

CREOL: College of Optics and Photonics

A Global View of Diffraction: Revisited

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Presented at

Fraunhofer IOF Physics Colloquium

Jena, Germany

March 10, 2010

Abstract

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 lead 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

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

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

Examples:

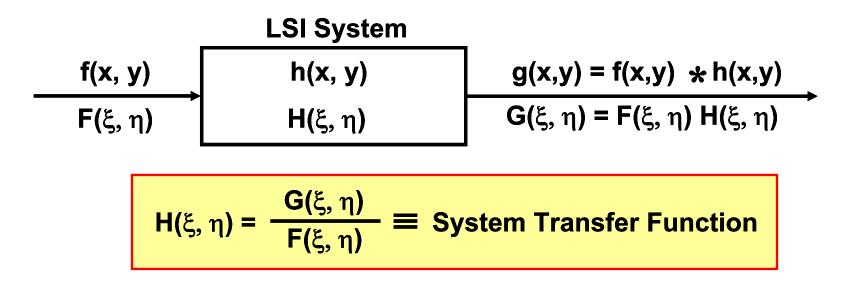
Transforming from Cartesian to spherical coordinates greatly simplifies solving Schrodinger's equation for the hydrogen atom.

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.

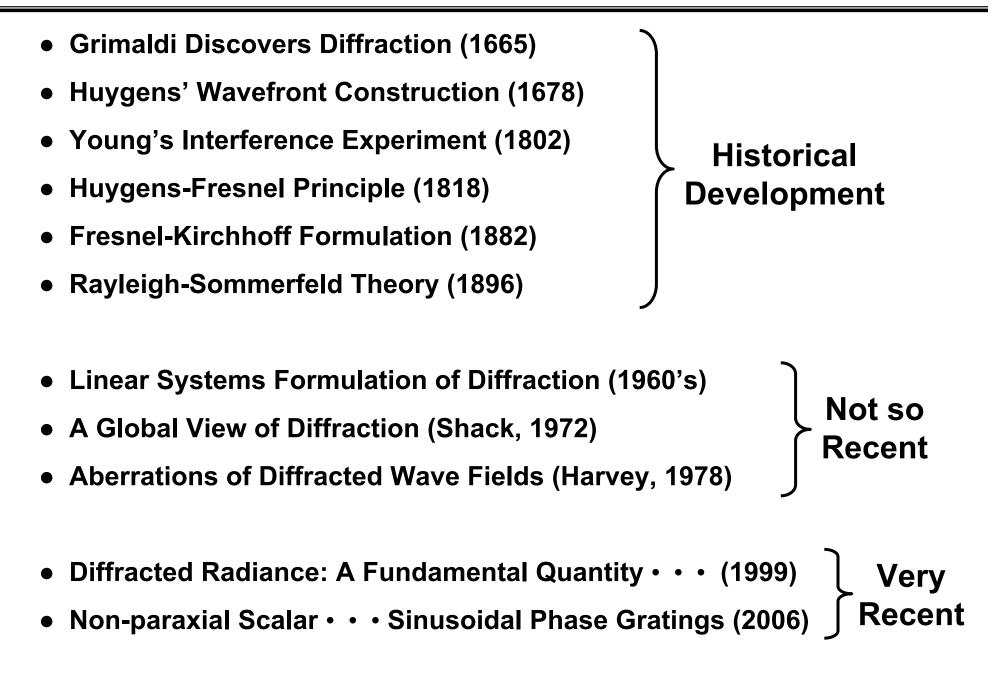
Natural Phenomena Exhibiting Linear, Shift-invariant Behavior are Readily Understood

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.



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



Outline

Paraxial Limitation in Conventional Fourier Optics

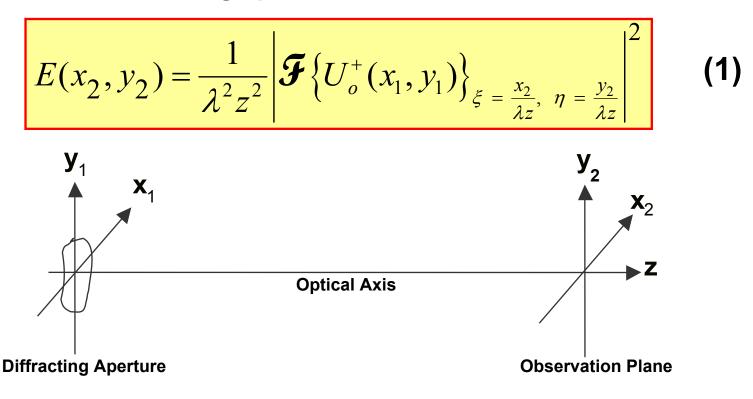
- Fraunhofer Diffraction and the Paraxial Limitation
- Diffraction Grating Behavior in Cartesian Space
- A Global View of Diffraction (1973-1979)
 - Aberrations of Diffracted Wave Fields
 - Non-paraxial Shift-invariance in Direction Cosine Space
- Radiometry/Scalar Diffraction (1999)
 - Diffracted Radiance: 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.^{1,2}



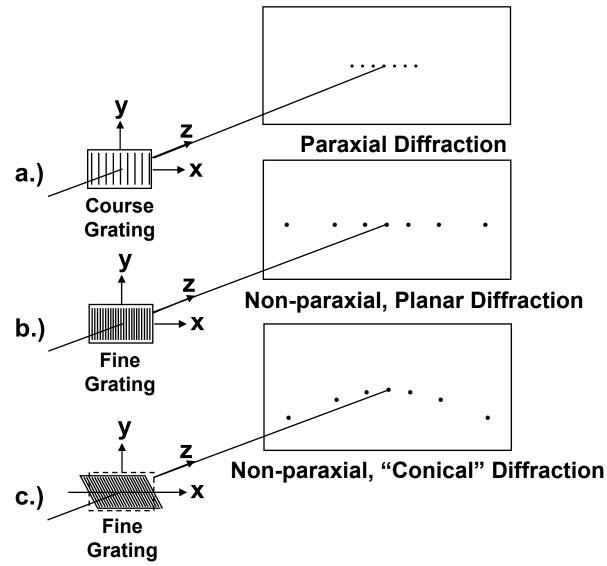
The Fraunhofer Approximation, and even Fresnel Approximation, Implicitly Contain a Paraxial Limitation!

* 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).

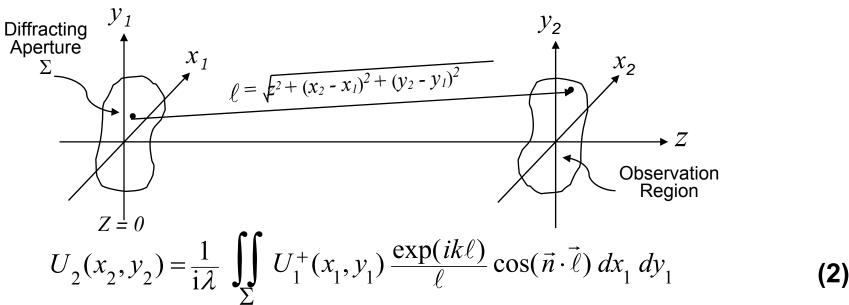
However, not all Diffraction Phenomena of Interest are limited to the Paraxial Regime

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



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 $z^3 >> \frac{\pi}{4\lambda} [(x_2 - x_1)^2 + (y_2 - y_1)^2]^2 \max$), then we obtain

$$U_{2}(x_{2}, y_{2}) = \frac{\exp(ikz)}{i\lambda z} \exp\left[i\frac{k}{2z}(x_{2}^{2} + y_{2}^{2})\right] \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_{1}^{+}(x_{1}, y_{1}) \exp\left[i\frac{k}{2z}(x_{1}^{2} + y_{1}^{2})\right] \exp\left[-i\frac{2\pi}{\lambda z}(x_{1}x_{2} + y_{1}y_{2})\right] dx_{1} dy_{1}$$

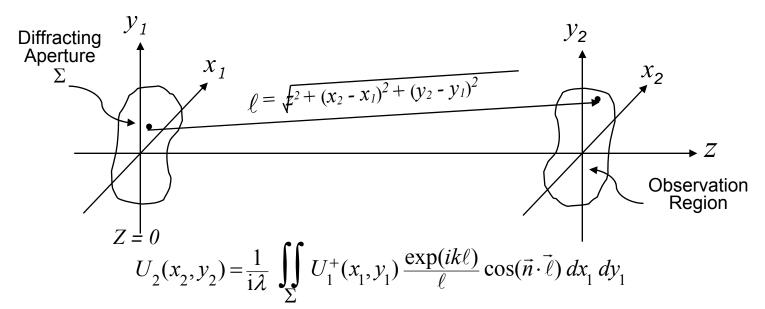
which we recognize as the following Fourier Transform integral.

$$U_{2}(x_{2}, y_{2}) = \frac{\exp(ikz)}{i\lambda z} \exp\left[i\frac{k}{2z}(x_{2}^{2} + y_{2}^{2})\right] \mathcal{F}\left\{U_{1}^{+}(x_{1}, y_{1}) \exp\left[i\frac{k}{2z}(x_{1}^{2} + y_{1}^{2})\right]\right\} \Big|_{\xi = \frac{x_{2}}{\lambda z}, \, \eta = \frac{y_{2}}{\lambda z}}$$

Fresnel Diffraction Formula

(3)

The Fraunhofer Approximation



Rayleigh-Sommerfeld Diffraction Formula for arbitrary illumination.

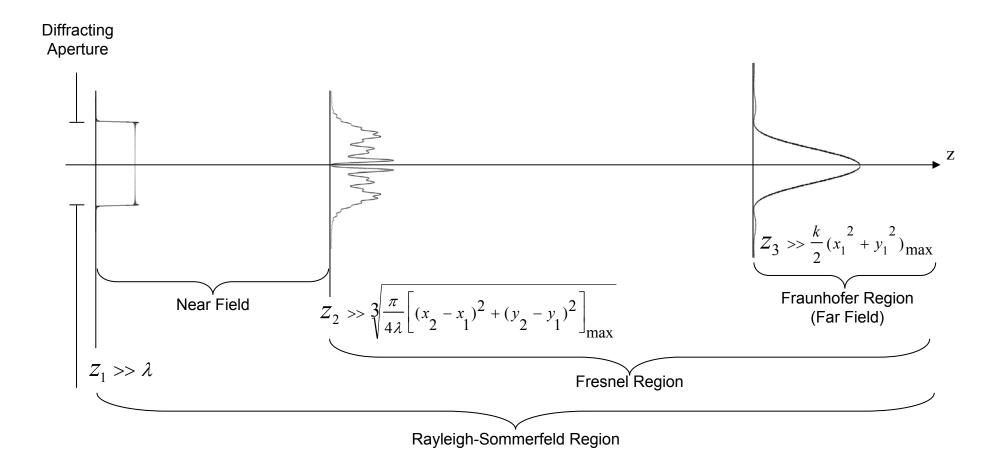
If the more stringent Fraunhofer criterion ($z >> k(x_1^2 + y_1^2)_{max}$) is satisfied, then the quadratic phase factor in the argument of the Fourier Transform operation is approximately unity over the entire aperture, and the complex amplitude distribution on the observation plane can be found directly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

$$U_{2}(x_{2}, y_{2}) = \frac{\exp(ikz)}{i\lambda z} \exp\left[i\frac{k}{2z}(x_{2}^{2} + y_{2}^{2})\right] \mathbf{\mathcal{F}}\left\{U_{1}^{+}(x_{1}, y_{1})\right\}\Big|_{\xi = \frac{x_{2}}{\lambda z}, \eta = \frac{y_{2}}{\lambda z}}$$

(4)

Fraunhofer Diffraction Formula

Fresnel and Fraunhofer Criteria* (and Regions of Validity)



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

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

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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 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.

$$A_{o}(\alpha,\beta;0) = \int_{-\infty-\infty}^{\infty} \int_{-\infty-\infty}^{\infty} U_{o}(\hat{x},\hat{y};0) \exp[-i2\pi(\alpha\hat{x}+\beta\hat{y})\,d\hat{x}\,d\hat{y}]$$
(5)
$$U_{o}(\hat{x},\hat{y};0) = \int_{-\infty-\infty}^{\infty} \int_{-\infty-\infty}^{\infty} A_{o}(\alpha,\beta;0) \exp[i2\pi(\alpha\hat{x}+\beta\hat{y})\,d\alpha\,d\beta]$$
(7)
$$U_{o}(\hat{x},\hat{y};2) = \int_{-\infty-\infty}^{\infty} \int_{-\infty-\infty}^{\infty} A(\alpha,\beta;\hat{z}) \exp[i2\pi(\alpha\hat{x}+\beta\hat{y})\,d\alpha\,d\beta]$$
(8)

* 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

$$\hat{\nabla}^2 + (2\pi)^2 \left[U(\hat{x}, \hat{y}; \hat{z}) = 0 \right]$$
(9)

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

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

$$\gamma = \sqrt{1 - (\alpha^2 + \beta^2)}$$
(10)

for $(\alpha^2 + \beta^2) \le 1$

where

Since Eq.(10) 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, $H(\alpha, \beta; \hat{z})$

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

(11)

where

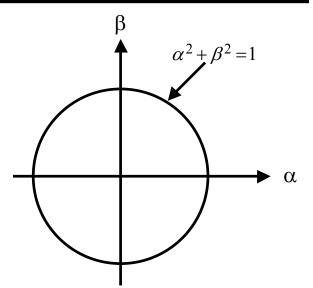
$$\gamma = \text{is imaginary} \quad \text{for}(\alpha^2 + \beta^2) \ge 1$$

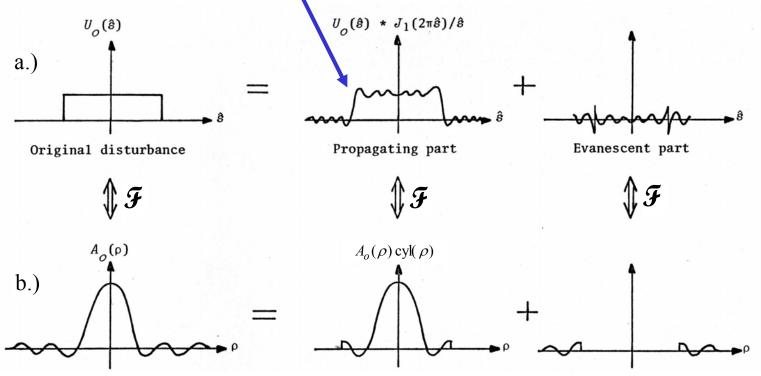
 $\gamma = is real$

Plane Wave Components in Direction Cosine Space

Consider a unit circle in direction cosine space as illustrated below. Inside the circle γ 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 γ 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.(10). 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.(11). Starting with the well-known Wehl expansion formula,* and following Lalor,** we obtain

$$h(\hat{x},\hat{y};\hat{z}) = \mathcal{F}^{-1}\left\{\exp(i2\pi\gamma\hat{z})\right\} = \left(\frac{1}{2\pi\hat{r}} - i\right)\frac{\hat{z}}{\hat{r}} \frac{\exp(i2\pi\hat{r})}{\hat{r}}$$
(12)

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 $\hat{r} >> 1$, 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.

$$h(\hat{x}, \hat{y}; \hat{z}) = -i\frac{\hat{z}}{\hat{r}}\frac{\exp(i2\pi\hat{r})}{\hat{r}} = \frac{\hat{z}}{\hat{r}}\frac{\exp[i2\pi(\hat{r}-1/4)]}{\hat{r}}$$
(13)

Impulse Response of Free Space \equiv Huygens' Wavelett

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.(12) for $h(\hat{x}, \hat{y}; \hat{z})$, we obtain the general Rayleigh-Sommerfeld Diffraction

Formula

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

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.(14); 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 $\hat{z} >> 1$

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

(14)

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 Helmholz 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

$$U(\hat{x}_{2},\hat{y}_{2};\hat{z}) = \frac{\exp(i2\pi\hat{z})}{i\hat{z}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathcal{U}_{o}(\hat{x}_{1},\hat{y}_{1};\hat{x}_{2},\hat{y}_{2}) \exp[-(i2\pi/\hat{z})(\hat{x}_{1}\hat{x}_{2}+\hat{y}_{1}\hat{y}_{2})] d\hat{x}_{1} d\hat{y}_{1}$$
(16)

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 (aberrations). These aberrations are precisely the effects ignored when making the usual Fresnel and Fraunhofer approximations.

$$\hat{W}(\hat{x}, \hat{y}) \equiv Wave front Aberation Function$$

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.

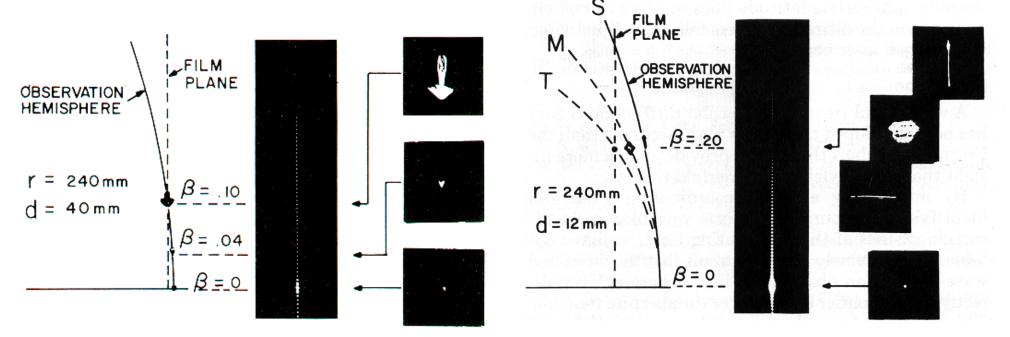
Aberration Coefficients for Different Configurations

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

	Geometrical Configuration Plane Sphere Sphere		
Aberrations	Plane Plane	Sphere Plane	Spnere Hemisphere
\hat{W}_{200} (Piston Error)	$\frac{\hat{z}}{2} \left(\frac{\hat{s}_{\text{max}}}{\hat{z}} \right)^2$	$\frac{\hat{z}}{2} \left(\frac{\hat{s}_{\max}}{\hat{z}}\right)^2$	0
\hat{W}_{020} (Defocus)	$rac{\hat{z}}{2} \left(rac{\hat{d}}{2\hat{z}} ight)^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
Ŵ ₁₃₁ (Coma)	$\frac{\hat{z}}{2} \left(\frac{\hat{s}_{\max}}{\hat{z}} \right) \left(\frac{\hat{d}}{2\hat{z}} \right)^3$	$\frac{\hat{z}}{2} \left(\frac{\hat{s}_{\max}}{\hat{z}} \right) \left(\frac{\hat{d}}{2\hat{z}} \right)^3$	$\frac{\hat{\mathbf{r}}}{2}\boldsymbol{\beta}_{\max}\left(\frac{\hat{d}}{2\hat{r}}\right)^{3}$
\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

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).

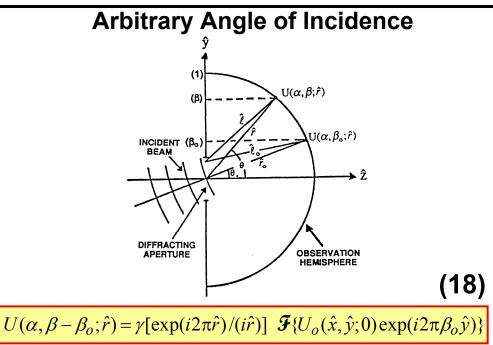


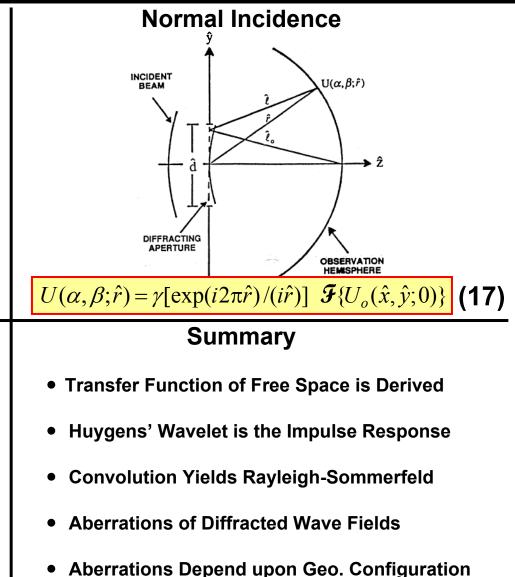
These aberrations are not; however, due to any "flaw" in the grating. They are inherent to the diffraction process. The grating merely concentrates light at field positions where the aberrations manifest themselves.

* 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 θ_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.





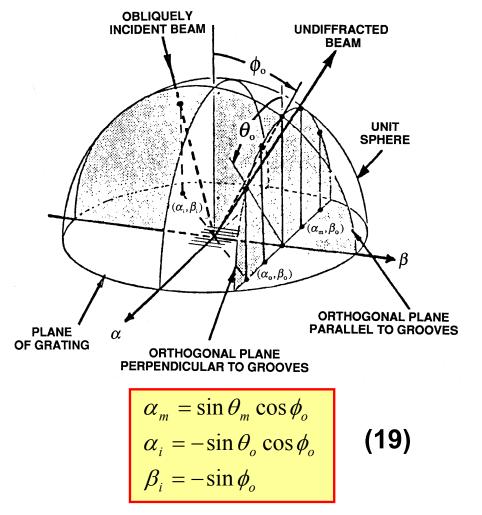
• Shift-invariance in Direction Cosine Space

* J. E. Harvey, "Fourier Treatment of Near-field Scalar Diffraction Theory", Am. J. Phys. 47 (11), 974-980, Nov 1979.

Shift-Invariance in Direction Cosine Space*

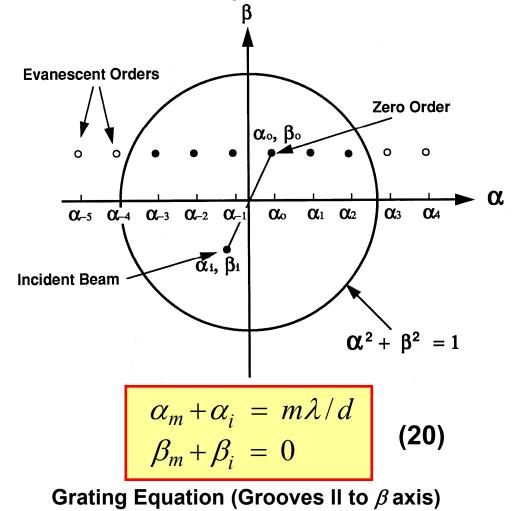
Global View of Diffraction

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



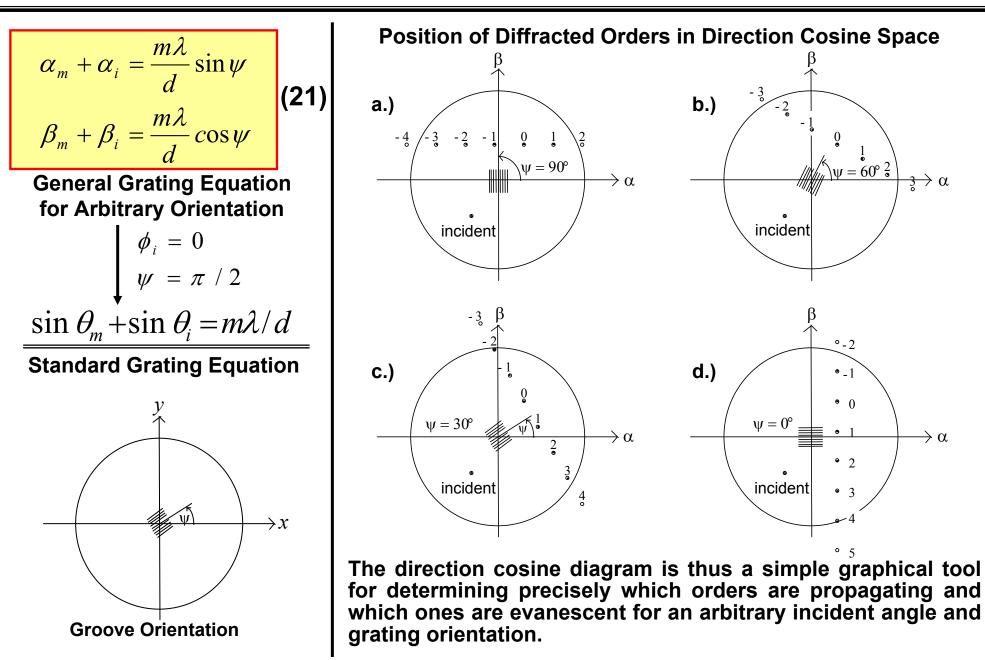
Direction Cosine Diagram

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



* J. E. Harvey and C. L. Vernold, "Description of Diffraction Grating Behavior in Direction Cosine Space", Appl. Opt. 37, 8158-8160 (Dec. 1, 1998).

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

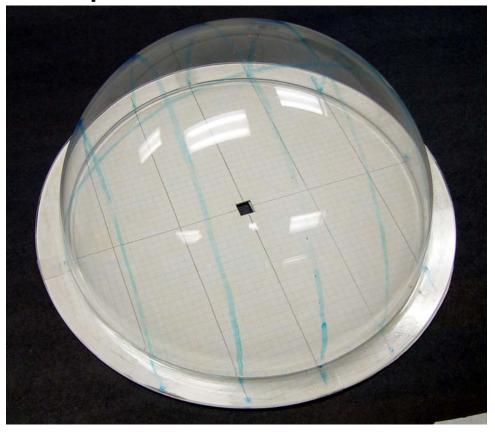


* H. A. Rowland, "Gratings in Theory and Practice", Phil. Mag., S.5. Vol. 35, No. 216, 397-419 (May 1893).

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.

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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*.

Irradiance
$$\equiv E = \frac{\partial P}{\partial A_c}$$
 (watts/area)
Radiant Exitance $\equiv M = \frac{\partial P}{\partial A_s}$ (watts/area)
Radiant Intensity $\equiv I = \frac{\partial P}{\partial \omega_c}$ (watts/steradian)
Radiance $\equiv L = \frac{\partial^2 P}{\partial \omega_c \partial A_s \cos \theta_s}$ (watts/steradian projected area)

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 today. 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) cm⁻¹/molecule-cm⁻², and finally (6) cm⁻²-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)

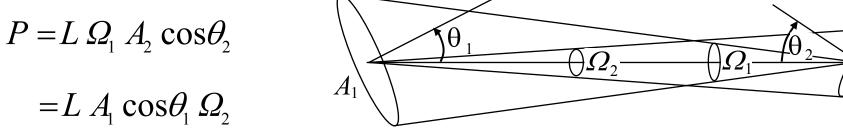
An extended source, that is, one whose dimensions are significant, must be treated differently than a point source. A small area of the source will radiate a certain amount of power per unit solid angle, thus, the radiation characteristics of a extended source are expressed in terms of power per unit 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 dA₁ and a receiver dA₂.

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

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

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.



Either $A_{\rho}\Omega$ product can be used. This is often a convenient flexibility in making calculations.

Diffracted Radiance: The Fundamental Quantity Predicted by Scalar Diffraction Theory*

The direction cosines α , β , and γ are related to the angular variables θ and ϕ in conventional spherical coordinates by the following expressions, where we have dropped the subscript *s* on the angles associated with the source

$$\alpha = \sin\theta \cos\varphi, \quad \beta = \sin\theta \sin\varphi, \quad \gamma = \cos\theta$$

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 *

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

From the shift theorem of Fourier Transform theory, we have

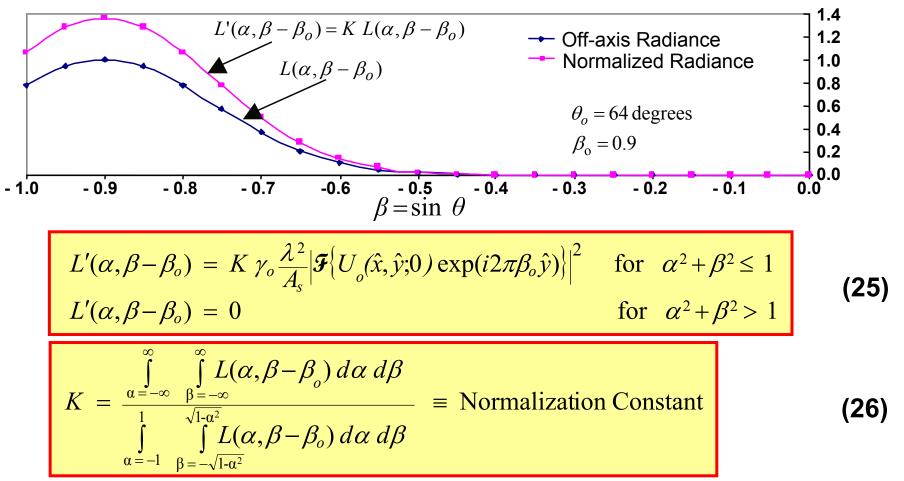
$$L(\alpha,\beta-\beta_o) = \gamma_o \frac{\lambda^2}{A_s} \left| \mathcal{F} \left\{ U_o(\hat{x},\hat{y};0) \exp(i2\pi\beta_o \hat{y}) \right\} \right|^2$$
(24)

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 cases 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.



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

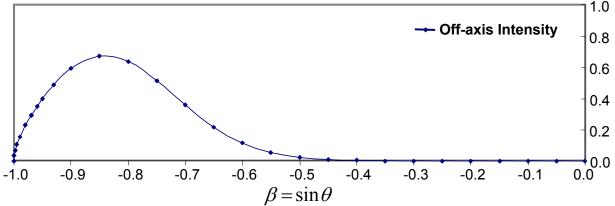
$$I(\alpha,\beta) = \int_{A_s} L(\alpha,\beta) \cos\theta_s \,\partial A_s$$

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

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

$$I(\alpha, \beta - \beta_o) = 0 \text{ for } \alpha^2 + \beta^2 > 1$$
(27)

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)

dA

(28)

 $d\omega_{r}$

Also, the bidirectional reflectance distribution $d\omega_{i}$ 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)

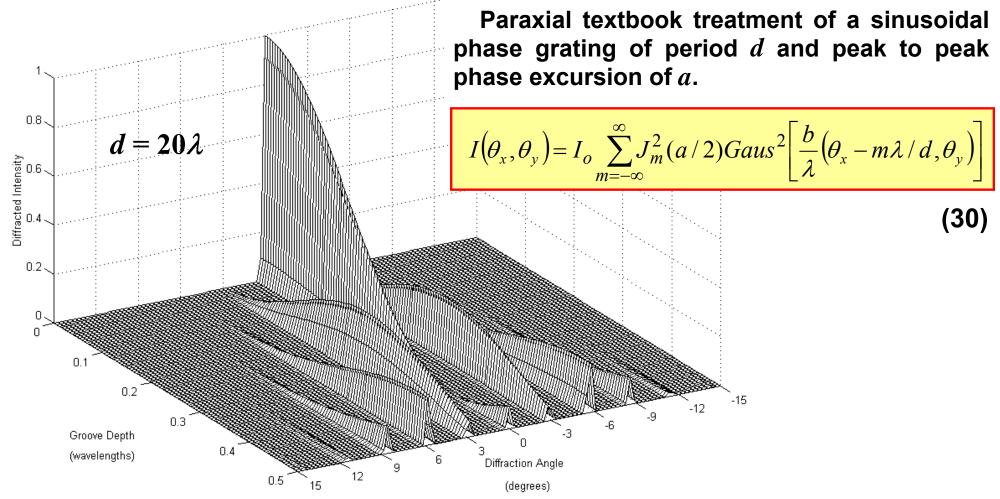
$$BRDF = f(\theta_r, \phi_r; \theta_i, \phi_i) = \frac{dL_r(\theta_r, \phi_r; \theta_i, \phi_i)}{dE_i(\theta_i, \phi_i)}$$
(29)

Outline

- 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

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

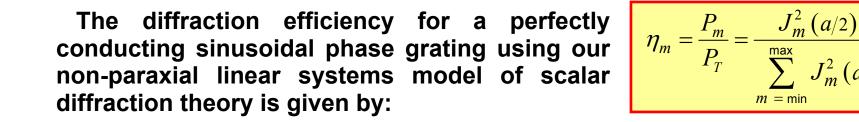
Scalar diffraction theory is frequently considered inadequate for predicting diffraction efficiencies for grating applications where $\lambda/d > 0.1$. It has also been stated that scalar theory imposes energy upon the evanescent diffracted orders.

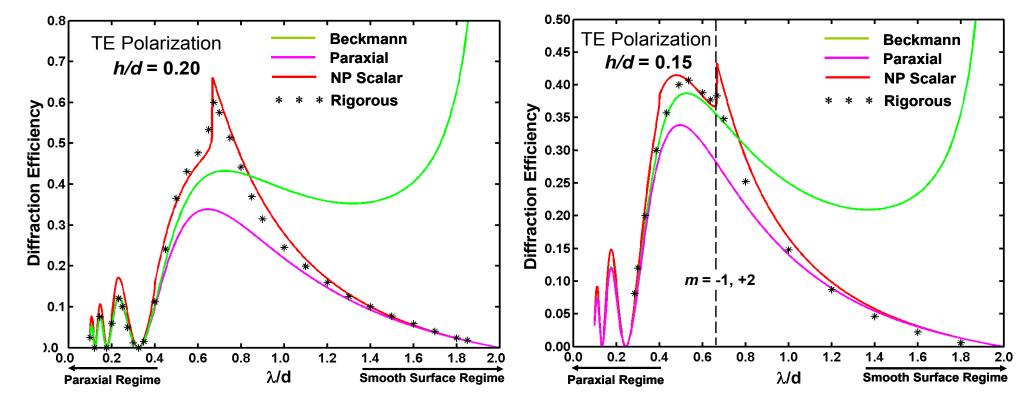


This leads to the common misconception that it is impossible to get more than 33.86% of the total reflected energy into the +1 diffracted order.

Diffraction Efficiency of a Perfectly Conducting Sinusoidal Phase Grating*

(31)



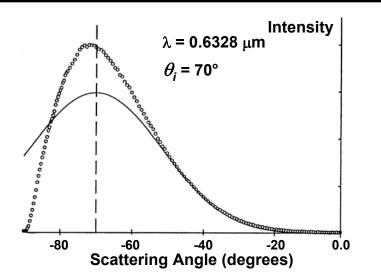


These figures show that using our non-paraxial scalar diffraction theory is able to predict efficiencies over a much larger range than previously thought possible.

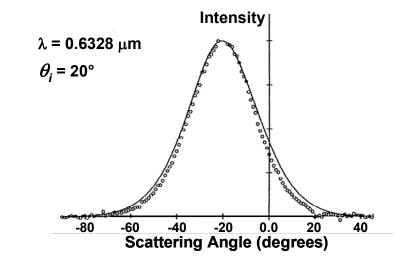
* J. E. Harvey, A. Krywonos and D. Bogunovic, "Non-paraxial Scalar Treatment of Sinusoidal Phase Gratings", JOSA A 23 (2006).

Example # 2: Explaining Non-Intuitive Experimental Surface Scatter Data*

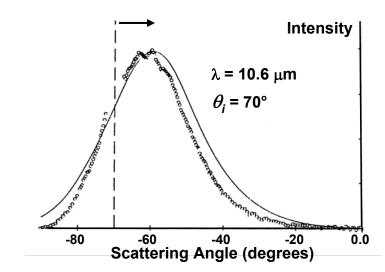
A detailed experimental investigation of light scattering from well-characterized random rough surfaces was reported by O'Donnell and Mendez in 1987. Several non-intuitive experimental results involving large scattering angles and large incident angles departed drastically from predictions using classical 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.

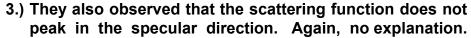


2.) Experimental data highly asymmetrical about the specular beam. B-K theory symmetrical but discontinuous at -90°.



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



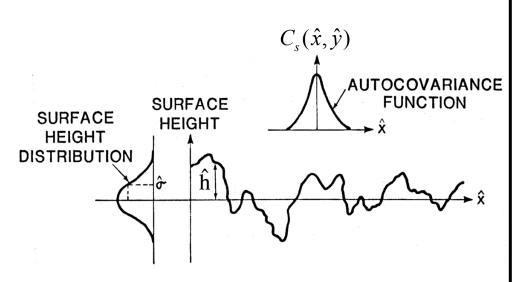


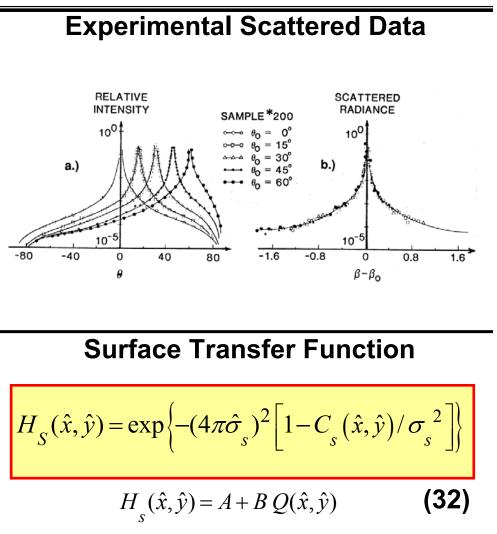
* O'Donnell and Mendez, "Experimental Study of Scattering from Characterized Random Surfaces", J. Opt. Soc. Am. A 4, 1194-1205 (1987).

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 merely rough surface imparts phase variations onto the incident wavefront upon No explicit "smooth surface" reflection. approximations were made.

Surface Characteristics



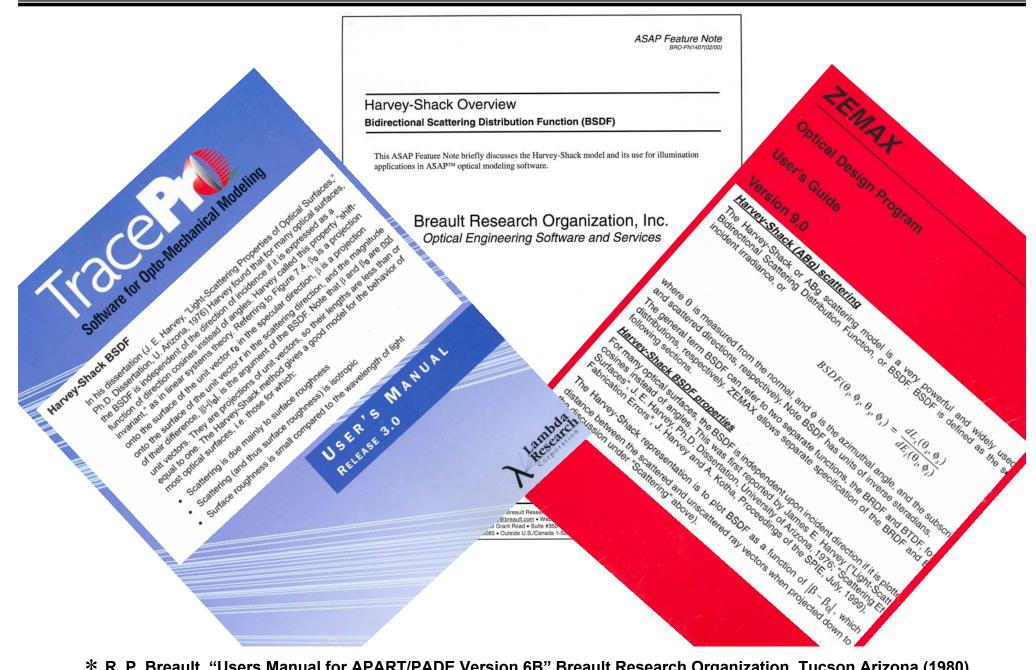


 $A = \exp[-(4\pi \hat{\sigma}_s)^2]$

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

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

Harvey-Shack Surface Scatter Model*



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

Modified Harvey-Shack Surface Scatter Theory*

During the 1980's the STF was generalized to include the extremely large incident angles inherent to grazing incidence Wolter Type I X-ray telescopes. The optical path difference (OPD) due to reflection from an irregular surface is illustrated here, and the assumed phase variation in the plane of the surface when the Kirchhoff approximation is invoked is presented. We have still made no explicit smooth surface approximation!

By Invoking the Kirchhoff Approximation

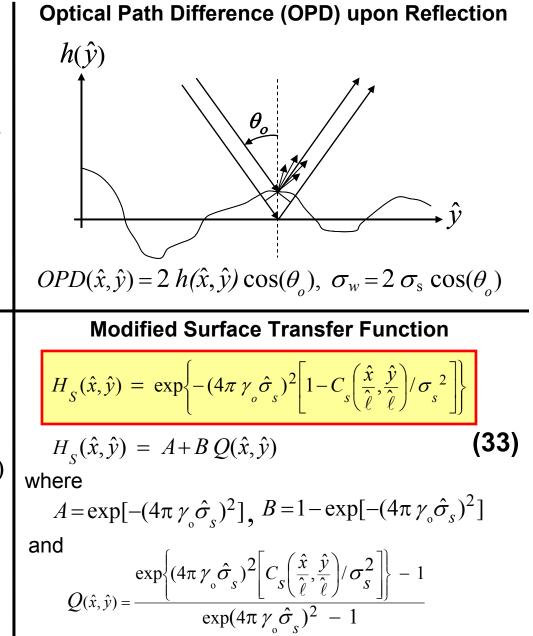
We can write the two-dimensional phase variation in the plane of the surface due to reflection from a rough surface at an arbitrary angle of incidence.

$$\phi(\hat{x}, \hat{y}) = (2\pi/\lambda) OPD = (4\pi/\lambda) h(\hat{x}, \hat{y}) \cos(\theta_o)$$

Of course, we must add to this the linear phase variation that results from the specularly reflected plane wavefront.

$$\phi_o = 2\pi\beta_o \hat{y}$$

Note that $\beta_o = \sin \theta_o$ and $\gamma_o = \cos \theta_o$.

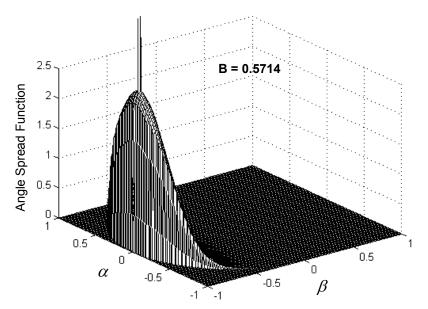


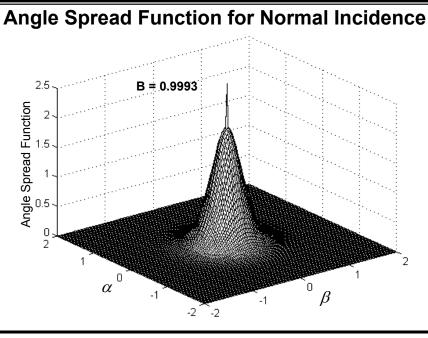
* J. E. Harvey, et. al., "Transfer Function Characterization of Grazing Incidence Optical Systems", Appl. Opt. 27, 1527-1533 (15 April 1988).

The Angle Spread Function (Scattered Radiance)

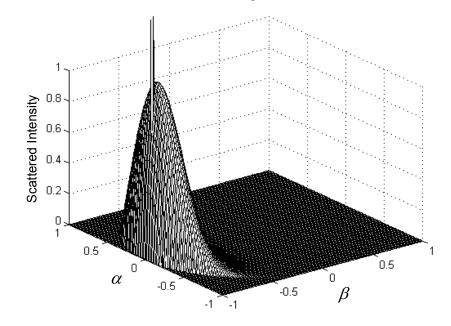
- For an isotropically rough surface, the scattered radiance function is rotationally symmetric for normal incidence.
- In accordance with our non-paraxial scalar diffraction theory, it is shift-invariant with respect to incident angle.
- For large incident angles it is truncated by the unit circle and 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).





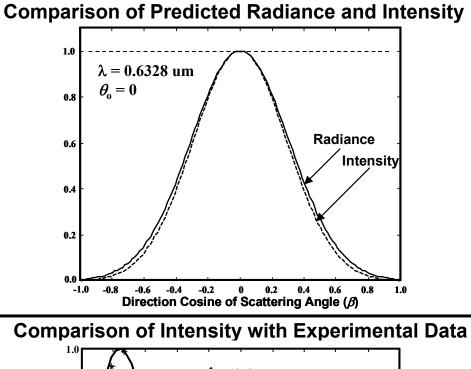


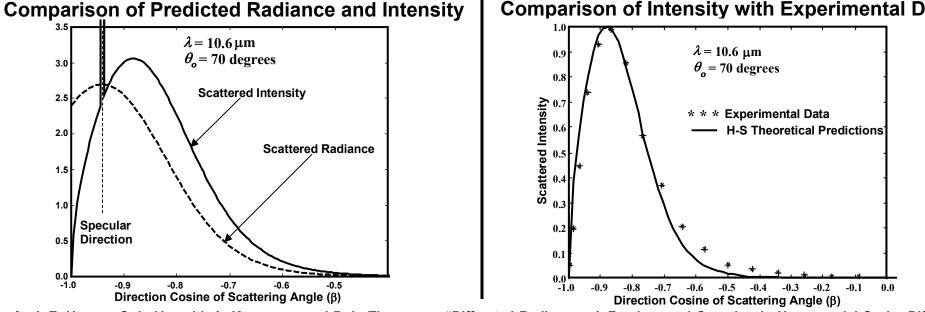
Scattered Intensity Distribution



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.





★ 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:

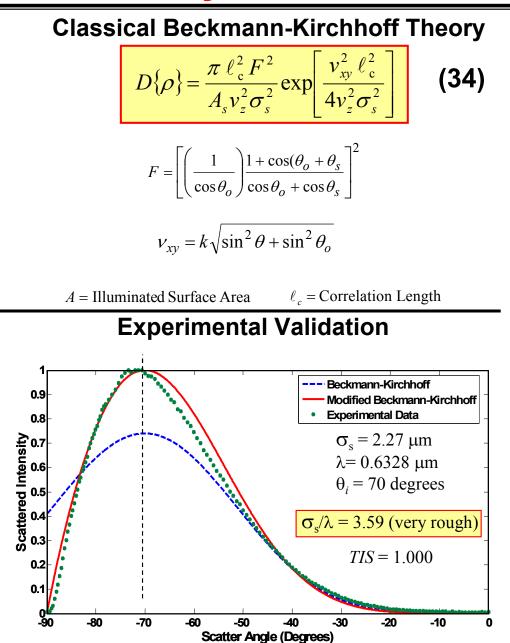
- Throw away the "F" factor.
- Equate to "Radiance".
- Apply the re-normalization factor, K.
- Multiply by Lambert's cosine function.

Modified Beckmann-Kirchhoff Theory

$$I(\theta,\phi) = K \frac{\pi \ell_c^2 \cos \theta}{v_z^2 \sigma_s^2} \exp\left[-\frac{v_{xy}^2 \ell_c^2}{4v_z^2 \sigma_s^2}\right]$$
(35)

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

 $I = L \cos \theta$ (Lambert's Cosine Law)



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

Summary and Conclusions

- 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.

However

In spite of the fact that this modified Beckmann-Kirchhoff surface scatter model seemed to provide the advantages of the classical Beckmann-Kirchhoff theory and the Rayleigh-Rice surface scatter theory—we got no respect from the scientific community.

Because it was only an *empirical modification*, not a *theoretical derivation*, the paper was rejected from two scientific journals before finally being published in Optical Engineering.*

During this time, the computer animation community started using (and referencing) our un-reviewed conference proceedings as it allowed them to render realistic objects and scenes.

Tomorrow I will discuss in detail a generalized Harvey-Shack surface scatter theory (theoretically-derived) that allows us to predict BRDFs from both smooth and rough surfaces, at large incident angles.

Joseph von Fraunhofer

(Father of Diffraction Grating Technology)

- First reported observation of grating effects by Francis Hopkinson, U.S. Sec. of Navy (1785).
- David Rittenhouse, an American astronomer, constructed the first grating (1786).
- Thomas Young used a diffraction grating to separate light into "an infinite number of colors" and investigate extensively the behavior of the dispersed light (1803).
- Joseph von Fraunhofer began his work on gratings (1821).
 - o Built the first grating ruling engine.
 - o Fabricated gratings of sufficient quality to measure the absorption lines of solar spectrum (which he discovered).
 - o Derived equations that governed the dispersive behavior of gratings.
 - o Noticed the presence of polarization effects.
 - o Was aware that groove shape affected the diffraction efficiency.

^{1.} D. Rittenhouse, "An Optical Problem Proposed by F. Hopkinson and Solved", J. Am. Phil. Soc. 201, 202-206 (1786).

^{3.} Young published most of his results in his Course of Lectures on Natural Philosophy and the Mechanical Arts (1807).

^{4.} J. Fraunhofer, "Kurtzer Bericht von the Resultaten neuerer Versuche uber die Gesetze des Lichtes, und die Theorie derselbem", Gilbert's Ann. Phys. 74, 337-378 (1823).