hat{k}^2 = \lambda^2 k^2 = (2\pi)^2$ ; hence, the Helmholtz wave equation becomes

$$\left[ \hat{\Delta}^2 + (2\pi)^2 \right] U(\hat{x}, \hat{y}; \hat{z}) = 0 \quad (10)$$

By requiring the individual plane wave components to satisfy the Helmholtz wave equation, we obtain

$$A(\alpha, \beta; \hat{z}) = A_o(\alpha, \beta; 0) \exp(i2\pi\gamma\hat{z}) \quad (11)$$

where

$$\gamma = \sqrt{1 - (\alpha^2 + \beta^2)}$$

Since Eq.(11) relates the Fourier transforms of the scalar fields in planes  $P_o$  and  $P$ , it can be rewritten in terms of a transfer function of free space,  $H(\alpha, \beta; \hat{z})$

$$H(\alpha, \beta; \hat{z}) = \frac{A(\alpha, \beta; \hat{z})}{A_o(\alpha, \beta; \hat{z})} = \exp(i2\pi\gamma\hat{z}) \quad (12)$$

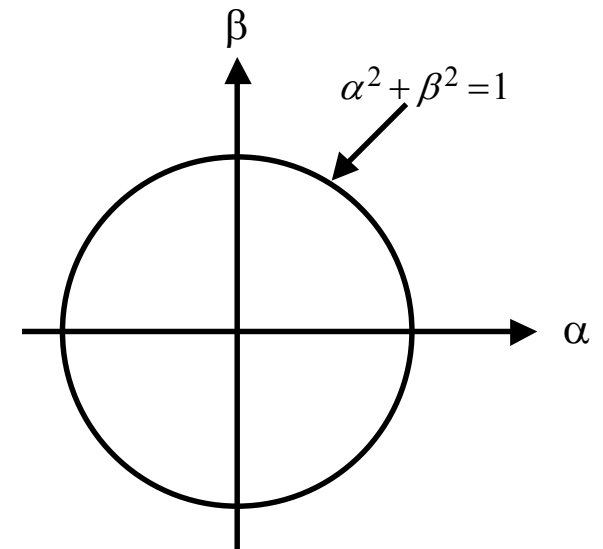
where

$$\gamma = \text{is real} \quad \text{for } (\alpha^2 + \beta^2) \leq 1$$

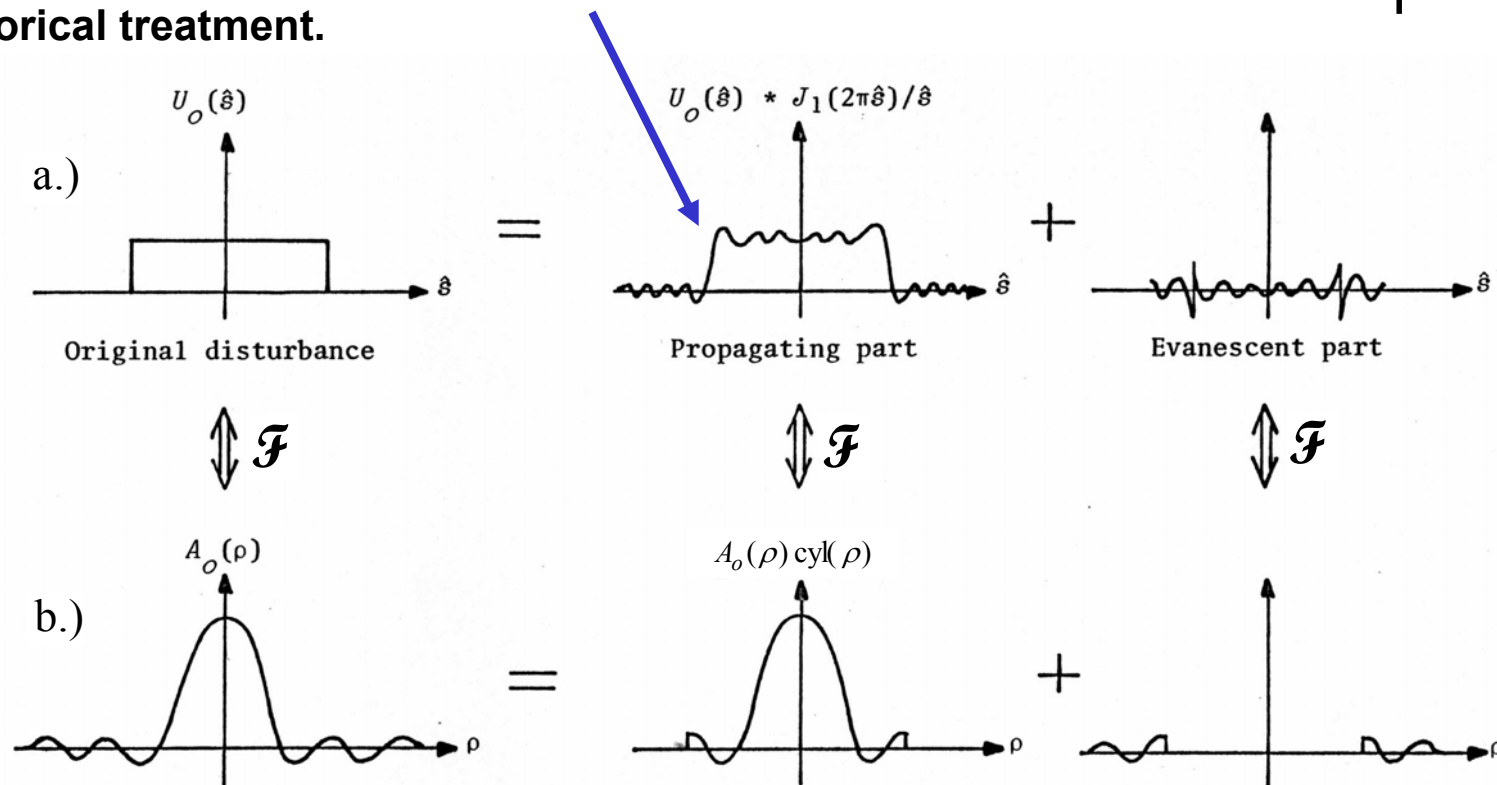
$$\gamma = \text{is imaginary} \quad \text{for } (\alpha^2 + \beta^2) \geq 1$$

# Plane Wave Components in Direction Cosine Space

Consider a unit circle in direction cosine space as illustrated below. Inside the circle  $\gamma$  is real and the corresponding part of the optical disturbance will propagate and contribute to the field in plane  $P$ . However those components of the direction cosine spectrum which lie outside of the unit circle have imaginary values of  $\gamma$  and represent that part of the optical disturbance which experiences a rapid exponential decay. These are referred to as *evanescent waves*.



This linear systems formulation provides considerable insight into diffraction phenomena (i.e., the Fresnel fringes) not provided by the historical treatment.





# The Huygens' Wavelett as an Impulse Response (Superposition of Spherical Waves)

The convolution theorem of Fourier transform theory requires that a convolution operation exists in the domain of real space that is equivalent to Eq.(11). We thus have an alternative method of expressing the complex amplitude distribution in the observation plane by convolving the disturbance emerging from the aperture with the *impulse response* of free space.

This impulse response is obtained by inverse Fourier transforming the transfer function of free space expressed in Eq.(12). Starting with the well-known Wehl expansion formula,\* and following Lalor,\*\* we obtain

$$h(\hat{x}, \hat{y}; \hat{z}) = \mathcal{F}^{-1} \{ \exp(i2\pi \gamma \hat{z}) \} = \left( \frac{1}{2\pi\hat{r}} - i \right) \frac{\hat{z}}{\hat{r}} \frac{\exp(i2\pi\hat{r})}{\hat{r}} \quad (13)$$

The above equation is an exact mathematical expression for a Huygens' wavelett that is valid right down to the actual disturbance emerging from the diffracting aperture; however, for  $\hat{r} \gg 1$ , it reduces to the familiar expression for a spherical wave with a cosine obliquity factor,  $\hat{z}/\hat{r}$ , and a  $\pi/2$  phase delay.

$$h(\hat{x}, \hat{y}; \hat{z}) = -i \frac{\hat{z}}{\hat{r}} \frac{\exp(i2\pi\hat{r})}{\hat{r}} = \frac{\hat{z}}{\hat{r}} \frac{\exp[i2\pi(\hat{r} - 1/4)]}{\hat{r}} \quad (14)$$

**Impulse Response of Free Space  $\equiv$  Huygens' Wavelett**

\* H. Wehl, Ann. Phys. 60, 481 (1919).

\*\* E. Lalor, J. Opt. Sci. Am. 58, 1235 (1968).

# The Rayleigh-Sommerfeld Diffraction Integral (Superposition of Spherical Waves)

If we write down the convolution integral for the disturbance in the observation plane, using the expression in Eq.(13) for  $h(\hat{x}, \hat{y}; \hat{z})$ , we obtain the *general Rayleigh-Sommerfeld Diffraction Formula*

$$U(\hat{x}, \hat{y}; \hat{z}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_o(\hat{x}', \hat{y}'; 0) \left( \frac{1}{2\pi\hat{\ell}} - i \right) \frac{\hat{z}}{\hat{\ell}} \frac{\exp(i2\pi\hat{\ell})}{\hat{\ell}} d\hat{x}' d\hat{y}' \quad (15)$$

where

$$\hat{\ell}^2 = (\hat{x} - \hat{x}')^2 + (\hat{y} - \hat{y}')^2 + \hat{z}^2 .$$

Note that we are now using  $\hat{x}'$  and  $\hat{y}'$  as dummy variables of integration (in the plane of the diffracting aperture). This is to avoid confusion since both the plane of the aperture and the observation plane contain the same  $\hat{x}$  and  $\hat{y}$  coordinates, differing only by the  $\hat{z}$  parameter.

No approximations have been made in deriving Eq.(15); hence, this expression for the diffracted wave field is valid throughout the entire space in which the diffraction occurs---right down to the aperture. This equation reduces to the less general but more familiar form of the Rayleigh-Sommerfeld diffraction formula when  $\hat{z} \gg 1$

$$U(\hat{x}, \hat{y}; \hat{z}) = -i \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_o(\hat{x}', \hat{y}'; 0) \frac{\hat{z}}{\hat{\ell}} \frac{\exp(i2\pi\hat{\ell})}{\hat{\ell}} d\hat{x}' d\hat{y}' \quad (16)$$

We have thus derived the general form of the Rayleigh-Sommerfeld diffraction integral from two basic assumptions; (i) that the Fourier transform of the optical disturbance exists, and (ii) that in propagating, each of the plane wave components obeys the Helmholtz wave equation.

# Aberrations of Diffracted Wave Fields\*

We have previously seen that performing a binomial expansion of the quantity  $\hat{\ell}$ , and retaining only the first two terms results in the Fresnel diffraction formula, which is invalid in the near field and also suffers from a paraxial limitation. In order *not* to impose these restrictions, all terms of the binomial expansion must be retained. This can be accomplished by re-writing the Rayleigh-Sommerfeld diffraction integral as the following Fourier transform integral

$$U(\hat{x}_2, \hat{y}_2; \hat{z}) = \frac{\exp(i2\pi\hat{z})}{i\hat{z}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{U}_o(\hat{x}_1, \hat{y}_1; \hat{x}_2, \hat{y}_2) \exp[-(i2\pi/\hat{z})(\hat{x}_1\hat{x}_2 + \hat{y}_1\hat{y}_2)] d\hat{x}_1 d\hat{y}_1 \quad (17)$$

Where the complex quantity

$$\mathcal{U}_o(\hat{x}_1, \hat{y}_1; \hat{x}_2, \hat{y}_2) = T_o(\hat{x}_1, \hat{y}_1; 0) \exp(i2\pi\hat{W})$$

can be regarded as a generalized pupil function that contains phase variations (wavefront aberrations). These aberrations are precisely the effects ignored when making the usual Fresnel and Fraunhofer approximations.

$$\hat{W}(\hat{x}, \hat{y}) \equiv \textit{Wavefront Aberration Function}$$

Thus near-field diffraction patterns are merely *aberrated* Fraunhofer diffraction patterns, and those aberrations are our old friends: spherical aberration, coma, astigmatism, etc.

\* J. E. Harvey and R. V. Shack, "Aberrations of Diffracted Wave Fields", Appl. Opt. 17 (18), 3003-3009, Sept 1978.

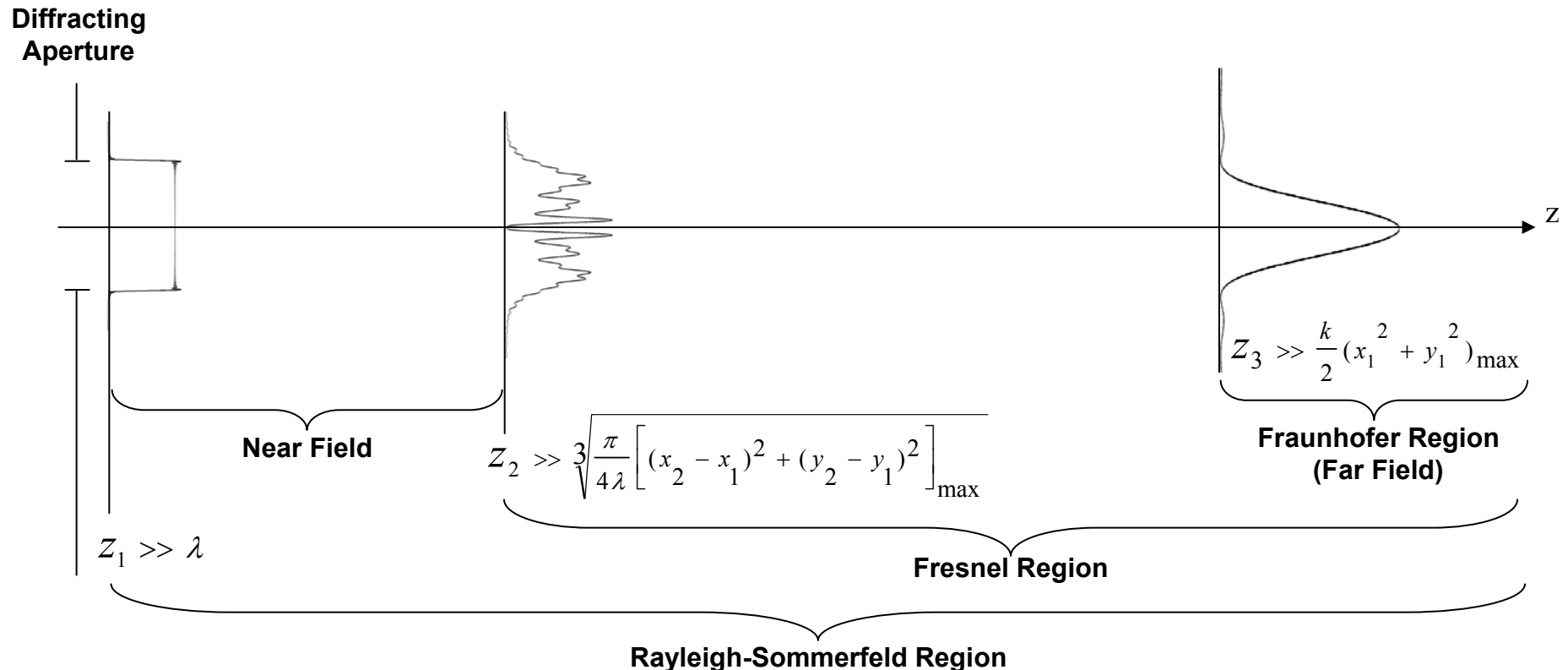
# Aberration Coefficients for Different Configurations

The individual terms of the binomial expansion are identical in form to the terms of the conventional wavefront aberration function, we can thus merely equate coefficients of like terms and obtain analytic expressions for the aberration coefficients.

Aberrations	Geometrical Configuration		
	Plane Plane	Sphere Plane	Sphere Hemisphere
$\hat{W}_{200}$ (Piston Error)	$\frac{\hat{z}}{2} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^2$	$\frac{\hat{z}}{2} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^2$	0
$\hat{W}_{020}$ (Defocus)	$\frac{\hat{z}}{2} \left( \frac{\hat{d}}{2\hat{z}} \right)^2$	0	0
$\hat{W}_{111}$ (Lateral Mag. Error)	0	0	0
$\hat{W}_{400}$ (3rd - order Piston)	$-\frac{\hat{z}}{8} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^4$	$-\frac{\hat{z}}{8} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^4$	0
$\hat{W}_{040}$ (Spherical Aberration)	$-\frac{\hat{z}}{8} \left( \frac{\hat{d}}{2\hat{z}} \right)^4$	0	0
$\hat{W}_{131}$ (Coma)	$\frac{\hat{z}}{2} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right) \left( \frac{\hat{d}}{2\hat{z}} \right)^3$	$\frac{\hat{z}}{2} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right) \left( \frac{\hat{d}}{2\hat{z}} \right)^3$	$\frac{\hat{r}}{2} \beta_{\max} \left( \frac{\hat{d}}{2\hat{r}} \right)^3$
$\hat{W}_{222}$ (Astigmatism)	$-\frac{\hat{z}}{2} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^2 \left( \frac{\hat{d}}{2\hat{z}} \right)^2$	$-\frac{\hat{z}}{2} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^2 \left( \frac{\hat{d}}{2\hat{z}} \right)^2$	$-\frac{\hat{r}}{2} \beta_{\max}^2 \left( \frac{\hat{d}}{2\hat{r}} \right)^2$
$\hat{W}_{220}$ (Field Curvature)	$-\frac{\hat{z}}{4} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^2 \left( \frac{\hat{d}}{2\hat{z}} \right)^2$	$-\frac{\hat{z}}{4} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^2 \left( \frac{\hat{d}}{2\hat{z}} \right)^2$	0
$\hat{W}_{311}$ (Distortion)	$\frac{\hat{z}}{2} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^3 \frac{\hat{d}}{2\hat{z}}$	$\frac{\hat{z}}{2} \left( \frac{\hat{s}_{\max}}{\hat{z}} \right)^3 \frac{\hat{d}}{2\hat{z}}$	0

# Tolerance on Defocus Precisely Locates the Far Field\*

Fresnel diffraction patterns are merely *defocused* Fraunhofer diffraction patterns.

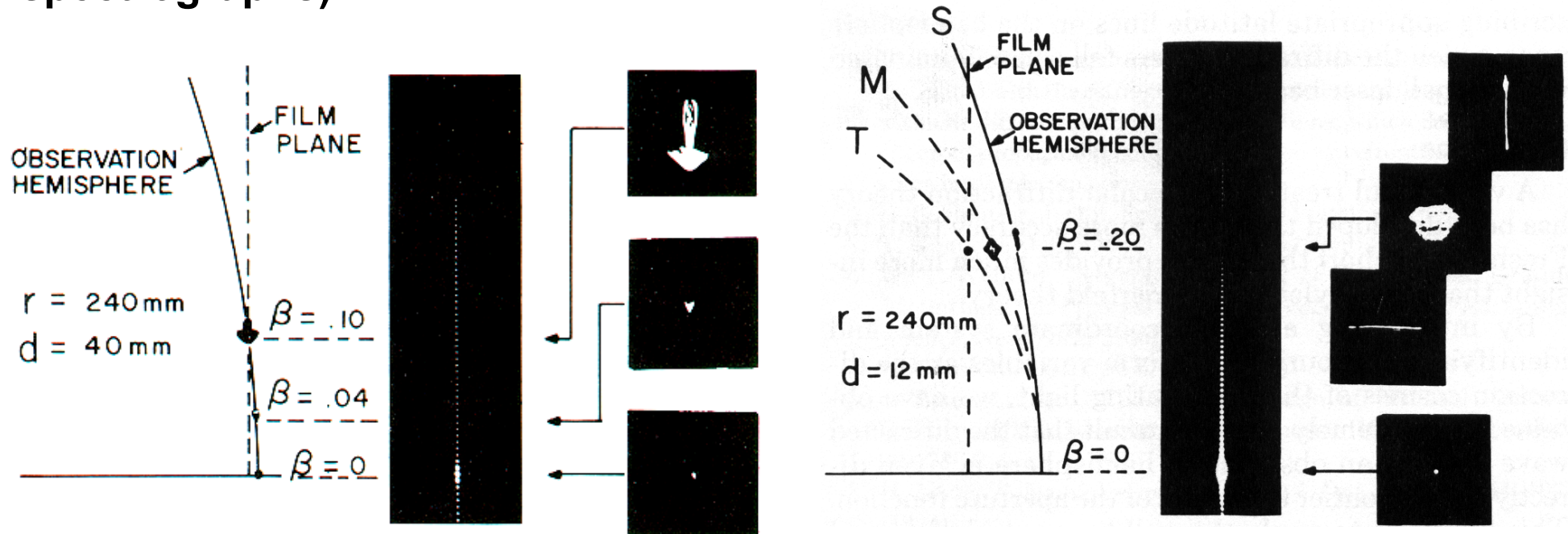


Optical engineers performing field tests or experiments can thus place a tolerance on the amount of defocus they are willing to allow (such as  $W_{020} \leq \lambda/4$ ), and calculate precisely where the boundary between the Fresnel Region and the Far Field is located.

\* J. E. Harvey, A. Krywonos, and D. Bogunovic, "Tolerance on Defocus precisely Locates the Far Field", Appl. Opt. 41, 2586-2588 (2002).

# Coma and Astigmatism\*

It is well known that *coma* and *astigmatism* are frequently present in diffracted orders produced when converging beams with a small focal ratio are incident upon a diffraction grating (such as in many grating spectrographs).



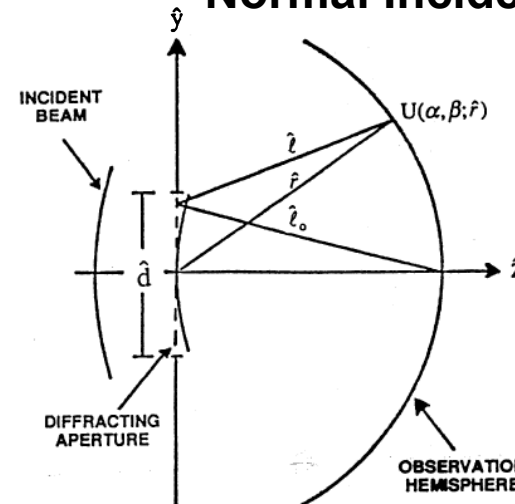
These aberrations are not; however, due to any “flaw” in the grating. They are *inherent to the diffraction process*. The grating merely concentrates light at field positions where the aberrations can manifest themselves.

\* J. E. Harvey and R. V. Shack, “Aberrations of Diffracted Wave Fields”, Appl. Opt. 17 (18), 3003-3009, Sept 1978.

# Shift-invariance in Direction Cosine Space\*

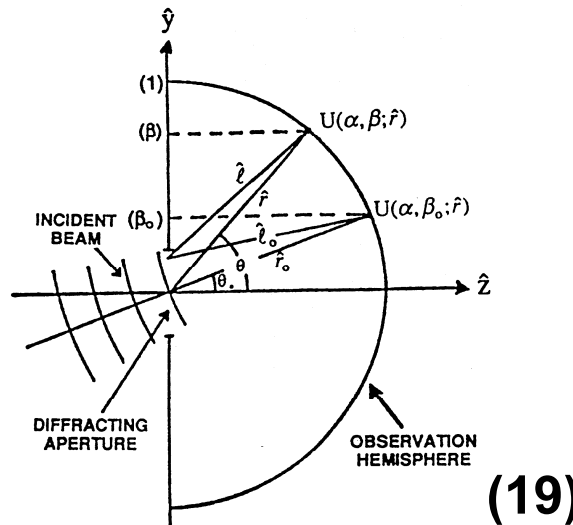
When a spherical wave is incident upon the diffracting aperture and the observation space is a hemisphere, the phase variations (coma and astigmatism) are frequently negligible and the diffracted wave field on the hemisphere is merely the Fourier transform of the aperture function multiplied by a spherical Huygen's wavelet. Furthermore, this Fourier transform relationship is valid not merely over a small region about the optical axis, but over the *entire* hemisphere. Adding a linear phase variation causes the spherical incident wavefront to strike the diffracting aperture at an arbitrary angle  $\theta_o$ . Application of the shift theorem thus indicates that the scalar diffraction process is shift-invariant with respect to incident angle when formulated in direction cosine space.

## Normal Incidence



$$U(\alpha, \beta; \hat{r}) = \gamma[\exp(i2\pi\hat{r})/(i\hat{r})] \mathcal{F}\{U_o(\hat{x}, \hat{y}; 0)\} \quad (18)$$

## Arbitrary Angle of Incidence



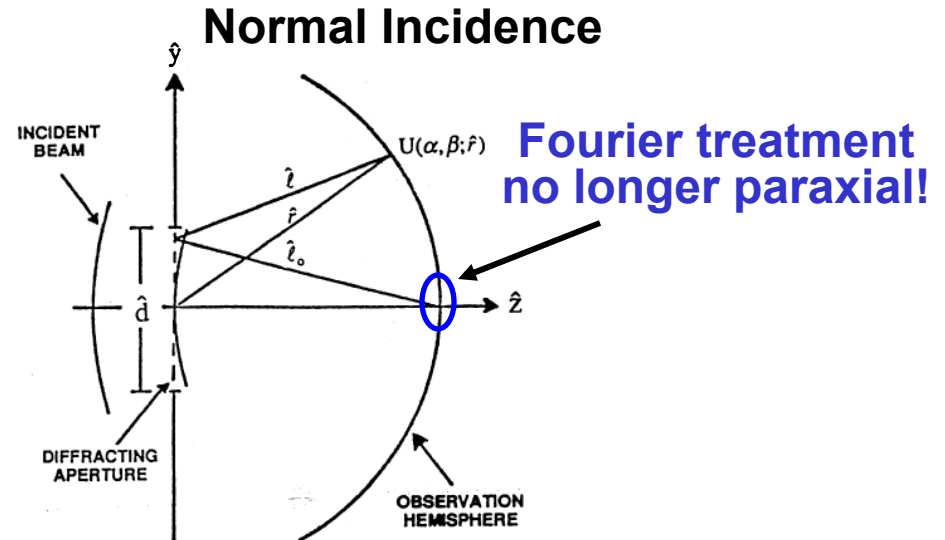
$$U(\alpha, \beta - \beta_o; \hat{r}) = \gamma[\exp(i2\pi\hat{r})/(i\hat{r})] \mathcal{F}\{U_o(\hat{x}, \hat{y}; 0)\exp(i2\pi\beta_o\hat{y})\} \quad (19)$$

## Summary

- Transfer Function of Free Space is Derived
- Huygens' Wavelet is the Impulse Response
- Convolution Yields Rayleigh-Sommerfeld Eq.
- Aberrations of Diffracted Wave Fields
- Aberrations Depend upon Geo. Configuration
- Shift-invariance in Direction Cosine Space

# Shift-invariance in Direction Cosine Space\*

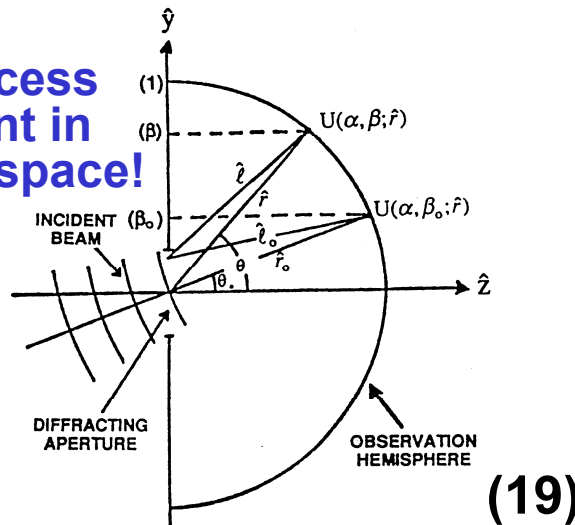
When a spherical wave is incident upon the diffracting aperture and the observation space is a hemisphere, the phase variations (coma and astigmatism) are frequently negligible and the diffracted wave field on the hemisphere is merely the Fourier transform of the aperture function multiplied by a spherical Huygen's wavelet. Furthermore, this Fourier transform relationship is valid not merely over a small region about the optical axis, but over the *entire* hemisphere. Adding a linear phase variation causes the spherical incident wavefront to strike the diffracting aperture at an arbitrary angle  $\theta_o$ . Application of the shift theorem thus indicates that the scalar diffraction process is shift-invariant with respect to incident angle when formulated in direction cosine space.



$$U(\alpha, \beta; \hat{r}) = \gamma[\exp(i2\pi\hat{r})/(i\hat{r})] \mathcal{F}\{U_o(\hat{x}, \hat{y}; 0)\} \quad (18)$$

## Arbitrary Angle of Incidence

**Diffraction Process is shift-invariant in direction cosine space!**



$$U(\alpha, \beta - \beta_o; \hat{r}) = \gamma[\exp(i2\pi\hat{r})/(i\hat{r})] \mathcal{F}\{U_o(\hat{x}, \hat{y}; 0)\exp(i2\pi\beta_o\hat{y})\} \quad (19)$$

## Summary

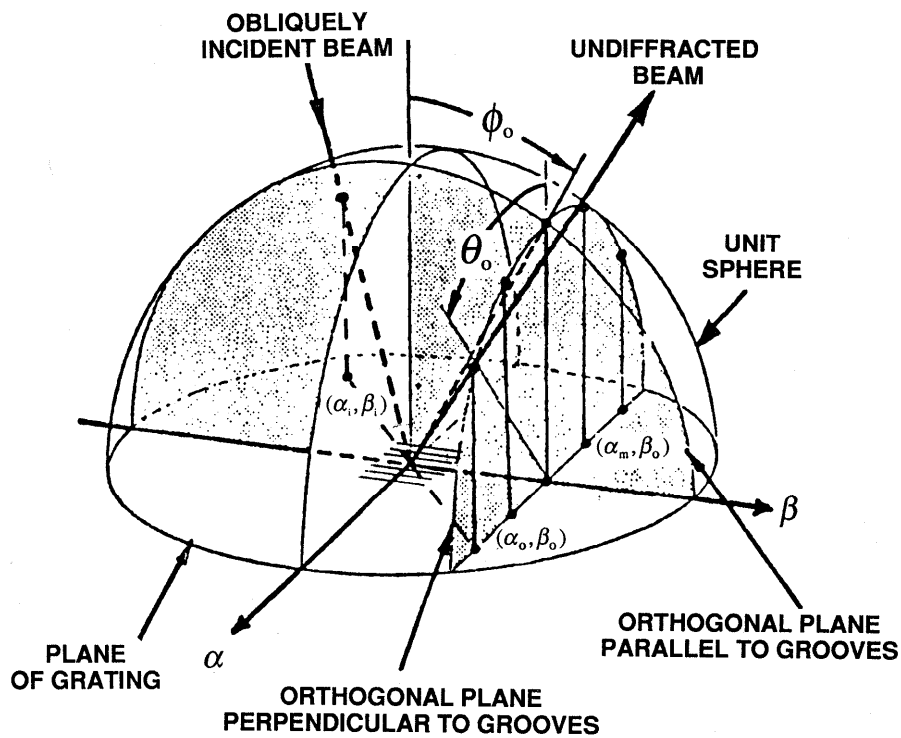
- Transfer Function of Free Space is Derived
- Huygens' Wavelet is the Impulse Response
- Convolution Yields Rayleigh-Sommerfeld Eq.
- Aberrations of Diffracted Wave Fields
- Aberrations Depend upon Geo. Configuration
- Shift-invariance in Direction Cosine Space



# Shift-Invariance in Direction Cosine Space\*

## Global View of Diffraction

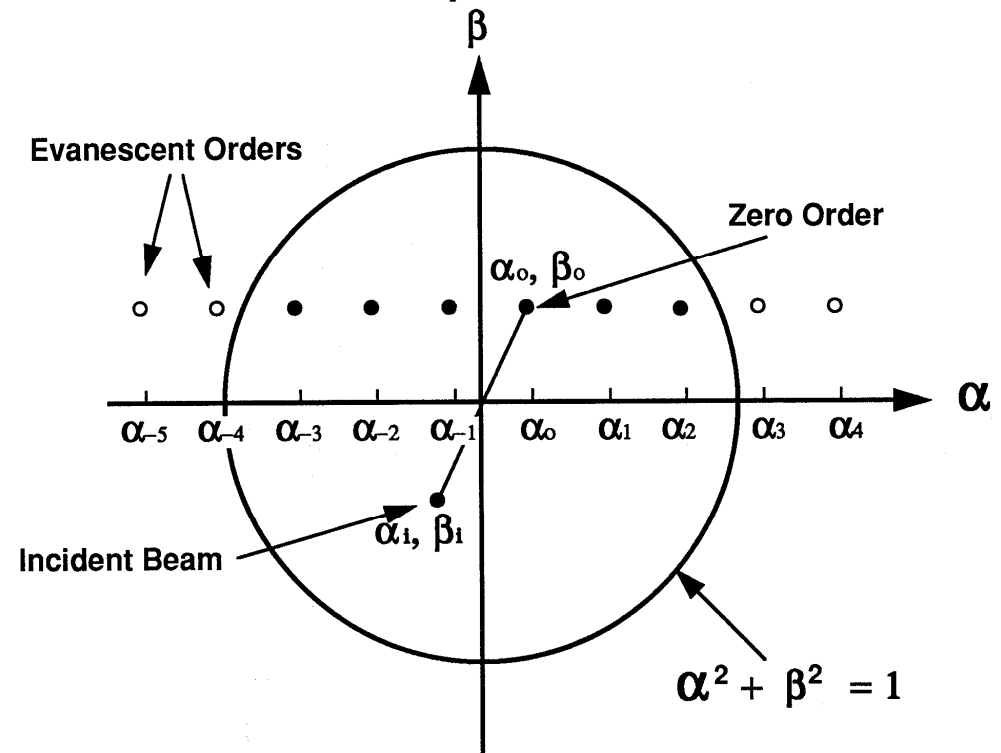
Illustration of the position of the diffracted orders in real space and direction cosine space for an arbitrary obliquely incident beam (conical diffraction).



$$\begin{aligned} \alpha_m &= \sin \theta_m \cos \phi_o \\ \alpha_i &= -\sin \theta_o \cos \phi_o \\ \beta_i &= -\sin \phi_o \end{aligned} \quad (20)$$

## Direction Cosine Diagram

Illustration of the evanescent and propagating orders. Diffraction angles are readily calculated from transformation equations.



$$\begin{aligned} \alpha_m + \alpha_i &= m\lambda/d \\ \beta_m + \beta_i &= 0 \end{aligned} \quad (21)$$

Grating Equation (Grooves II to  $\beta$  axis)

# Arbitrary Incident Angle and Orientation of Grating (number and position of propagating orders)

$$\alpha_m + \alpha_i = \frac{m\lambda}{d} \sin \psi \quad (22)$$

$$\beta_m + \beta_i = \frac{m\lambda}{d} \cos \psi$$

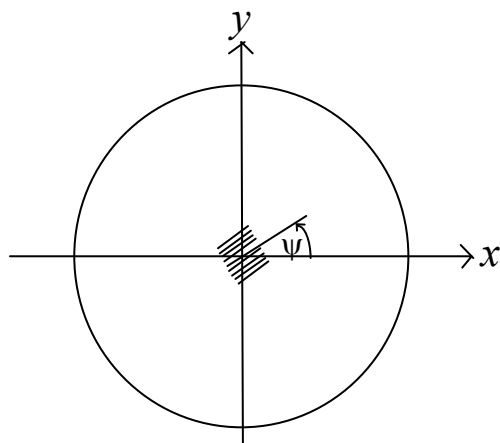
General Grating Equation  
for Arbitrary Orientation

$$\phi_i = 0$$

$$\psi = \pi / 2$$

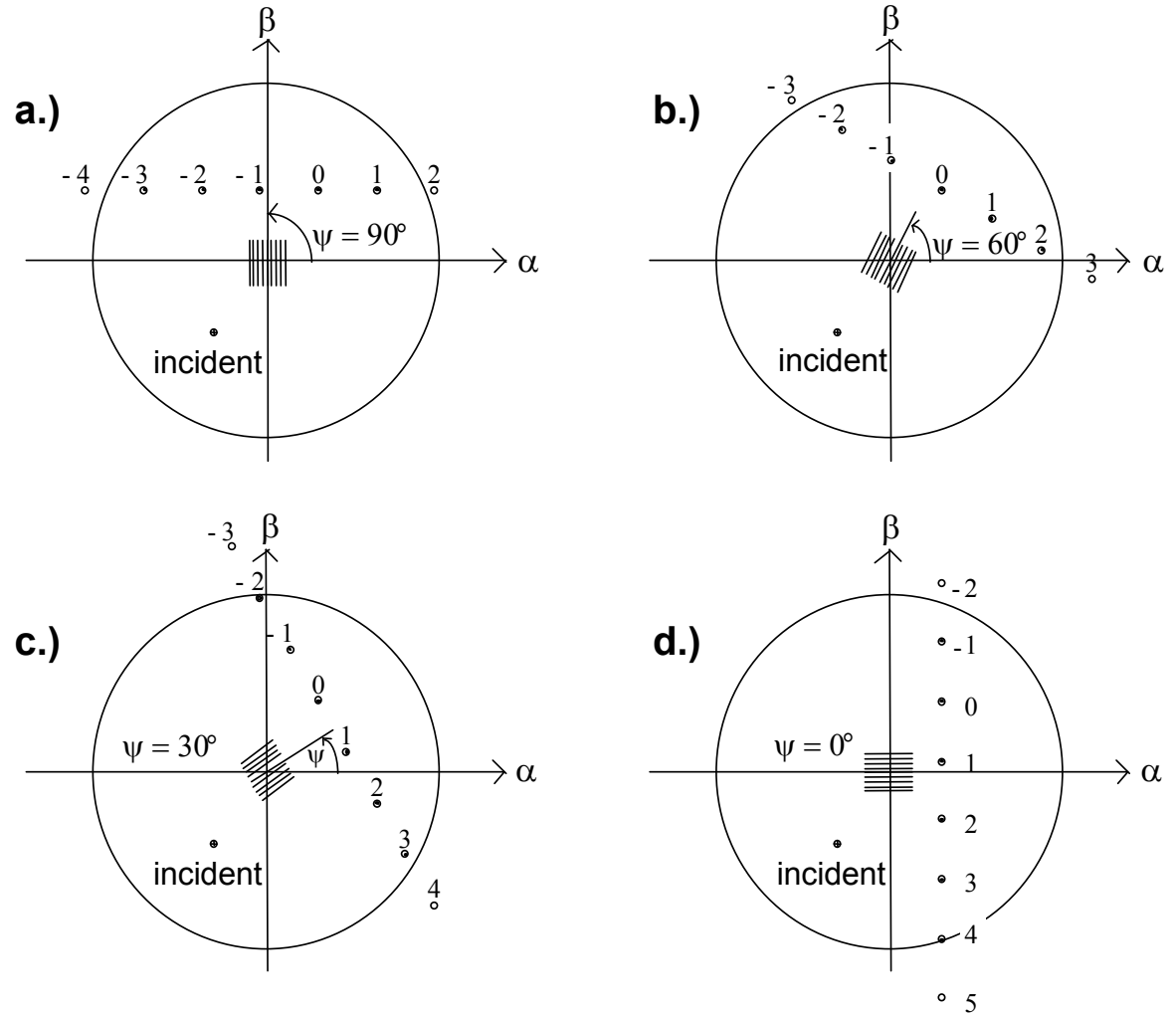
$$\sin \theta_m + \sin \theta_i = m\lambda / d$$

Standard Grating Equation



Groove Orientation

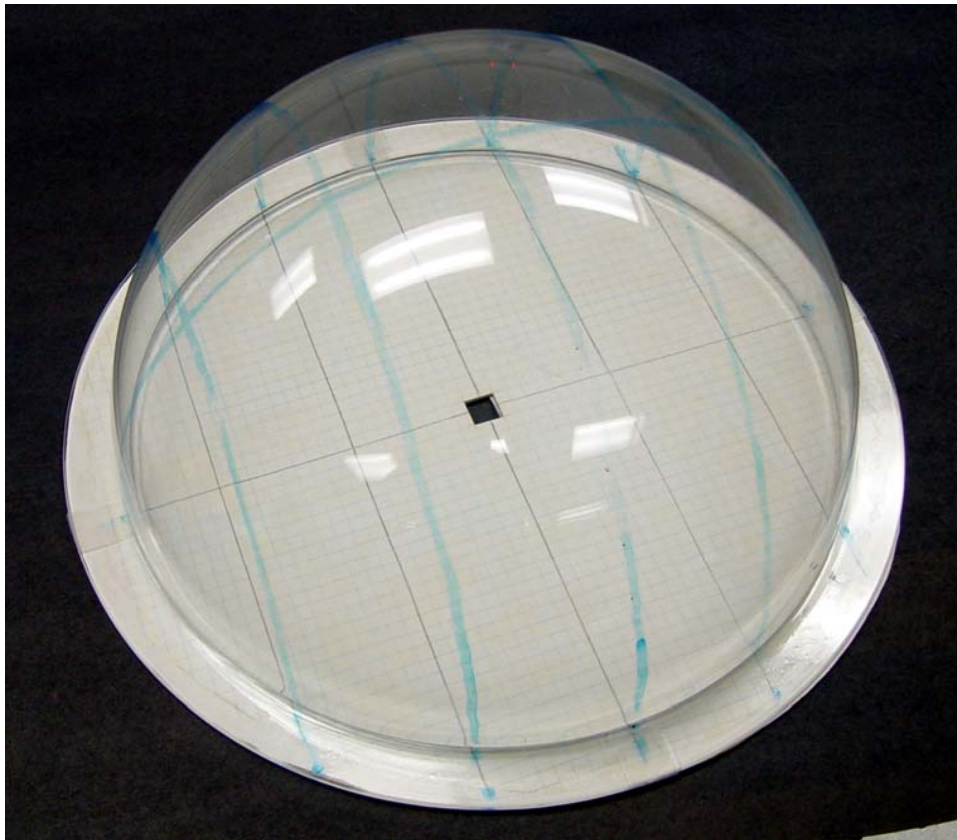
Position of Diffracted Orders in Direction Cosine Space



The direction cosine diagram is thus a simple graphical tool for determining precisely which orders are propagating and which ones are evanescent for an arbitrary incident angle and grating orientation.

# Classroom Prop used to Observe “Shift-invariance” in Direction Cosine Space

A plastic dome serves as a convenient observation hemisphere to help students observe the “shift-invariant” behavior in direction cosine space. Graph paper is placed on its base and latitude lines marked on the observation hemisphere. A transmission grating is located at its center, and with a laser beam incident from the back, the diffracted orders are observed where they strike the hemisphere.



# Quantitative Distribution of Radiant Power among the Diffracted Orders

---


We now know the number and angular distribution of propagating diffracted orders; however, suppose we want to know the quantitative distribution of radiant power among the propagating diffracting orders.

- It is widely believed, even among diffraction experts, that scalar theory is incapable of accurately predicting the diffraction efficiencies for non-paraxial diffracted orders, and that a rigorous electromagnetic (vector) theory is required!
- In fact, it is widely (and erroneously) believed that scalar diffraction theory is synonymous with paraxial theory; i.e., scalar diffraction theory is *inherently limited* to making predictions in the paraxial regime!

Of course, what I am about to show you is that, if you make the transformation into direction cosine space, and if you choose the proper radiometric quantity, even non-paraxial diffraction efficiencies can be predicted (and intuitively understood) using simple scalar diffraction theory.

# Outline

---

- **Paraxial Limitation in Conventional Fourier Optics**
  - Fraunhofer Diffraction and the Paraxial Limitation
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# Radiometry: The Neglected Stepchild of Physics

---

Let us briefly review the definitions of a few radiometric quantities. In the past physicists have frequently used the word *intensity* to mean the flow of *energy per unit area per unit time*. However, by international, if not universal agreement, that term is slowly being replaced by the word *irradiance*.

$$\text{Irradiance} \equiv E = \frac{\partial P}{\partial A_c} \quad (\text{watts/area})$$

$$\text{Radiant Exitance} \equiv M = \frac{\partial P}{\partial A_s} \quad (\text{watts/area})$$

$$\text{Radiant Intensity} \equiv I = \frac{\partial P}{\partial \omega_c} \quad (\text{watts/steradian})$$

$$\text{Radiance} \equiv L = \frac{\partial^2 P}{\partial \omega_c \partial A_s \cos \theta_s} \quad (\text{watts/steradian projected area})$$

(23)

**Radiance**, the radiometric analog to the more familiar photometric term *brightness*, is defined as radiant power per unit solid angle per unit *projected source area*.

# Getting Intense about Intensity\*

---

Jim Palmer has stated that: “The term *intensity* is probably the most misused and abused word in the technical literature. It can be found to be used in at least six (6) contexts: (1) watts per steradian, (2) watts per unit area, (3) watts per unit area per steradian, (4) just plain watts, and most bizarre (5)  $\text{cm}^{-1}/\text{molecule}\cdot\text{cm}^{-2}$ , and finally (6)  $\text{cm}^{-2}\cdot\text{amagat}^{-1}$ . These last two are used to describe spectral line strengths.”

**Intensity is an International System of Units (SI) Base Quantity!**

As an SI Base Quantity, it has the same stature as the other six SI Base Quantities: length (meter), mass (kilogram), time (second), electric current (ampere), thermodynamic temperature (Kelvin), and amount of substance (mole), and finally, **intensity carries the units of watts per steradian!** All other physical quantities are derived from these seven SI Base Quantities.

*Intensity* is properly used when describing the radiation emanating from a *point source*, or a source small compared to the distance between the source and the collector. For *extended sources*, one must use the radiometric quantity *radiance*.

**And most diffracting apertures should be considered to be extended sources!**

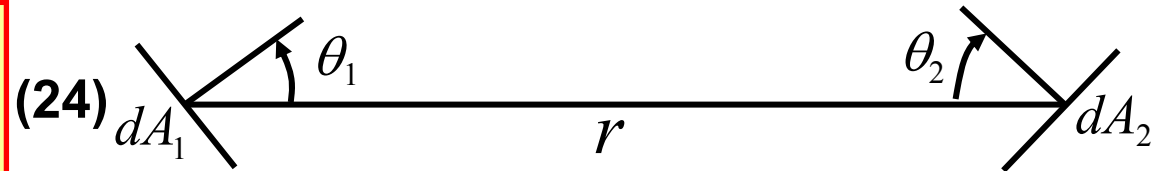
\* James M. Palmer, “Getting Intense about Intensity”, Optics & Photonics News, (Feb 1995).

# The Fundamental Theorem of Radiometry (Derived from the Definition of Radiance)

An extended source, that is, one whose dimensions are significant, must be treated differently than a point source. A small area of the source will radiate a certain amount of power per unit solid angle, thus, the radiation characteristics of an extended source are expressed in terms of power per unit solid angle *per unit projected area*. This is called *radiance*.

The definition of radiance provides the *Fundamental Theorem of Radiometry* which describes the radiant power transfer between a radiant source  $dA_1$  and a receiver  $dA_2$ .

$$d^2P = L \frac{dA_1 \cos\theta_1 dA_2 \cos\theta_2}{r^2} \quad (24)$$

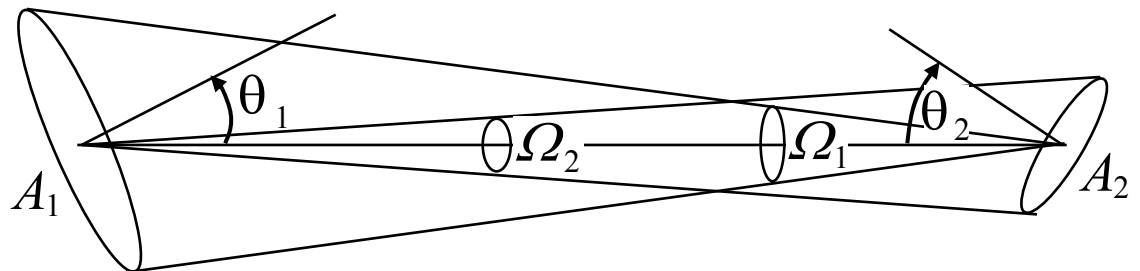


Assuming small angles, we can group the  $r^2$  with either the source or the receiver projected area and obtain two equivalent expressions

$$d^2P = L d\Omega_1 dA_2 \cos\theta_2 = L dA_1 \cos\theta_1 d\Omega_2$$

Dropping the differentials, the radiant power transmitted to the collector from the source is given by the product of the source radiance and either of the two *projected area, solid angle* “ $A_p\Omega$ ” products.

$$\begin{aligned} P &= L \Omega_1 A_2 \cos\theta_2 \\ &= L A_1 \cos\theta_1 \Omega_2 \end{aligned}$$



Either  $A_p\Omega$  product can be used. This is often a convenient flexibility in making calculations.



# Diffracted Radiance is the Quantity that is Shift-invariant in Direction Cosine Space\*

The direction cosines  $\alpha$ ,  $\beta$ , and  $\gamma$  are related to the angular variables  $\theta$  and  $\phi$  in conventional spherical coordinates by the following expressions, where we have dropped the subscript  $s$  on the angles associated with the source

$$\alpha = \sin\theta \cos\phi, \quad \beta = \sin\theta \sin\phi, \quad \gamma = \cos\theta .$$

For this coordinate transformation, the Jacobian determinant in the well-known change of variables theorem is given by  $\sin\theta \cos\theta$  and the differential solid angle can be expressed as

$$d\omega_c = \sin\theta d\theta d\phi = d\alpha d\beta/\gamma$$

Applying the change of variables theorem for an arbitrary solid angle, we find that, if the source is a uniformly illuminated diffracted aperture, the diffracted radiance distribution in direction cosine space is given by \*

$$L(\alpha, \beta) = \frac{\lambda^2}{A_s} \left| \mathcal{F}\{U_o(\hat{x}, \hat{y}; 0)\} \right|^2$$

From the shift theorem of Fourier Transform theory, we have

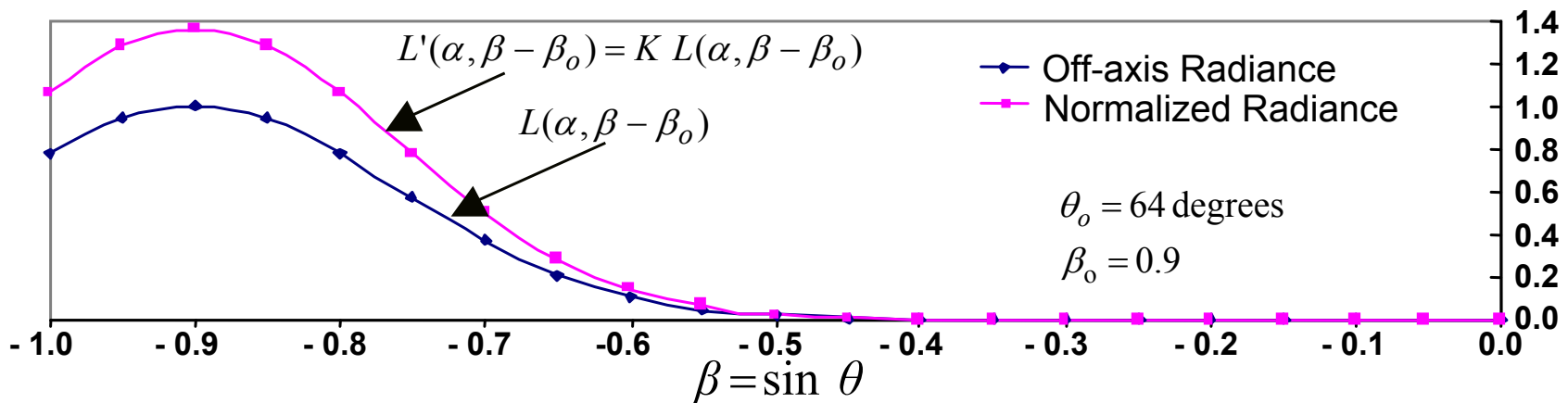
$$L(\alpha, \beta - \beta_o) = \gamma_o \frac{\lambda^2}{A_s} \left| \mathcal{F}\{U_o(\hat{x}, \hat{y}; 0) \exp(i2\pi\beta_o \hat{y})\} \right|^2 \quad (25)$$

We have thus shown that the squared modulus of the Fourier transform of the complex amplitude distribution emerging from the diffracting aperture yields *diffracted radiance*, not *irradiance* or *intensity*. This realization greatly extends the range of parameters over which simple Fourier techniques can be used to make accurate calculations of wide-angle diffraction phenomena.

\* J. E. Harvey, et.al., "Diffracted Radiance: A Fundamental Quantity in Non-Paraxial Scalar Diff. Theory", Appl. Opt. 38, 6469 (1999).

# Re-Normalization Conserves Energy in the Presence of Evanescent Waves

In extreme non-paraxial applications, the diffracted radiance distribution function will extend beyond the unit circle in direction cosine space. This can occur due to high spatial frequency content in the diffracting aperture resulting in very large diffracted angles, or due to large incident angles that shifts a radiance distribution function of modest width such that it extends beyond the unit circle. In either case, evanescent waves are produced and the above equations for radiance must be re-normalized. This is not done in a heuristic manner to conserve energy, but is a direct result of Parseval's theorem from Fourier transform theory.



$$\begin{aligned}
 L'(\alpha, \beta - \beta_0) &= K \gamma_o \frac{\lambda^2}{A_s} \left| \mathcal{F}\{U_o(\hat{x}, \hat{y}; 0) \exp(i2\pi\beta_o \hat{y})\} \right|^2 & \text{for } \alpha^2 + \beta^2 \leq 1 \\
 L'(\alpha, \beta - \beta_0) &= 0 & \text{for } \alpha^2 + \beta^2 > 1
 \end{aligned} \tag{26}$$

$$K = \frac{\int_{\alpha=-\infty}^{\infty} \int_{\beta=-\infty}^{\infty} L(\alpha, \beta - \beta_0) d\alpha d\beta}{\int_{\alpha=-1}^1 \int_{\beta=-\sqrt{1-\alpha^2}}^{\sqrt{1-\alpha^2}} L(\alpha, \beta - \beta_0) d\alpha d\beta} \equiv \text{Normalization Constant} \tag{27}$$

The well-known Wood's anomalies that occur in diffraction grating efficiency measurements are entirely consistent with this predicted re-normalization in the presence of evanescent waves.

# Diffracted Intensity is Definitely not Shift-Invariant

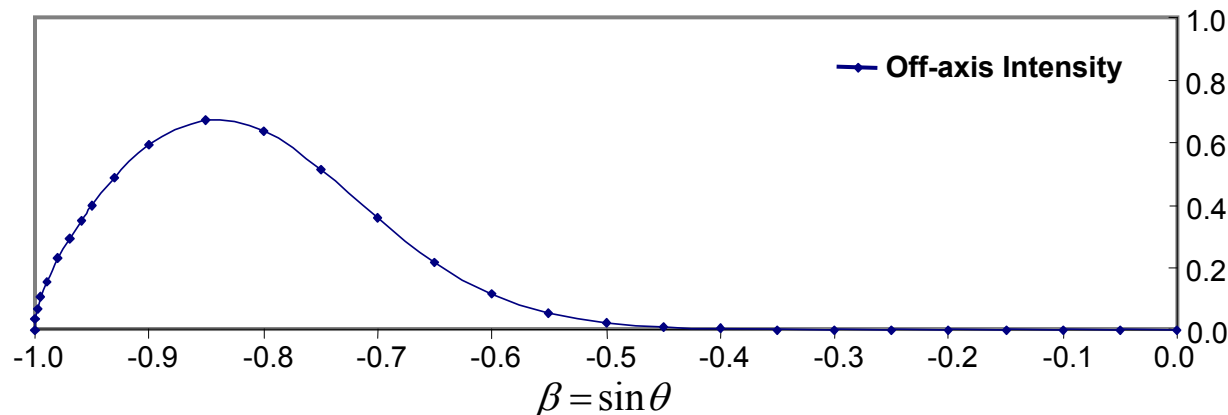
In order to calculate radiant intensity to compare with experimental measurements (radiance is not a directly measurable quantity), one needs only to apply Lambert's cosine law (i.e., multiply the radiance by  $\gamma = \cos \theta_s$ ) and integrate over the source area

$$I(\alpha, \beta) = \int_{A_s} L(\alpha, \beta) \cos \theta_s \, \partial A_s$$

Again, if the source is a uniformly illuminated diffracting aperture, we obtain diffracted intensity by multiplying by  $A_s \cos \theta_s$

$$\begin{aligned} I(\alpha, \beta - \beta_o) &= K \gamma_o \gamma \lambda^2 \left| \mathcal{F}\{U_o(\hat{x}, \hat{y}; 0) \exp(i2\pi\beta_o \hat{y})\} \right|^2 & \text{for } \alpha^2 + \beta^2 \leq 1 \\ I(\alpha, \beta - \beta_o) &= 0 & \text{for } \alpha^2 + \beta^2 > 1 \end{aligned} \quad (28)$$

Although diffracted radiance can exhibit a discontinuity at the edge of the unit circle (for a Lambertian emitter the radiance is constant and drops discontinuously to zero at the edge of the unit circle), Lambert's Cosine Law assures that diffracted intensity never exhibits such discontinuities. The figure below illustrates the diffracted intensity profile of the current example in direction cosine space. Note the asymmetry in this intensity profile that is characteristic of diffraction patterns at large incident angles.



# Radiance as a Fundamental Quantity (Should we be Surprised?)

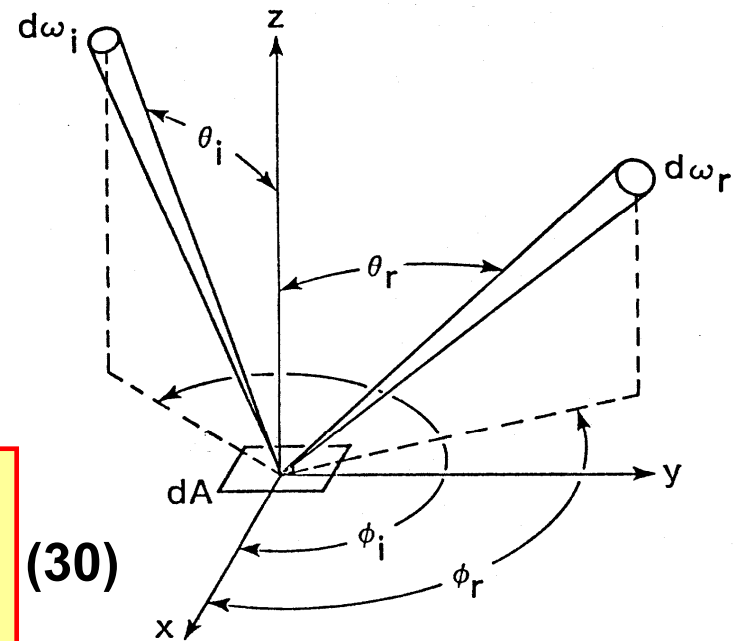
In geometrical optics we have the “Brightness Theorem” which states that the brightness of an image can never exceed the brightness of the object. *Brightness* is merely the photometric analog of the radiometric quantity *radiance*. Stated another way, if the radiant power transmitted through an optical system is constant (no losses), then

$$\frac{L}{n^2} = \frac{L'}{n'^2} = \text{Const.}$$

Brightness Theorem  
(Radiance is Conserved) (29)


Also, the bidirectional reflectance distribution function (BRDF) is a fundamental quantity that completely describes the scattering properties of a surface. It is defined as the *reflected radiance* (radiant power per unit solid angle per unit projected area) in a given direction divided by the *incident irradiance* (radiant power per unit area)

$$BRDF = f(\theta_r, \phi_r; \theta_i, \phi_i) = \frac{dL_r(\theta_r, \phi_r; \theta_i, \phi_i)}{dE_i(\theta_i, \phi_i)} \quad (30)$$



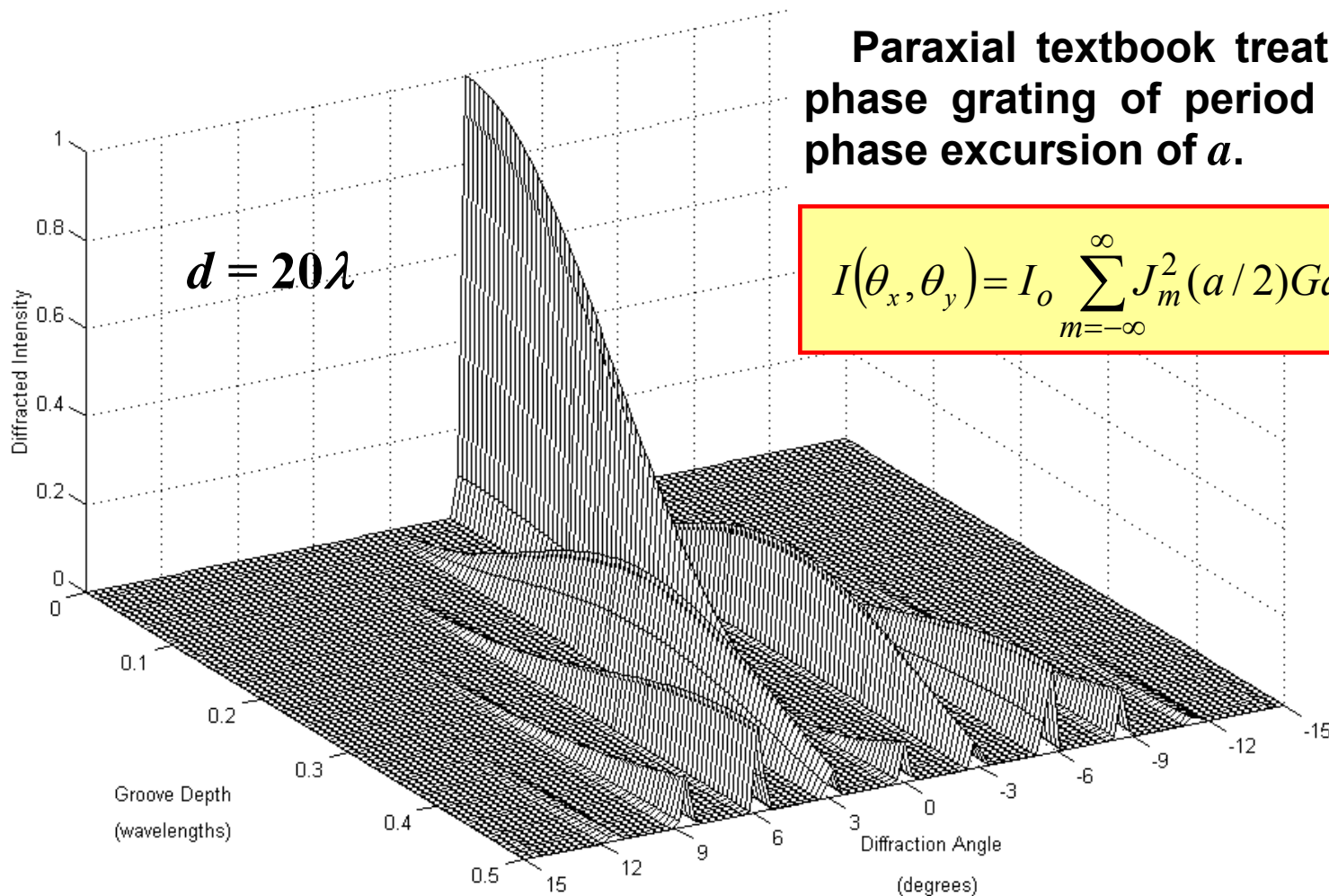
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# Example # 1: Non-paraxial Behavior of Sinusoidal Phase Gratings

Scalar diffraction theory is frequently considered inadequate for predicting diffraction efficiencies for grating applications where  $\lambda/d > 0.1$ . It has also been stated that scalar theory imposes energy upon the evanescent diffracted orders.



Paraxial textbook treatment of a sinusoidal phase grating of period  $d$  and peak to peak phase excursion of  $a$ .

$$I(\theta_x, \theta_y) = I_o \sum_{m=-\infty}^{\infty} J_m^2(a/2) \text{Gaus}^2 \left[ \frac{b}{\lambda} (\theta_x - m\lambda/d, \theta_y) \right]$$

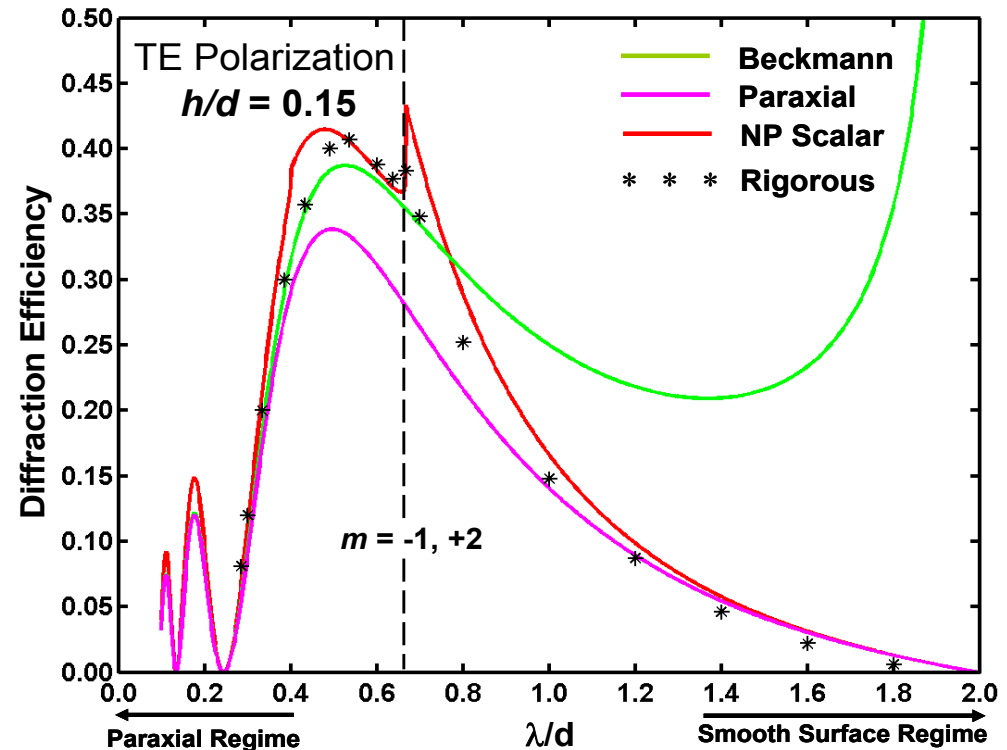
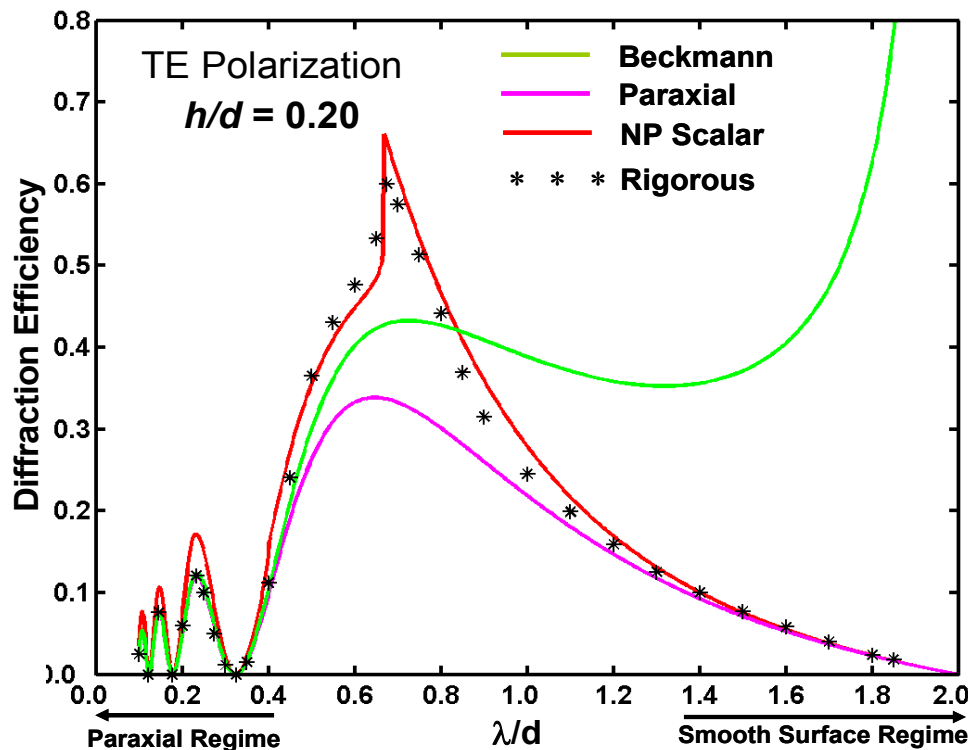
(31)

This leads to the common misconception that it is impossible to get more than 33.86% of the total reflected energy into the +1 diffracted order.

# Diffraction Efficiency of a Perfectly Conducting Sinusoidal Phase Grating\*

The diffraction efficiency for a perfectly conducting sinusoidal phase grating using our non-paraxial linear systems model of scalar diffraction theory is given by:

$$\eta_m = \frac{P_m}{P_T} = \frac{J_m^2(a/2)}{\sum_{m=\min}^{\max} J_m^2(a/2)} \quad (32)$$

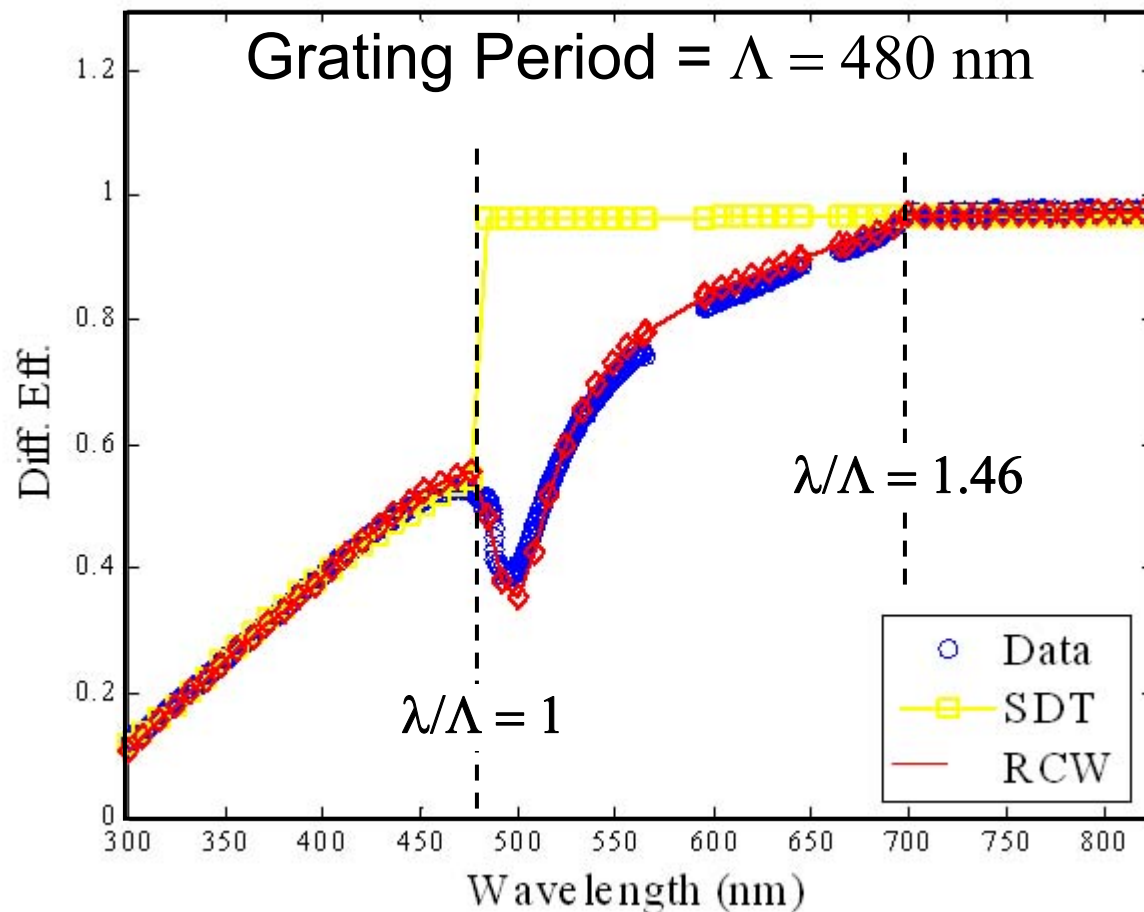


These figures show that using our non-paraxial scalar diffraction theory is able to accurately predict diffraction efficiencies over a much larger range than previously thought possible.

# Grating Characterization using Scatterometry\*

Harvey's renormalized scalar diffraction theory makes it possible to extend the useful range of scalar diffraction theory from  $0.1 < \lambda/\Lambda < 1.0$  and for  $\lambda/\Lambda > 1.0$ .

Using the SDT as a seed function for grating characterization results in a fast and robust two-step hybrid method that is a factor of eight (8) faster than a pure vector calculation code.



\* P.- E. Hansen and L. Neilsen, "Combined optimization and hybrid scalar-vector diffraction method for grating topography parameters determination", Materials Science and Engineering B 165, 165-168 (December 2009).



## Example # 2: Surface Scatter Behavior

---

In the Optical Design and Image Analysis Laboratory we must be able to perform a complete systems engineering analysis of image quality as degraded not only by diffraction and aberrations but surface scatter effects from residual optical fabrication errors as well.

- **Diffraction Effects** (Fundamental Physics)
- **Geometrical Aberrations** (Optical Design Errors)
- **Surface Scatter Effects** (Optical Fabrication Errors)
- **Detector Effects** (Film Grain Size, Finite Pixel Size, etc.)
- **Plus many other potential error sources**  
(Provided by Error Budget Tree)

# Optical Design and Analysis Codes

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**Commercially-available optical design and analysis codes model image degradation due to geometrical aberrations very well as they are based upon geometrical ray trace techniques.**

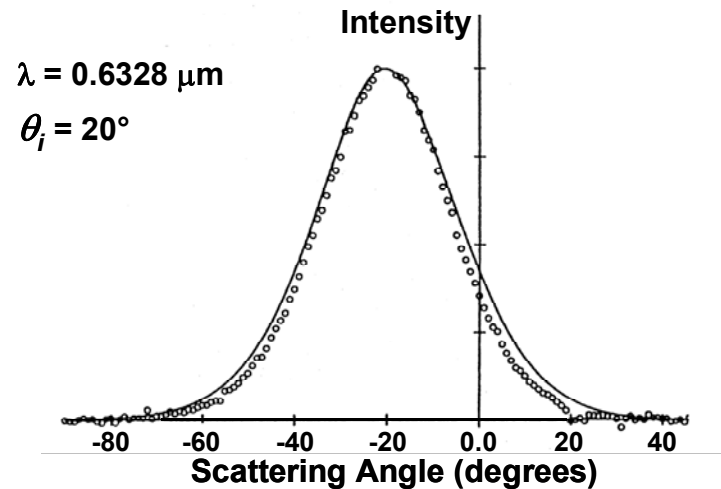
**And most of those codes have an adequate diffraction analysis capability; however, none of them have an adequate surface scatter analysis capability.**

**ZEMAX, Code V, ASAP, and FRED all claim to be able to model image degradation due to surface scatter effects. However, you must provide the scatter behavior (BRDF) as input; i.e., they cannot predict image degradation from optical surface metrology data.**

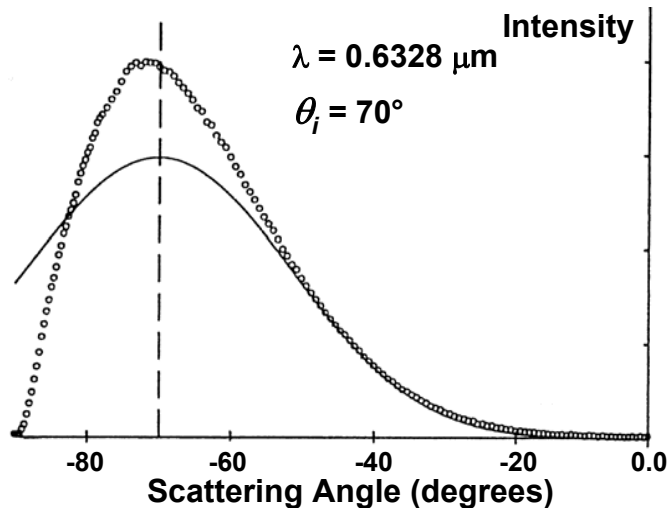
**The problem is further compounded by the fact that wide-angle surface scatter behavior resulting from obliquely-incident beams is often rather complicated and non-intuitive.**

# Non-Intuitive Surface Scatter Behavior\*

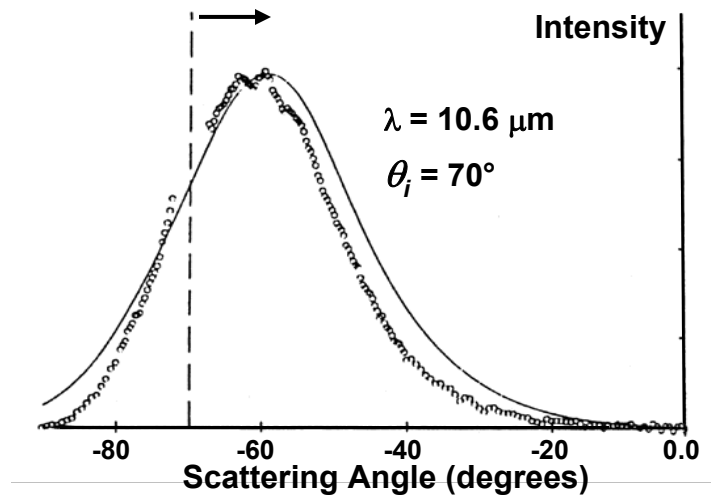
A detailed experimental investigation of light scattering from well-characterized random rough surfaces was reported by O'Donnell and Mendez in 1987. Several non-intuitive experimental results involving large scattering angles and large incident angles departed drastically from predictions using classical B-K scattering theory. These results were presented without adequate explanation, and the authors stated that “as far as we know, there is no theory available to compare with the results”. These non-intuitive experimental results became the basis for a significant advancement in our understanding of non-paraxial surface scatter (diffraction) behavior.



- 1.) A persistent tendency for experimental data to be narrower than that predicted by the Beckmann-Kirchhoff theory.



- 2.) Experimental data highly asymmetrical about the specular beam. B-K theory symmetrical but discontinuous at  $-90^\circ$ .



- 3.) They also observed that the scattering function does not peak in the specular direction. Again, no explanation.

\* O'Donnell and Mendez, “Experimental Study of Scattering from Characterized Random Surfaces”, J. Opt. Soc. Am. A 4, 1194-1205 (1987).

# Historical Review of Surface Scatter Theory

- **Rayleigh (1896, 1907)**  
Investigated scattering of acoustic waves.  
Developed vector perturbation theory for gratings.
- **Fano (1941)**  
Expanded on the Rayleigh approach to explain anomalous grating behavior.
- **Rice (1951)**  
Applied the Rayleigh perturbation approach to the problem of radar scatter from the sea.
- **Brekhovskikh (1952)**  
Introduced use of the Kirchhoff Approximation (KA) in scattering problems.
- **Isakovich (1952)**  
First to apply KA to scattering from rough surfaces.
- **Beckmann (1963)**  
Published extensive monograph on scattering from rough surfaces using the KA.  
Most widely used Western reference.
- **Nicodemus (1970)**  
Introduced the Bidirectional Reflectance Distribution Function (BRDF).
- **Church (1970's)**  
Introduced the vector perturbation approach to the optics literature.
- **Harvey and Shack (1976)**  
Developed a linear systems formulation of surface scatter theory.

## Recent Approximate Approaches

This is still a very active area of research (over 200 references since 1980).

In 2004, Elfouhailey and Guerin\* wrote a critical review including over thirty (30) different approximate approaches of predicting surface scatter behavior. These were divided into three categories:

- Small Perturbation Methods
- Kirchhoff Approaches
- Unified Methods

They concluded that

*“there does not seem to be a universal method that is to be preferred systematically. All methods present a compromise between versatility, simplicity, numerical efficiency, accuracy and robustness, with a different weighting in these various fields...There is still room for improvement in the development of approximate scattering methods.”*

\* T. M. Elfouhaily and C. A. Guerin, “A Critical Survey of approximate Scattering Wave Theories from Random Rough Surfaces”, Waves in Random Media 14, R1-R40 (2004).

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# Rayleigh-Rice Surface Scatter Theory\*

The Rayleigh-Rice scattering theory is based on the vector perturbation approach first done by Rayleigh for gratings. Using a perturbation of the surface height and solving for the exact boundary conditions at the scattering surface leads to an infinite number of equations and unknowns which is only practically solved when the roughness is small.

The Rayleigh-Rice surface scatter theory agrees well with experimental wide angle scatter measurements and large incident angles for smooth surfaces, however not all surfaces of interest satisfy this requirement.

The scattered intensity (normalized by incident power) is given by

$$\frac{(dP / d\Omega_s)}{P_i} = \left( \frac{16\pi^2}{\lambda^4} \right) \cos \theta_i \cos^2 \theta_s Q S(f_x, f_y) \quad (33)$$

$S(f_x, f_y)$  is the two-sided, two-dimensional surface *PSD* function expressed in terms of the sample spatial frequencies

$$f_x = \frac{\sin \theta_s \cos \phi_s - \sin \theta_i}{\lambda} \quad \text{and} \quad f_y = \frac{\sin \theta_s \sin \phi_s}{\lambda}$$

$Q$  is the polarization dependent reflectance of the surface. For *TE* polarization and measurements in the plane of incidence  $Q$  is given exactly by the geometric mean of the sample specular reflectances at  $\theta_i$  and  $\theta_s$

$$Q = [R_s(\theta_i) R_s(\theta_s)]^{1/2}$$

\* S. O. Rice, "Reflection of Electromagnetic Waves from Slightly Rough Surfaces", Commun. Pure Appl. Math, 4, p 351 (1951).

# Historical Review of Surface Scatter Theory

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\* T. M. Elfouhaily and C. A. Guerin, “A Critical Survey of approximate Scattering Wave Theories from Random Rough Surfaces”, Waves in Random Media 14, R1-R40 (2004).

# Beckmann-Kirchhoff Scattering Theory\*

Beckmann used a Kirchhoff diffraction approach to solving the surface scatter problem. Instead of solving for the exact boundary conditions, he approximated the fields and normal derivatives at a point on the scattering surface with the fields and normal derivatives that would exist on a plane tangent to that point. This allows the Beckmann-Kirchhoff theory to be used for rougher surfaces, however it also requires the radius of curvature of the surface features to be much larger than the wavelength. In addition, the Beckmann-Kirchhoff theory contains a built-in paraxial limitation.

Beckmann only provides a closed-form solution for the case of moderately rough and very rough surfaces when the surface can be described by a Gaussian autocovariance function. In that case, the scattered intensity is given by

$$I(\theta, \phi) = \frac{\pi \ell_c^2 F^2 \exp(-g)}{A} \sum_{m=1}^{\infty} \frac{g^m}{m! m} \exp\left[-\frac{v_{xy}^2 \ell_c^2}{4m}\right] \quad (34)$$

For smooth and moderately rough surfaces

$$I(\theta, \phi) = \frac{\pi F^2 \ell_c^2}{A^2 g} \exp\left(-\frac{v_{xy} \ell_c^2}{4g}\right) \quad (35)$$

For very rough surfaces

where

$$F = \left[ \left( \frac{1}{\cos \theta_o} \right) \frac{1 + \cos(\theta_o + \theta_s)}{\cos \theta_o + \cos \theta_s} \right]^2$$

$$g = \left( \frac{2\pi\sigma}{\lambda} \right)^2 (\cos \theta_o + \cos \theta_s)$$

$$v_{xy} = k \sqrt{\sin^2 \theta_s + \sin^2 \theta_o}$$

$A$  = Illuminated Surface Area

$\ell_c$  = Correlation Length

\* P. Beckmann and A. Spizzichino, *Scattering of Electromagnetic Waves from Rough Surfaces*, Pergamon Press, New York, 1963.



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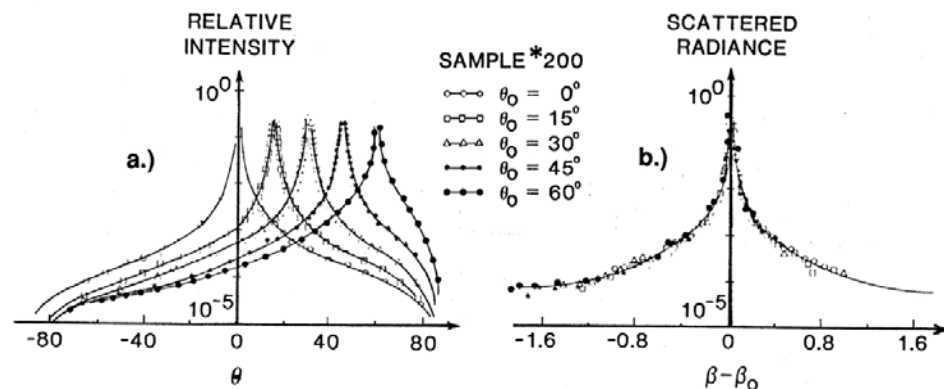
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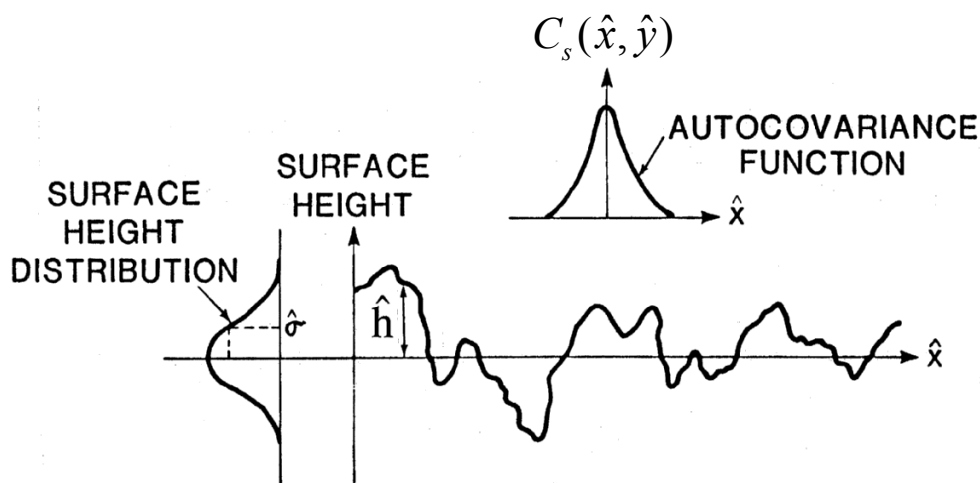
# Transfer Function Characterization of Surface Scatter\*

In 1976 Harvey and Shack formulated a scattering theory in a linear systems format resulting in a surface transfer function (STF) that relates scattering behavior to surface topography. Surface scatter phenomena was modeled as a simple scalar diffraction process, where the diffracting “aperture” is a random phase “aperture” rather than the conventional binary amplitude aperture. The rough surface merely imparts phase variations onto the incident wavefront upon reflection. *No explicit “smooth surface” approximations were made.*

## Experimental Scattered Data



## Surface Characteristics



## Surface Transfer Function

$$H_S(\hat{x}, \hat{y}) = \exp\left\{-\left(4\pi\hat{\sigma}_s\right)^2\left[1 - C_s(\hat{x}, \hat{y})/\sigma_s^2\right]\right\}$$

$$H_S(\hat{x}, \hat{y}) = A + B Q(\hat{x}, \hat{y}) \quad (36)$$

$$A = \exp[-(4\pi\hat{\sigma}_s)^2]$$

$$B = 1 - \exp[-(4\pi\hat{\sigma}_s)^2]$$

\* J. E. Harvey, “Light-Scattering Characteristics of Optical surfaces”, Ph.D. Dissertation, Univ. of Arizona (1976).

# Harvey-Shack BRDF Model\*

**TracePro**  
Software for Opto-Mechanical Modeling

**Harvey-Shack BSDF**

In his dissertation (J. E. Harvey, "Light-Scattering Properties of Optical Surfaces," Ph.D. Dissertation, U. Arizona, 1976) Harvey found that for many optical surfaces, the BSDF is independent of the direction of incidence if it is expressed as a function of direction cosines instead of angles. Harvey called this property "shift-invariant," as in linear systems theory. Referring to Figure 7.4,  $\beta_0$  is a projection onto the surface of the unit vector  $\mathbf{r}_0$  in the specular direction, and the magnitude of their difference,  $|\beta - \beta_0|$ , is the argument of the BSDF. Note that  $\beta$  and  $\beta_0$  are not unit vectors. They are projections of unit vectors, so their lengths are less than or equal to one. The Harvey-Shack method gives a good model for the behavior of most optical surfaces, i.e. those for which:

- Scattering is due mainly to surface roughness
- Scattering (and thus surface roughness) is isotropic
- Surface roughness is small compared to the wavelength of light

**USER'S MANUAL**  
RELEASE 3.0

**Lambda Research Corporation**

ASAP Feature Note  
BRO-FN1407(02/00)

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**Harvey-Shack Overview**

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**Bidirectional Scattering Distribution Function (BSDF)**

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This ASAP Feature Note briefly discusses the Harvey-Shack model and its use for illumination applications in ASAP™ optical modeling software.

Breault Research Organization, Inc.  
Optical Engineering Software and Services

**ZEMAX**  
Optical Design Program

**User's Guide**  
Version 9.0

**Harvey-Shack (ABg) scattering**

The Harvey-Shack or ABg scattering model is a very powerful and widely used Bidirectional Scattering Distribution Function, or BSDF. BSDF is defined as the scattered irradiance, or

where  $\theta$  is measured from the normal, and  $\phi$  is the azimuthal angle, and the subscripts and scattered directions, respectively. Note BSDF has units of inverse steradians. The general term BSDF can refer to two separate functions, the BRDF and BTDF, for distributions, respectively. ZEMAX allows separate specification of the BRDF and BTDF in following sections.

**Harvey-Shack BSDF properties**

For many optical surfaces, the BSDF is independent upon incident direction if it is plotted as cosines instead of angles. This was first reported by James E. Harvey ("Light-Scattering Surfaces", J. E. Harvey Ph.D. Dissertation, University of Arizona, 1976; "Scattering Error Fabrication Errors", J. Harvey and A. Kofha, Proceedings of the SPIE, July, 1999).

The Harvey-Shack representation is to plot BSDF as a function of  $|\beta - \beta_0|$ , which is the distance between the scattered and unscattered ray vectors when projected down to the discussion under "Scattering" above).

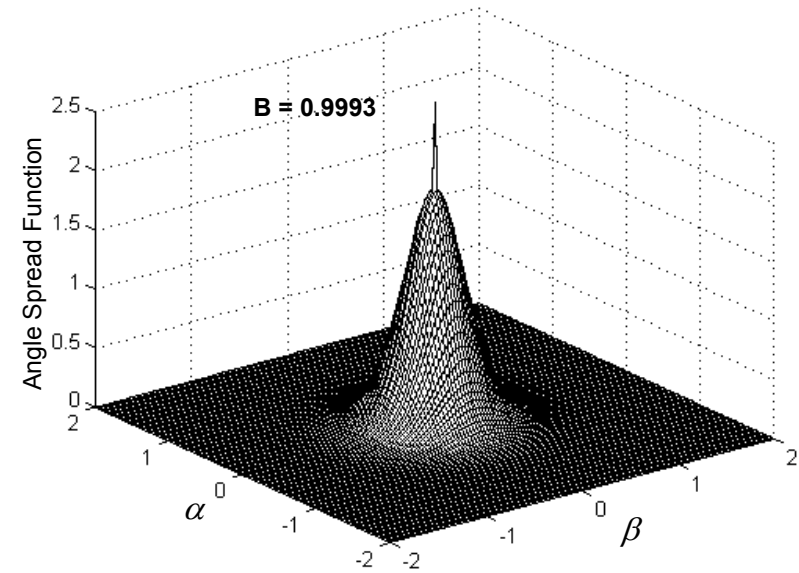
$$BSDF(\theta_i, \phi_i, \theta_s, \phi_s) = \frac{dL_s(\theta_s, \phi_s)}{d\Omega_s(\theta_s, \phi_s)}$$

\* R. P. Breault, "Users Manual for APART/PADE Version 6B", Breault Research Organization, Tucson Arizona (1980).

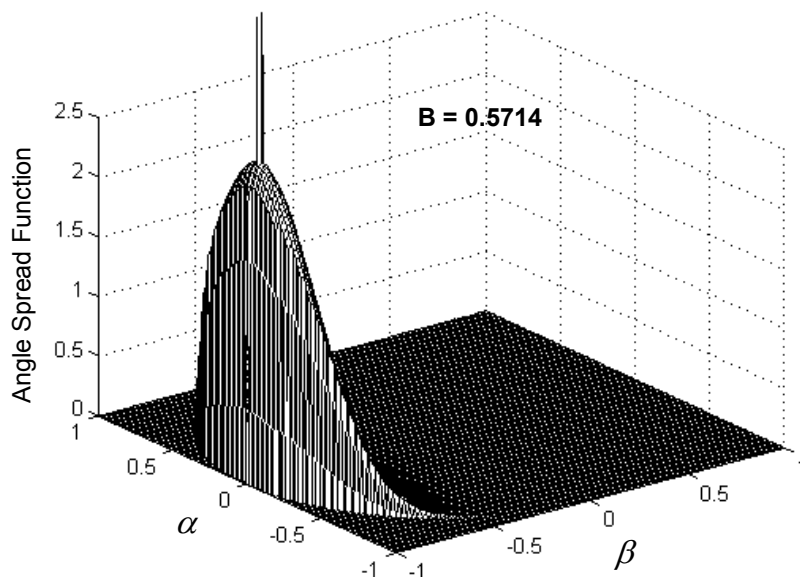
# The Angle Spread Function (Scattered Radiance)

- For an isotropically rough surface, the scattered radiance function is rotationally symmetric for normal incidence.
- In accordance with our non-paraxial scalar diffraction theory, it is shift-invariant with respect to incident angle.
- For large incident angles it is truncated by the unit circle and re-normalized (conserves energy).
- Finally, the scattered intensity distribution is obtained by applying Lambert's Cosine Law (makes asymmetrical and shifts peak from specular beam).

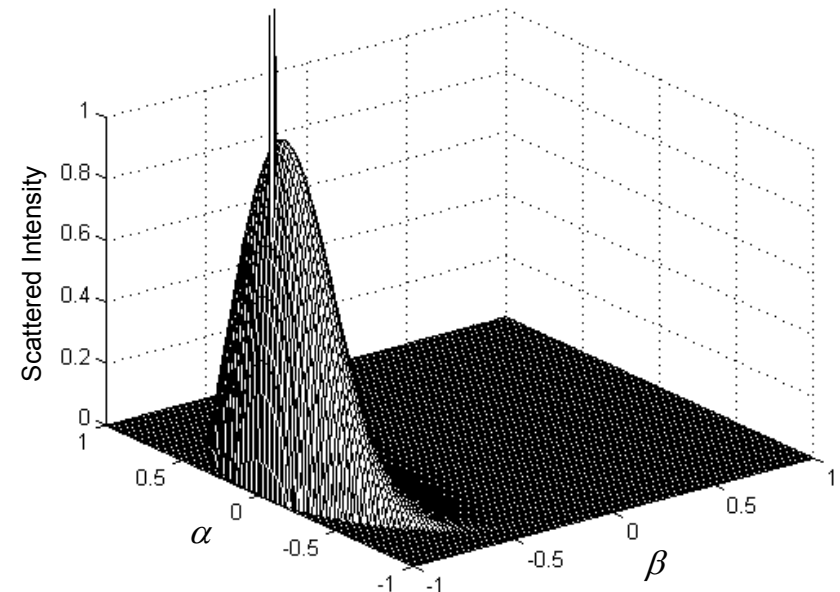
## Angle Spread Function for Normal Incidence



## Angle Spread Function for Large Incident Angle (Truncated and re-normalized)



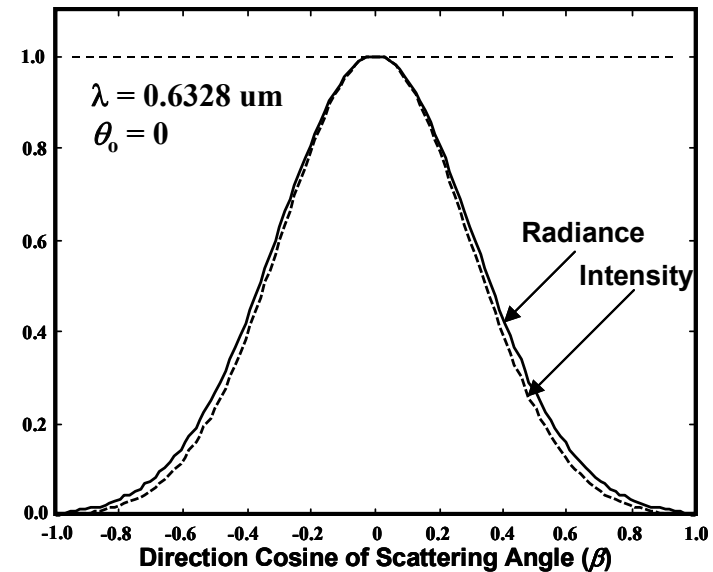
## Scattered Intensity Distribution



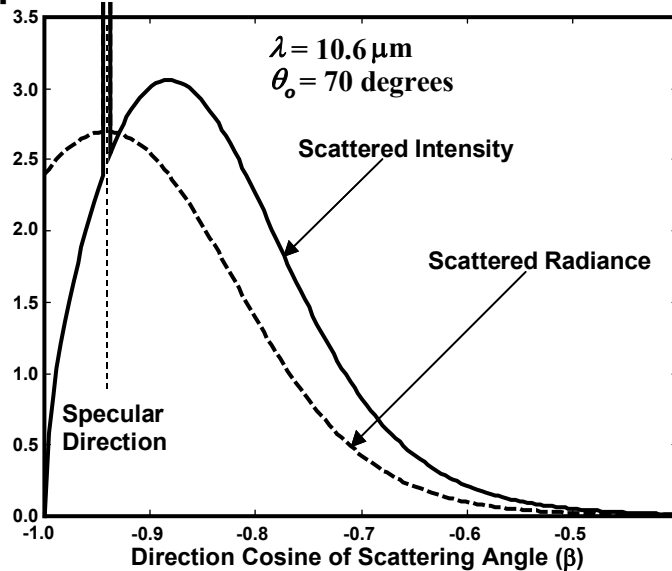
# Radiometry Matters—O'Donnell and Mendez were Comparing Apples and Oranges\*

- Compare scattered radiance and intensity predictions for the O'Donnell-Mendez surface.
- The O'Donnell-Mendez non-intuitive results are obviously the result of comparing different radiometric quantities!
- Finally, we compare the Harvey-Shack prediction for scattered intensity with the O'Donnell-Mendez experimental data. Excellent agreement is indicated except at the knee of the curve.

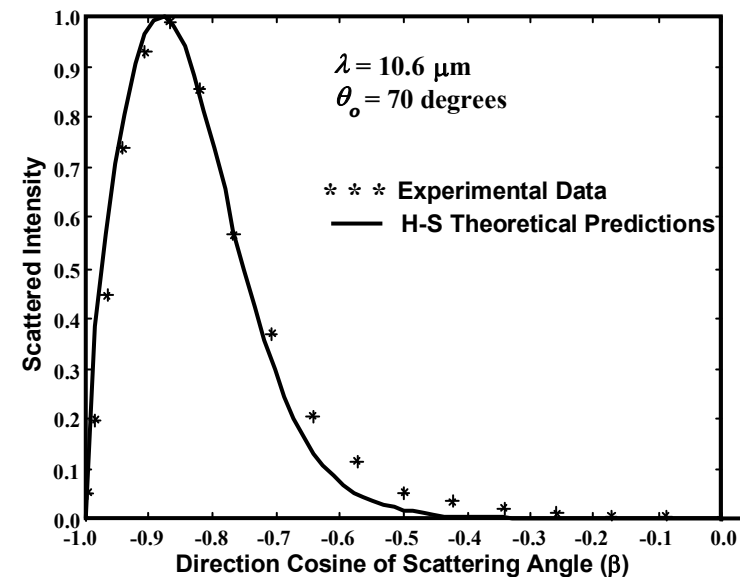
### Comparison of Predicted Radiance and Intensity



### Comparison of Predicted Radiance and Intensity



### Comparison of Intensity with Experimental Data



\* J. E. Harvey, C. L. Vernold, A. Krywonos, and P. L. Thompson, "Diffracted Radiance: A Fundamental Quantity in Non-paraxial Scalar Diffraction Theory", Appl. Opt. 38, 6469-6481 (1 Nov 1999).

# Empirically Modified Beckmann-Kirchhoff Surface Scatter Theory\*

Our new understanding of non-paraxial scalar diffraction theory, and our knowledge that diffracted radiance is shift-invariant in direction cosine space leads us to make the following empirical modifications:

- Throw away the “F” factor.
- Equate to “Radiance”.
- Apply the re-normalization factor, K.
- Multiply by Lambert’s cosine function.

## Classical Beckmann-Kirchhoff Theory

$$D\{\rho\} = \frac{\pi \ell_c^2 F^2}{A_s v_z^2 \sigma_s^2} \exp\left[\frac{v_{xy}^2 \ell_c^2}{4v_z^2 \sigma_s^2}\right] \quad (37)$$

$$F = \left[ \left( \frac{1}{\cos \theta_o} \right) \frac{1 + \cos(\theta_o + \theta_s)}{\cos \theta_o + \cos \theta_s} \right]^2$$

$$v_{xy} = k \sqrt{\sin^2 \theta + \sin^2 \theta_o}$$

$A$  = Illuminated Surface Area       $\ell_c$  = Correlation Length

## Modified Beckmann-Kirchhoff Theory

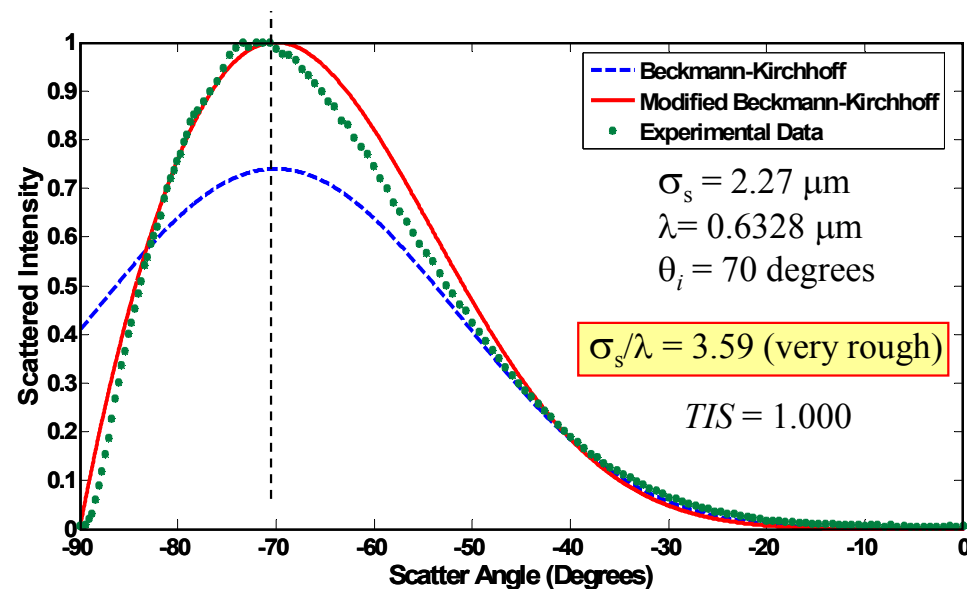
$$I(\theta, \phi) = K \frac{\pi \ell_c^2 \cos \theta}{v_z^2 \sigma_s^2} \exp\left[-\frac{v_{xy}^2 \ell_c^2}{4v_z^2 \sigma_s^2}\right] \quad (38)$$

$K$  = Re-normalization Factor  
(Assures Conservation of Energy)

$$I = L \cos \theta$$

(Lambert’s Cosine Law)

## Experimental Validation



\* J. E. Harvey, A. Krywonos, and C. Vernold, “Modified Beckmann-Kirchhoff Scattering Theory”, submitted to Opt. Eng.



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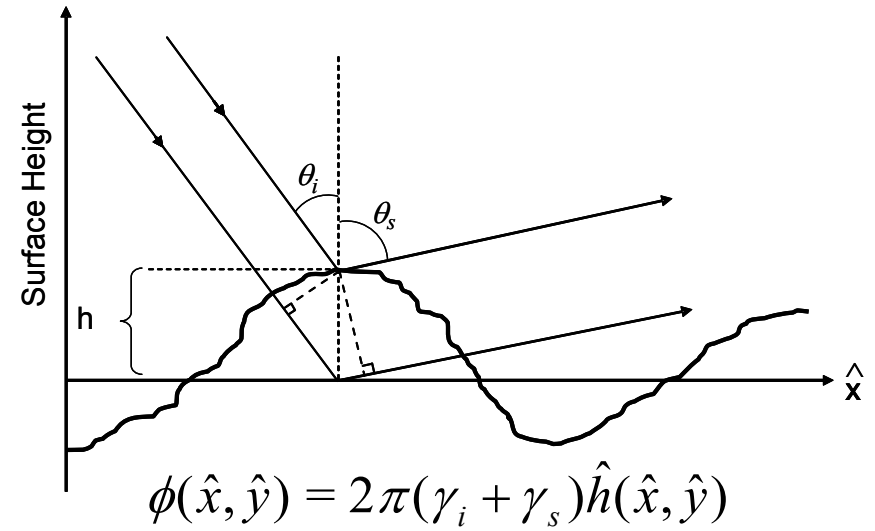
# Development of a Unified Surface Scatter Theory\*

## (Arbitrarily Rough Surfaces, Large Incident and Scatter Angles)

### Limitations of the Original Harvey-Shack

- Scalar theory (no polarization effects).
- Does not account for redistribution of energy from evanescent to propagating waves.
- Surface transfer function has a built-in paraxial limitation.

### Phase Variation Depends on Scattering Angle



### New Surface Transfer Function

$$H_s(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = \exp\left\{-\left[2\pi\hat{\sigma}_s(\gamma_i + \gamma_s)\right]^2\left[1 - C_s(\hat{x}, \hat{y})/\sigma_s^2\right]\right\}$$

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$$B = 1 - \exp\left\{-\left[2\pi\hat{\sigma}_s(\gamma_i + \gamma_s)\right]^2\right\}$$

$$\gamma_i = \cos\theta_i \quad \gamma_s = \sqrt{1 - \alpha_s^2 - \beta_s^2} = \cos\theta_s$$

$$BRDF = Q \mathcal{F}\{H(\hat{x}, \hat{y}; \gamma_i, \gamma_s)\} \quad (40)$$

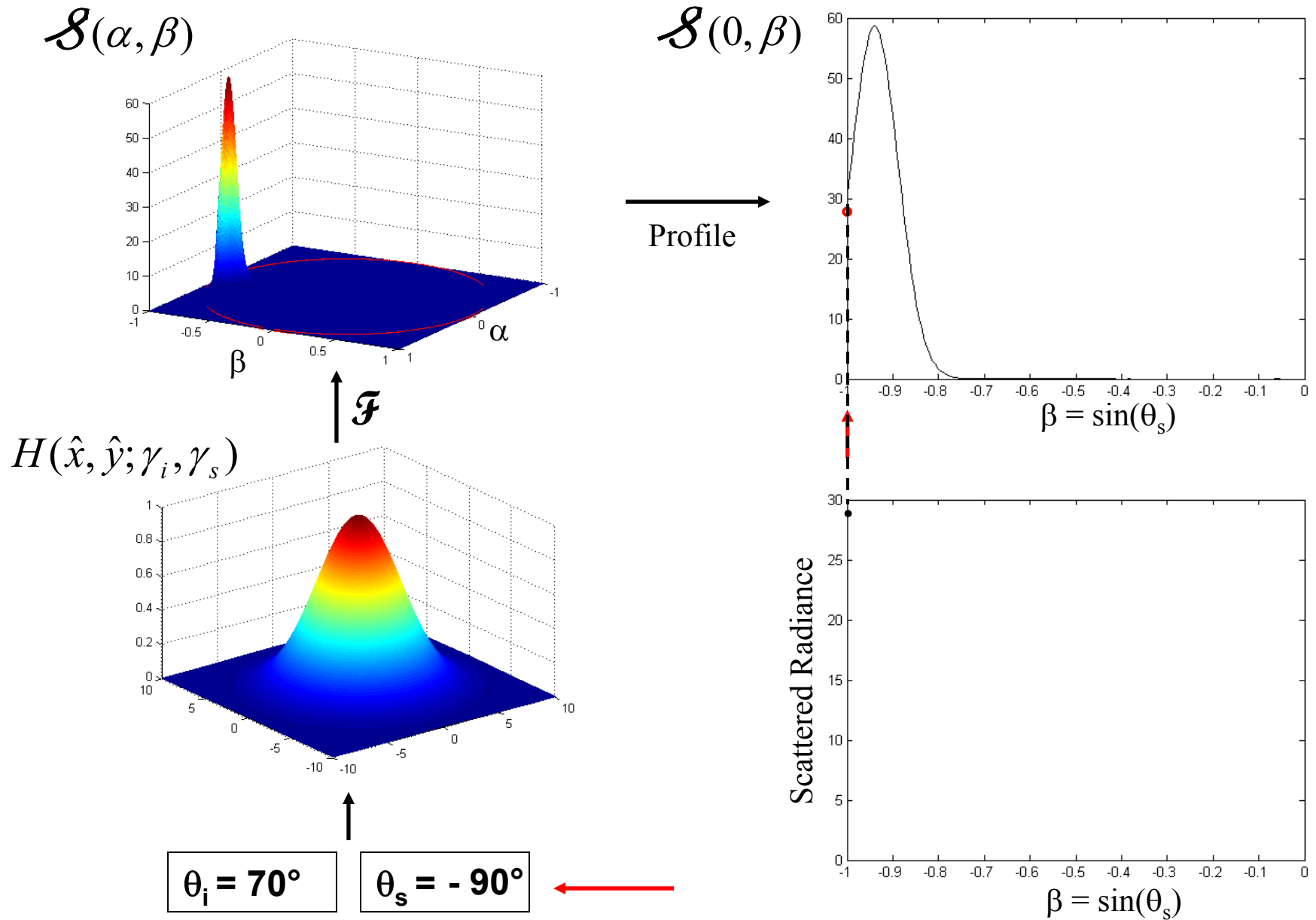
### New Generalized Harvey-Shack Theory

The system is no longer shift invariant (requires a different transfer function for each incident and scattering angle).

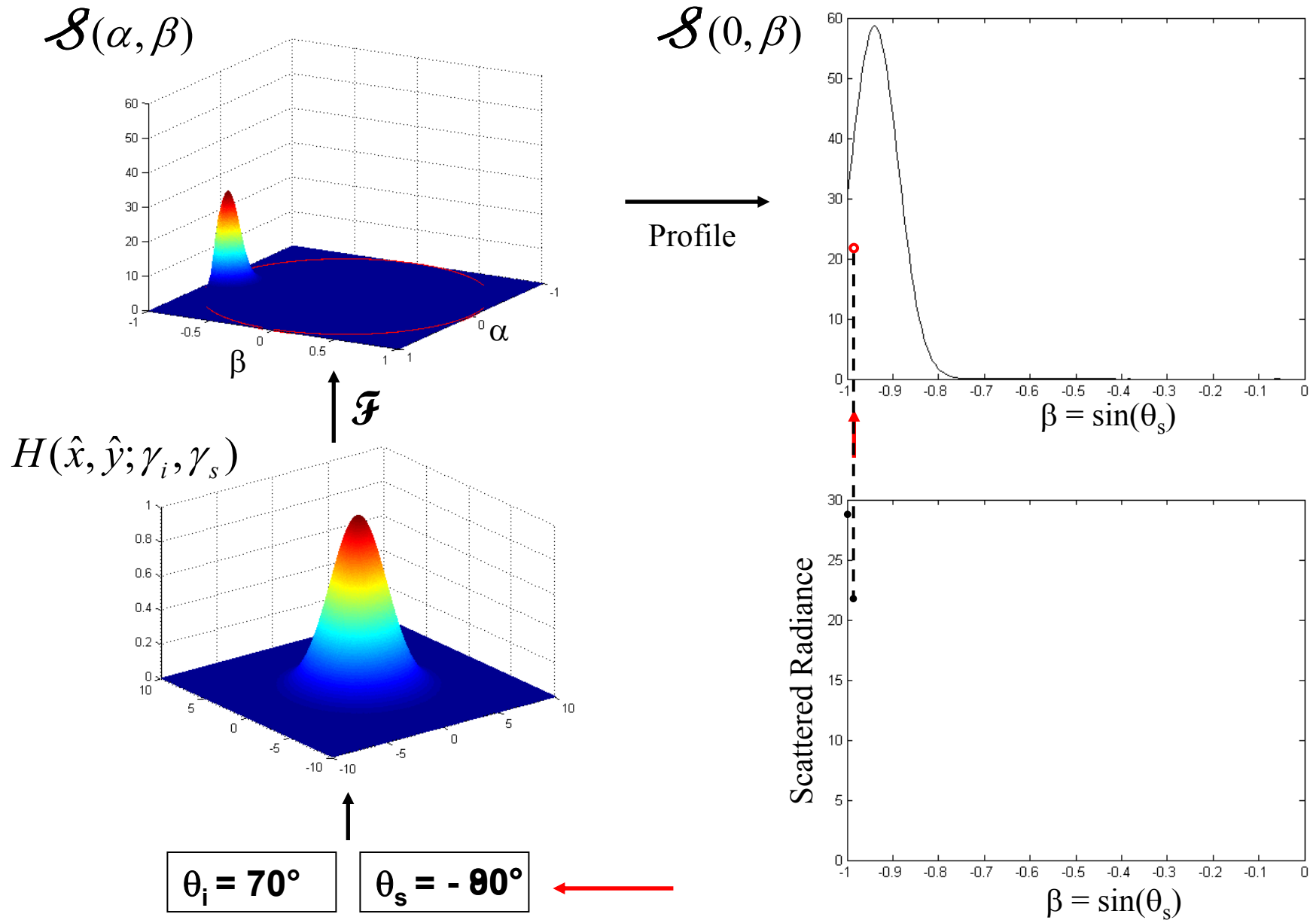
This is similar to imaging systems with field-dependent aberrations, where a different MTF is used for each field angle.

This new surface scatter model has been quasi-vectorized by merely substituting Stover's polarization reflectance factor,  $Q$ , for the reflectance,  $R$ , in the scalar treatment.

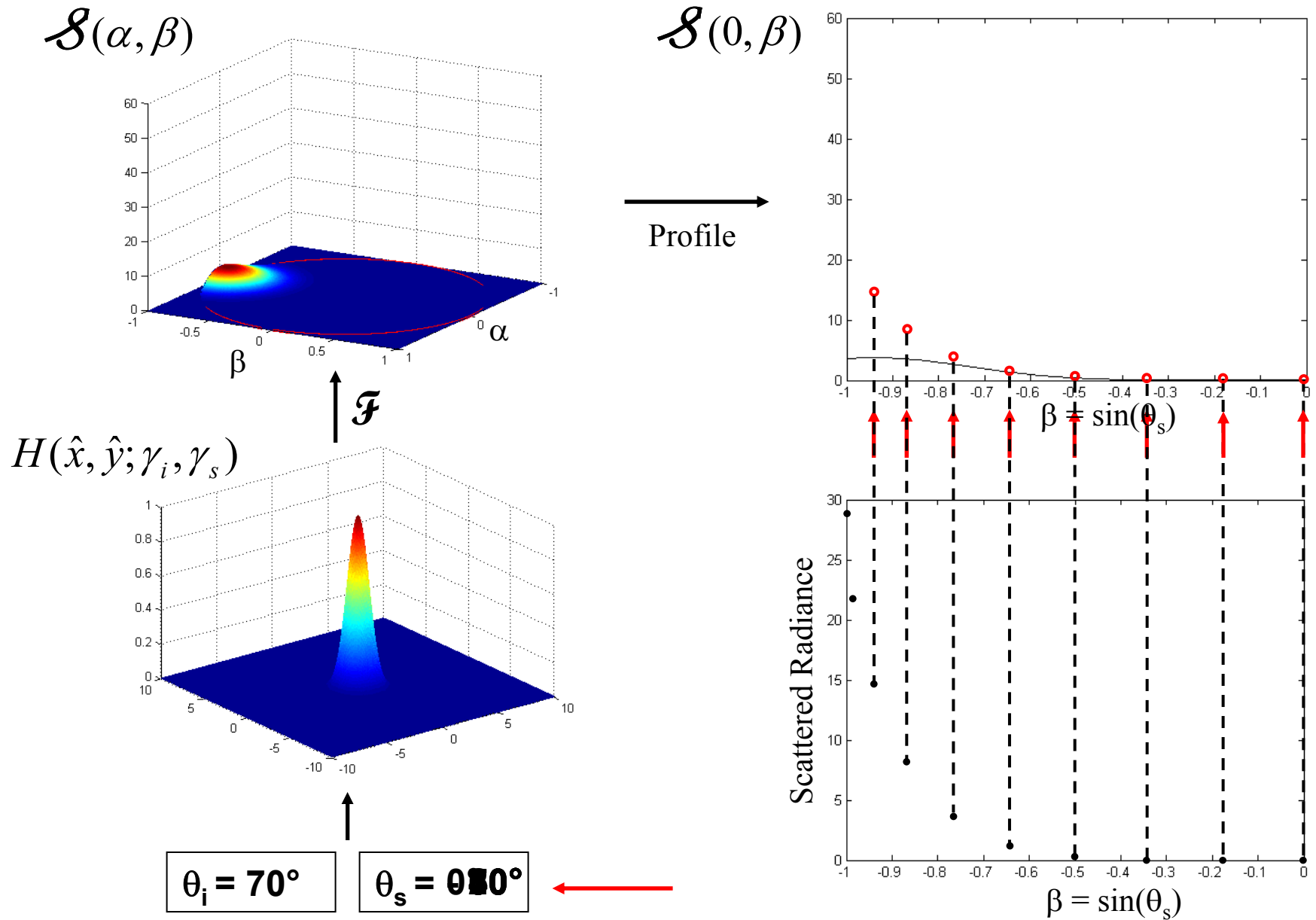
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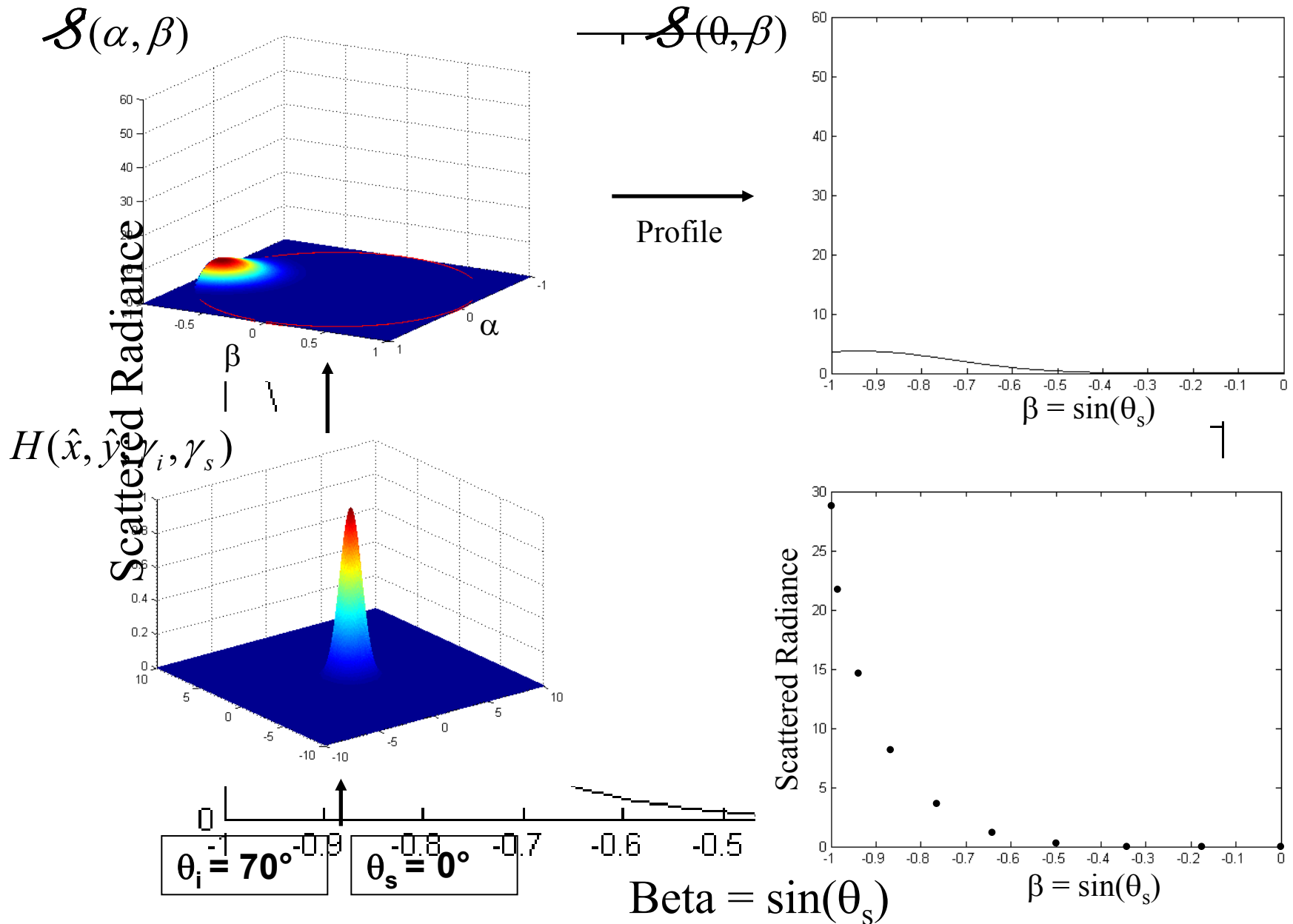
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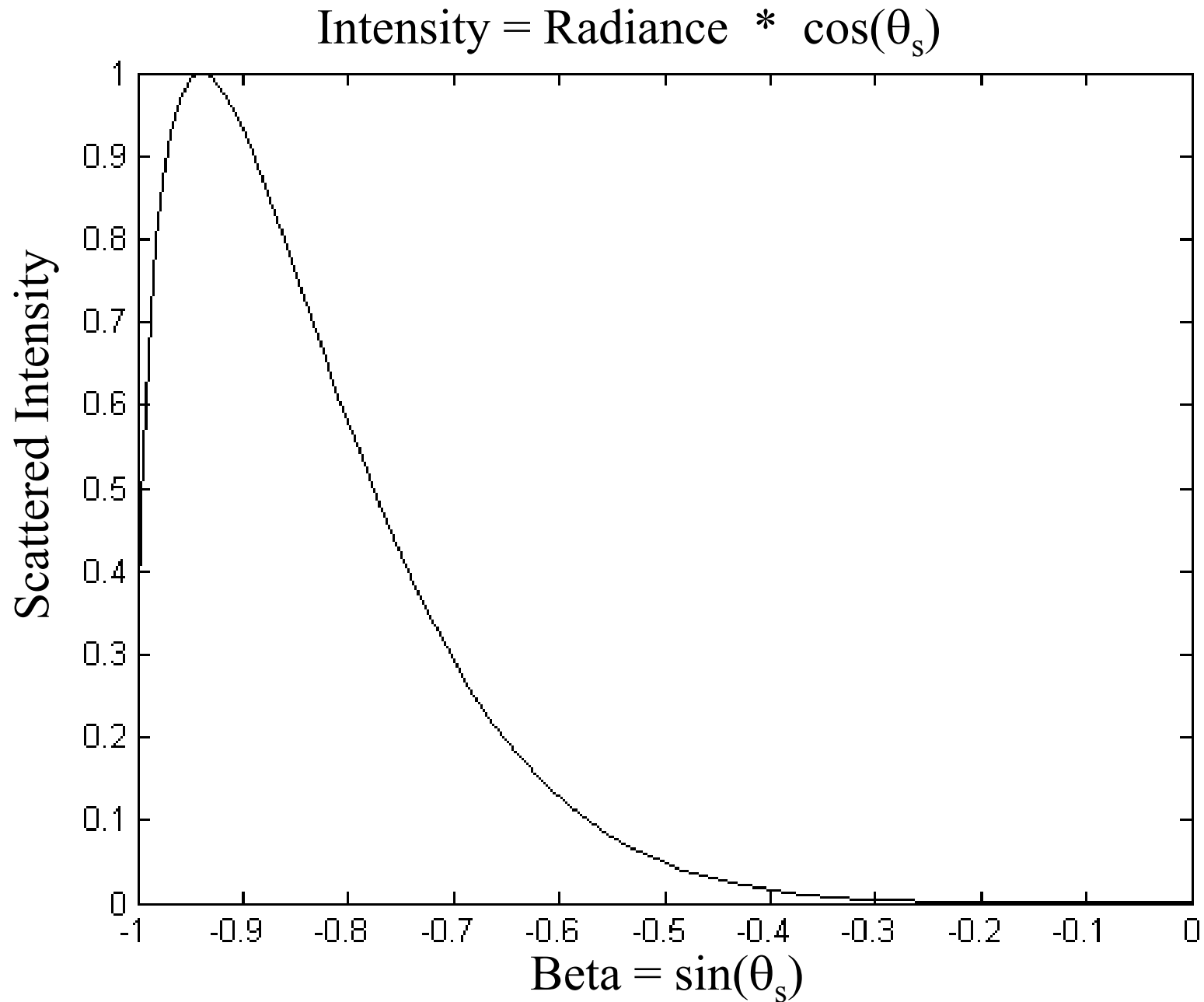


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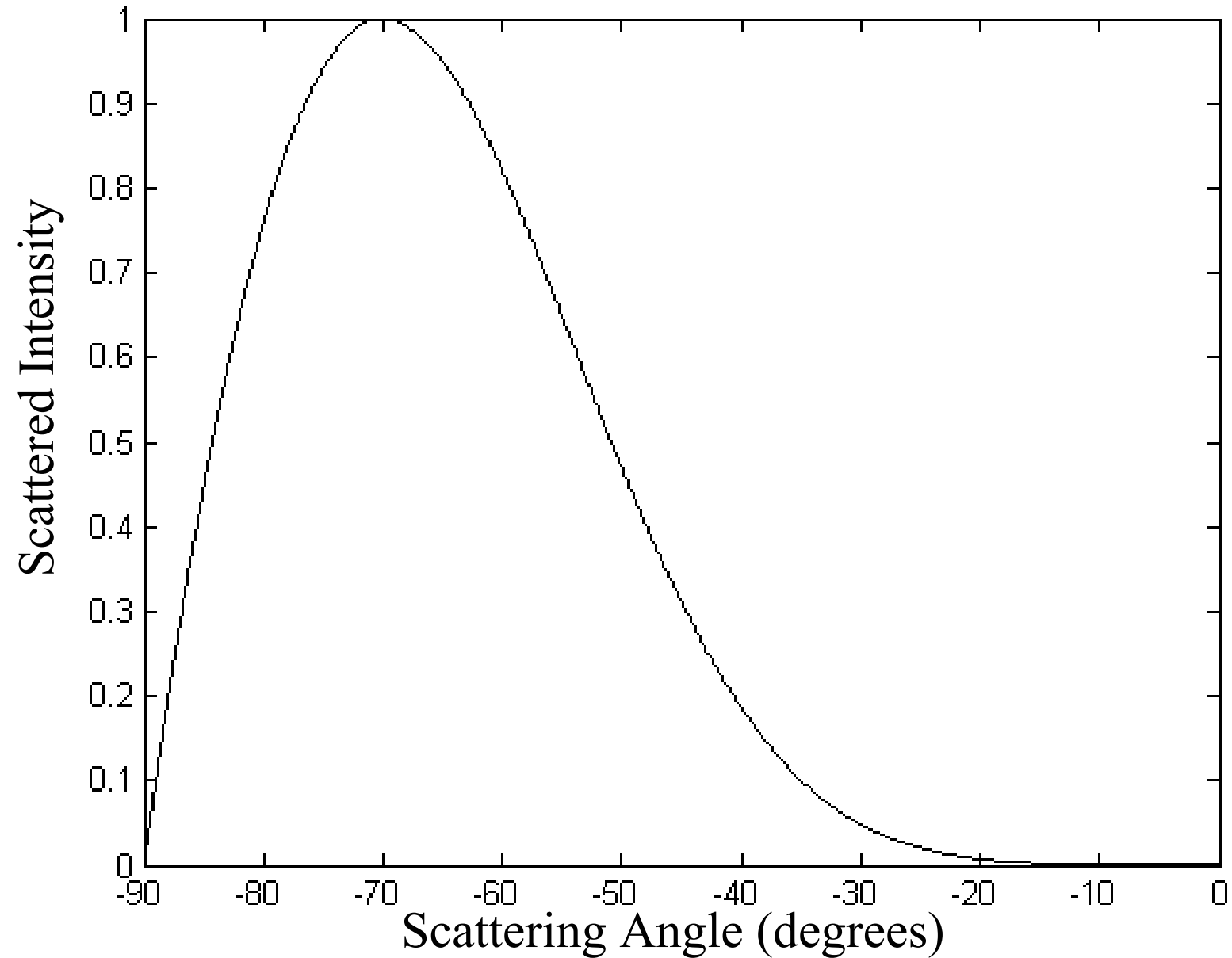
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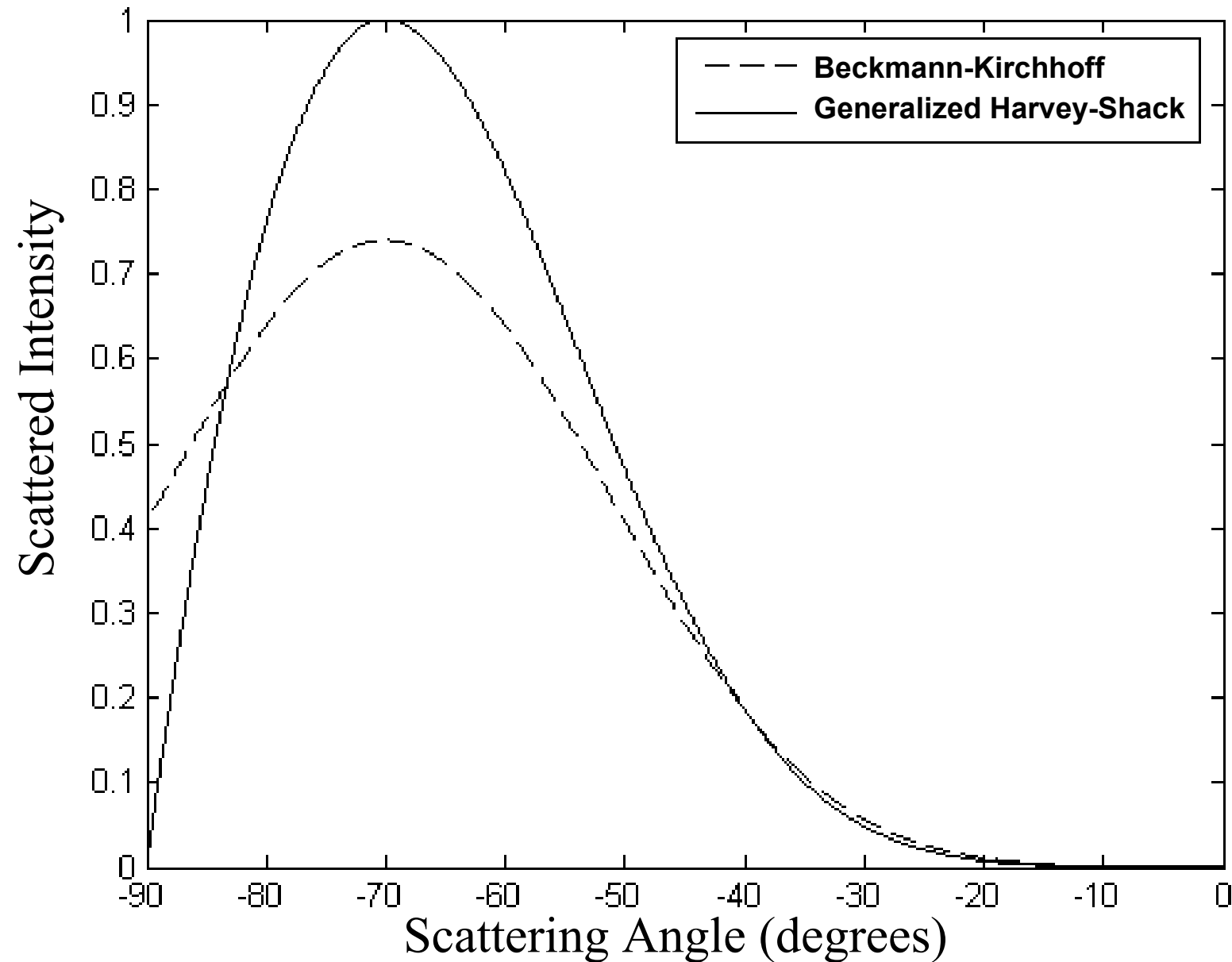
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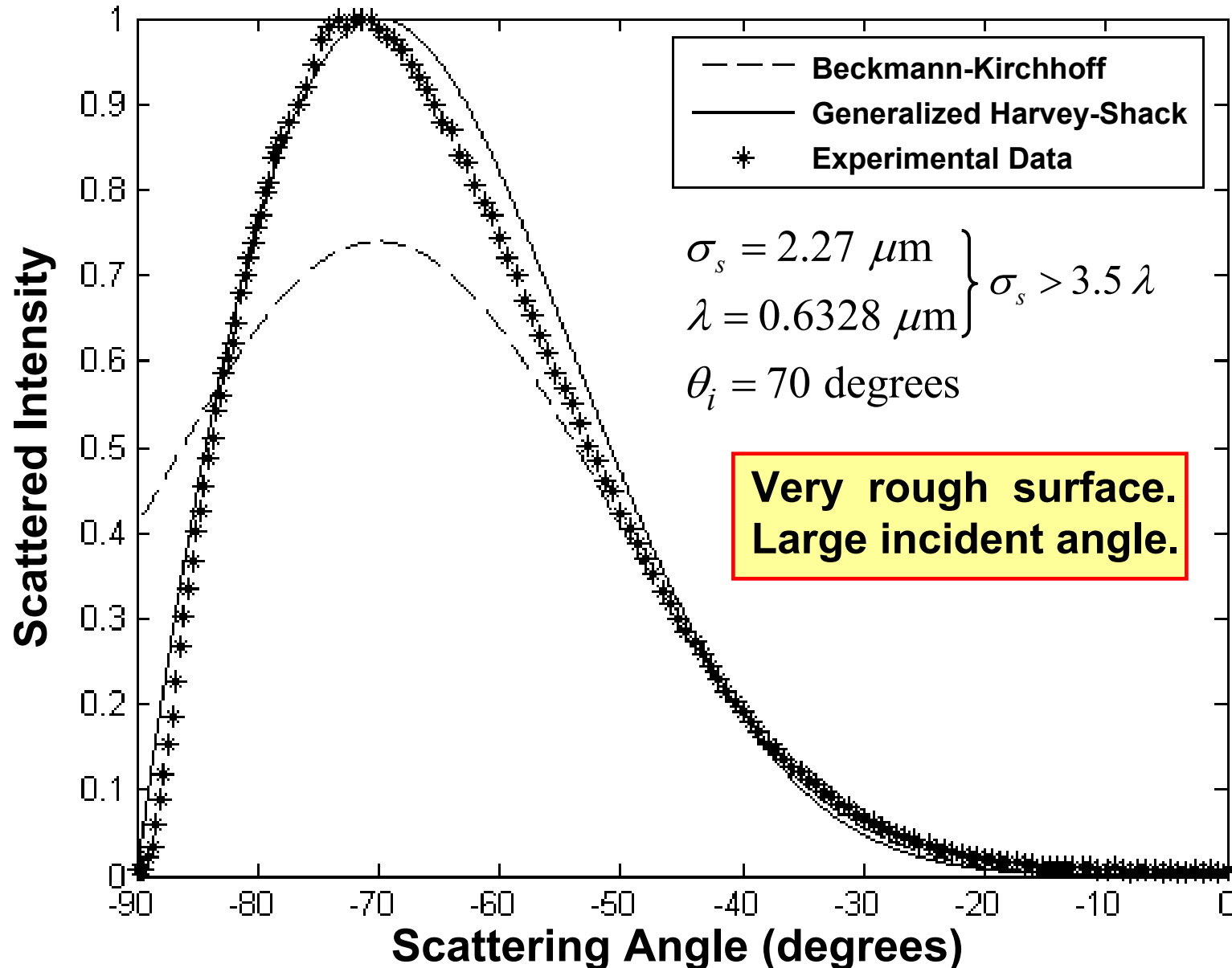
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# Unified Surface Scatter Theory

(Experimentally Validated by O'Donnell-Mendez Data)\*

\* K. A. O'Donnell and E. R. Mendez, "Experimental study of scattering from characterized random surfaces", J. Opt. Soc. Am. A, 4, 1194-1205 (1987).



# Summary and Conclusions

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- Reviewed the historical development of scalar diffraction theory.
- Emphasized the paraxial limitation of the conventional linear systems formulation of scalar diffraction theory.
- Demonstrated that diffraction phenomena is shift-invariant in direction cosine space.
- Discussed the importance of using proper radiometric terminology and nomenclature.
- Showed that *radiance* is the fundamental quantity for describing the diffraction and propagation of radiation; i.e., diffracted radiance is shift-invariant in direction cosine space, even for non-paraxial diffraction from nanostructures.
- Provided two examples that back up the above claims.
  1. The sinusoidal phase grating.
  2. Wide-angle scatter from rough surfaces at large incident angles.