

# Biomedical Optics

## Light Scattering by Particles Theoretical Aspects

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[www.demul.net/frits](http://www.demul.net/frits)

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Dept. Appl. Physics, 1981 - 2003; revised 2017

# Light Scattering by Particles

## Theoretical Aspects

Contents: (movie part I)

1. Overview of scattering functions
2. Plots of various examples

Appendices: (movie part II)

- A. Derivation of the dipole radiation formula
- B. Derivation of the general scattering equation.

Literature: (most important)

H.C. van de Hulst: “Light scattering by small particles”,  
1957, 1981, ISBN 0486642283, Dover Publ. New York.

# Contents: (movie part I)

1. Overview of scattering functions
  - a) Huygens' principle of spherical waves
  - b) General scattering expression
  - c) Dipole (Rayleigh) scattering
  - d) Rayleigh-Gans scattering
  - e) Mie scattering
  - f) Various other expressions
2. Plots of various examples  
Dipole, Rayleigh-Gans, Mie, etc.

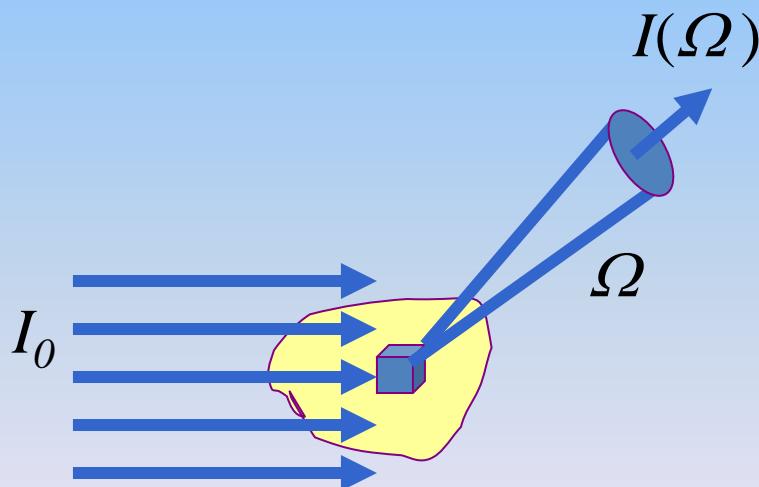
# Definitions

## Definitions:

**Incident intensity:**  $I_0$

**Scattered intensity:**  $I(\Omega)$

**$\Omega$  = solid scattering angle**



**Scattering cross section  $\sigma$**

per particle [m<sup>2</sup>]

= apparent effective “shadow area”  
for scattering

$\sigma$  may be dependent on the angle  
of scattering

$$\frac{d\sigma}{d\Omega}$$

**differential scattering  
cross section**

$$I(\Omega) = \frac{d\sigma}{d\Omega} I_0$$

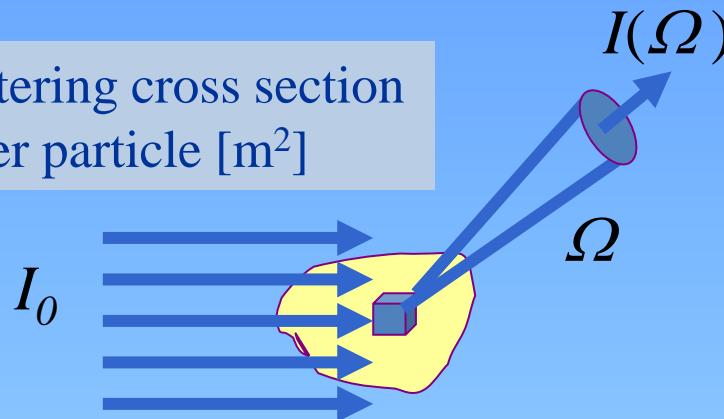
$$\left[ \frac{W}{sr} \right] = \left[ \frac{m^2}{sr} \right] \left[ \frac{W}{m^2} \right]$$

$$\sigma_{tot} = \iint_{\Omega} \left( \frac{\partial \sigma}{\partial \Omega} \right) d\Omega$$

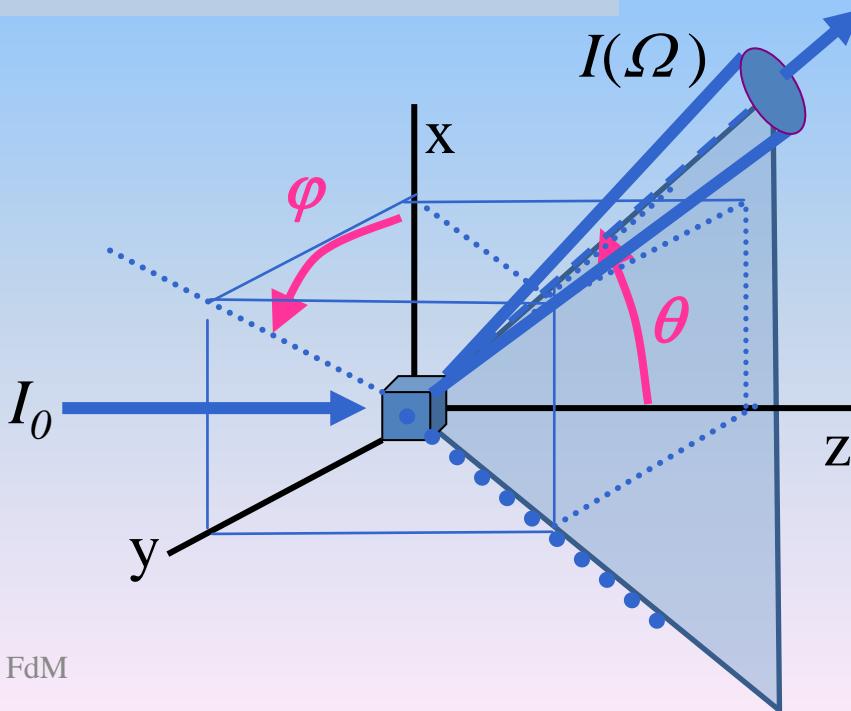
**total scattering  
cross section**

# Definitions

Scattering cross section  
 $\sigma$  per particle [m<sup>2</sup>]



Incident beam // +Z-axis



$$I(\Omega) = \frac{d\sigma}{d\Omega} I_0$$

Scattering angles:

$\theta$  = polar angle (from Z-axis)

$\varphi$  = azimuthal angle (in XY-plane)

Scattering function:

$$p(\theta, \varphi) = \frac{\partial \sigma}{\partial \Omega}$$

$$I(\Omega) = p(\theta, \varphi) I_0$$

Normalization:

$$\frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} p(\theta, \varphi) \cdot \sin \theta \cdot d\theta d\varphi = 1$$

# Definitions

Wave vectors:  $\mathbf{k}_0$  and  $\mathbf{k}_s$  (or  $\mathbf{k}$ )

$$k = \frac{2\pi}{\lambda} \quad ; \quad \lambda_{medium} = \frac{\lambda_{vacuum}}{n}$$

Scattering / Absorption coefficients:  $\mu$  [m<sup>-1</sup>]

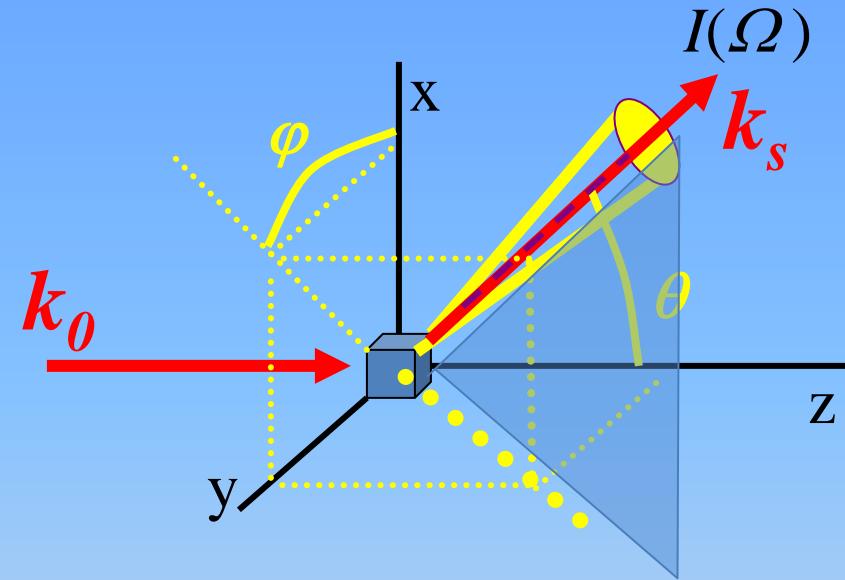
$$\mu = n \sigma$$

$$[\text{m}^{-1}] = [\text{m}^{-3}] [\text{m}^2]$$

$$n = \text{nr. of particles per m}^3$$

Lambert-Beer Law:

$$I(z) = I_0 \cdot \exp(-\mu z)$$



Beam attenuation coefficients:

- scattering:  $\mu_s$  [m<sup>-1</sup>]
- absorption:  $\mu_a$
- total:  $\mu_t = \mu_s + \mu_a$

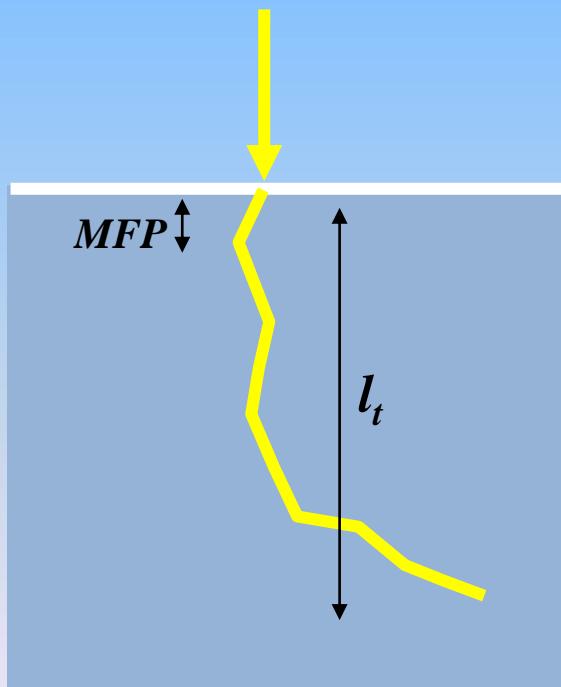
Mean-free-path:  $MFP = \mu_t^{-1}$  [m]

Albedo :  $\mu_s / \mu_t$  [-]

# Definitions

Scattering in tissue is predominantly forward:

$$g = \langle \cos \theta \rangle > \approx 0.9$$



Reduced scattering coefficient:  
 $\mu_s' = (1 - g) \mu_s \quad \ll \mu_s$

Transport mean-free-path:  
 $l_t = 1 / [\mu_s' + \mu_a] \gg MFP$

$$MFP = 1 / [\mu_s + \mu_a]$$

# Overview

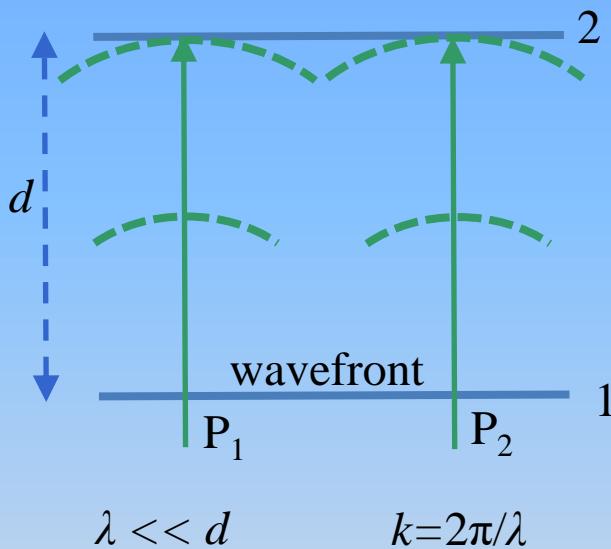
Overview of theories:

EM	Basic: Electromagnetic Theory from Maxwell's Equations
D	Dipolar (Rayleigh) scattering
RG	Rayleigh-Gans scattering
M	Mie scattering
HG	Other Scattering Functions: Henyey-Greenstein
I	Isotropic
PF	Peaked-forward
G	Advanced Models: Groenhuis
B	Bonner
P	Patterson
F	Farrell
FdM	Fundamental: (not in this presentation) Transport Equation and Diffusion Scattering

# Basic Theories: Principle of Huygens

Field propagation by spherical waves, emitted by all points of the wavefront

EM  
D  
RG  
M  
  
HG  
I  
PF  
  
G  
B  
P  
F



Fresnel (1818) derived:

“Disturbance”

from any point of plane 1 to any point of plane 2 (at mutual distance  $r$ ):

~ spherical wave  $\Phi$ :

$$\Phi = \frac{e^{-ikr}}{r}$$

Integrate over plane 2:

**Result:** “Disturbance”  $E$  caused by a “disturbance”  $E_0$ , present at a wavefront area element  $dS$ , in a point at a distance  $r$  from  $dS$  :

$$E = \frac{i}{r\lambda} e^{-ikr} dS \cdot E_0$$

Factor  $i$  ( $= e^{i\pi/2}$ ) causes phase shift  $1/2 \pi$  in scattered wave ( $\cos \leftrightarrow \sin$ ).

This is the basic formula for all light scattering theories.

# Basic EM Scattering Theory (1)

EM  
D  
RG  
M

HG  
I  
PF

G  
B  
P  
F

Electromagnetic Theory from Maxwell's Equations  $\rho = 0 ; j = 0$

$$\nabla \bullet \vec{D} = 0 \quad ; \quad \nabla \bullet \vec{B} = 0 \quad ; \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad ; \quad \nabla \times \vec{B} = \mu_0 \frac{\partial \vec{D}}{\partial t}$$

Wave Equation:

$$\nabla \times \nabla \times \vec{E} = -\mu_0 \frac{\partial^2 \vec{D}}{\partial t^2}$$

Insert material properties:  
dielectric constant  
 $\epsilon_I = \epsilon_0 \cdot (\epsilon_r - 1) = f(r, t)$

$$\vec{D}(\vec{r}, t) = \epsilon(\vec{r}, t) \cdot \vec{E}(\vec{r}, t)$$

$$\epsilon(\vec{r}, t) = \epsilon_0(\vec{r}, t) + \epsilon_1(\vec{r}, t) + \dots$$

Fields: incident:  $E_0$   
scattered:  $E_1$   
total:  $E = E_0 + E_1$

$$\vec{E}_0(r, t) = \vec{E}_{0m} \exp[i(\vec{k}_0 \bullet \vec{r} - \omega_0 t)]$$

$$k = 2\pi/\lambda \quad ; \quad \omega = 2\pi f$$

Assume:  $\epsilon_I \ll \epsilon_0$  and  $E_1 \ll E_0$  ; 1<sup>st</sup> order approximation

# Basic EM Scattering Theory (2)

EM  
D  
RG  
M

HG  
I  
PF

G  
B  
P  
F

Wave Equation:

$$\nabla \times \nabla \times \vec{E} = -\mu_0 \frac{\partial^2 \vec{D}}{\partial t^2} ; \quad \vec{D} = \epsilon \vec{E}$$

Assume:  $\epsilon_I \ll \epsilon_0$  and  $E_I \ll E_0$  ; 1<sup>st</sup> order approximation

Insert:  $E_0 + E_I$  for  $E$ , and of  $\epsilon_0 + \epsilon_I$  for  $\epsilon$  in the Wave Equation

Use:  $\nabla \times \nabla \times \vec{E} = -\nabla^2 \vec{E} + \nabla(\nabla \bullet \vec{E}) = -\nabla^2 \vec{E}$  since  $\nabla \bullet \vec{E} = 0$

0<sup>th</sup> order:

$$\nabla^2 \vec{E}_0 = \epsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} \vec{E}_0 \quad \Rightarrow \text{Incoming field } \vec{E}_0$$

1<sup>st</sup> order:

$$\nabla^2 \vec{E}_1 - \epsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} \vec{E}_1 = \mu_0 \frac{\partial^2}{\partial t^2} (\epsilon_1 \vec{E}_0) - \frac{1}{\epsilon_0} \nabla(\nabla \bullet (\epsilon_1 \vec{E}_0))$$

so:

$$f_1(\vec{E}_1) = f_0(\epsilon_1 \vec{E}_0)$$

Problem: Find  $E_I = f(\epsilon_1 E_0)$

# Basic EM Scattering Theory (3)

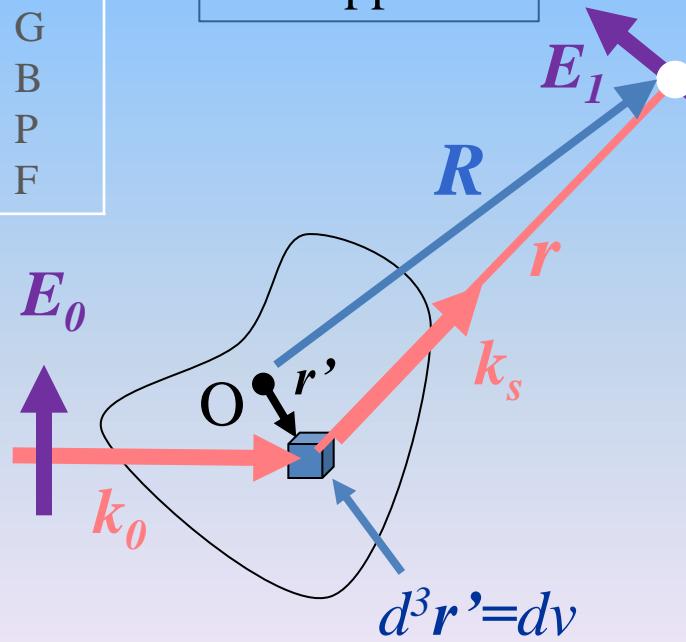
EM  
D  
RG  
M  
  
 HG  
I  
PF  
  
 G  
B  
P  
F

**Problem:** Find  $\vec{E}_I = f(\epsilon_I \vec{E}_0)$

**Solution:**

$$\vec{E}_I(\vec{R}, t) = \frac{1}{4\pi\epsilon_0 R} \iiint_{vol} d^3\vec{r}' \vec{k}_s \times \vec{k}_s \times \left\{ \epsilon_I(\vec{r}', t') \cdot \vec{E}_0(\vec{r}', t') \right\}$$

**Derivation:**  
See Appendix



Volume integration

$\epsilon$  : Material properties

$1/R$  : Spherical outgoing wave

Polarization direction

$E_0$ : Incident field vector

Retarded time:  $t' = t - (\vec{r} - \vec{r}')/c$   
due to flight time towards detector.  
This retarded time accounts for phase differences

$$\exp [-i(\vec{k}_s - \vec{k}_0) \bullet (\vec{R} - \vec{r}') - i\omega_0 t]$$

# Basic EM Scattering Theory (4)

EM  
D  
RG  
M  
HG  
I  
PF  
G  
B  
P  
F

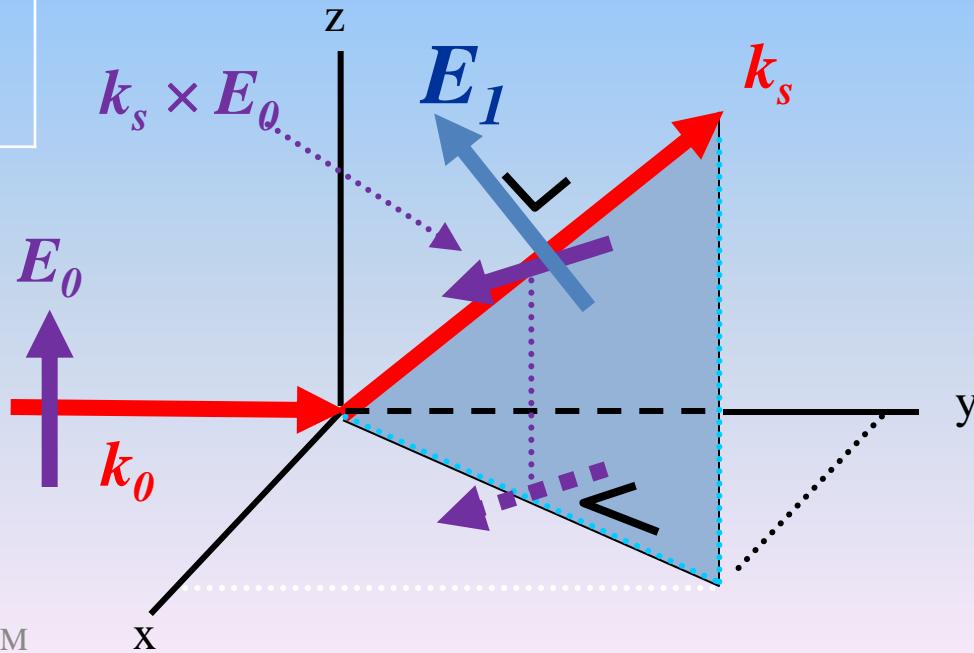
Determine direction of Polarization:

Here  $\varepsilon(\vec{r}', t')$  is scalar function

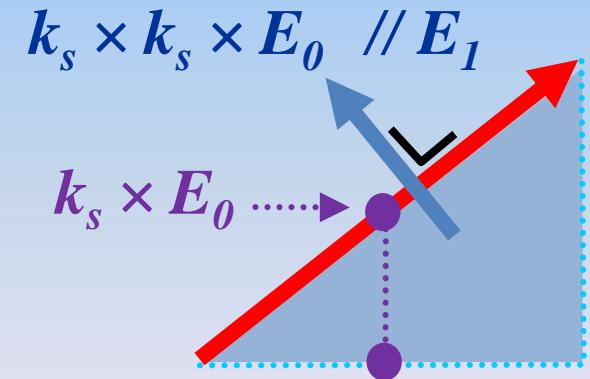
Solution:

$$\vec{E}_1(\vec{r}, t) = \frac{1}{4\pi\varepsilon_0 r} \iiint_{vol} d^3\vec{r}' [\vec{k}_s \times \vec{k}_s \times \left\{ \varepsilon_1(\vec{r}', t') \cdot \vec{E}_0(\vec{r}', t') \right\}]$$

$$\vec{E}_1 \parallel [\vec{k}_s \times \vec{k}_s \times \vec{E}_0]$$



$\vec{E}_0$ : vertical polarization



$\vec{k}_s \times \vec{E}_0$  pointing out-of-plane

# Basic EM Scattering Theory (5)

EM  
D  
RG  
M  
HG  
I  
PF  
  
G  
B  
P  
F

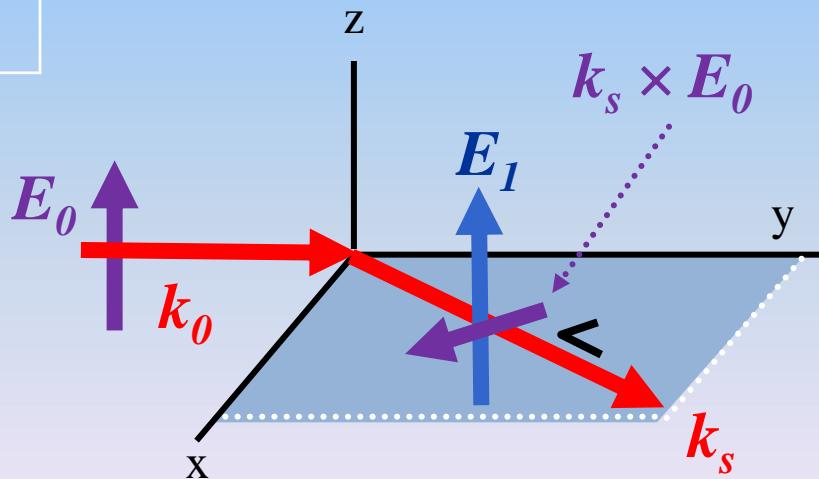
## Determine direction of Polarization

Here  $\varepsilon(\vec{r}', t')$  is scalar function

Solution:

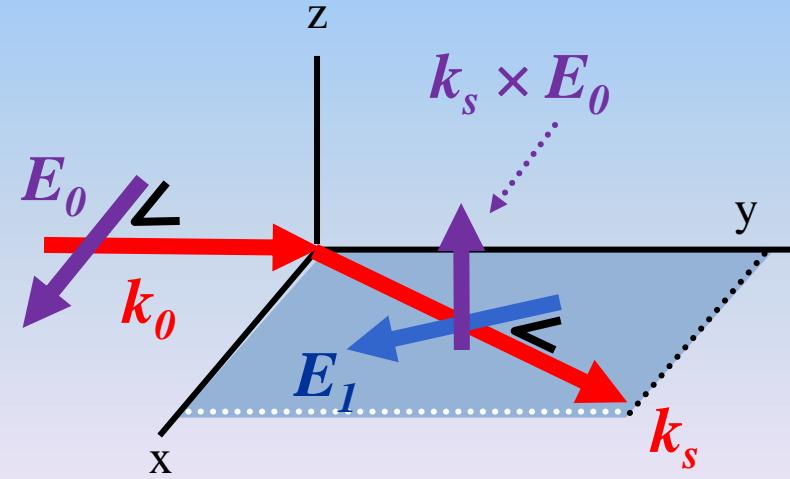
$$\vec{E}_1(\vec{r}, t) = \frac{1}{4\pi\varepsilon_0 r} \iiint_{vol} d^3\vec{r}' \cdot \vec{k}_s \times \vec{k}_s \times \left\{ \varepsilon_1(\vec{r}', t') \cdot \vec{E}_0(\vec{r}', t') \right\}$$

In-plane scattering:  
vertical polarization



No depolarization

In-plane scattering:  
horizontal polarization



Depolarization present

# Basic EM Scattering Theory (6)

EM  
D  
RG  
M

HG  
I  
PF

G  
B  
P  
F

## Solution: Electric Field Strength:

Here  $\varepsilon(\vec{r}', t')$  is scalar function

$$\vec{E}_I(\vec{r}, t) = \frac{1}{4\pi\varepsilon_0 r} \iiint_{vol} d^3\vec{r}' \cdot \vec{k}_s \times \vec{k}_s \times \left\{ \varepsilon_1(\vec{r}', t') \cdot \vec{E}_0(\vec{r}', t') \right\}$$

Intensity =  
autocorrelation  
function of  
Field Strength:

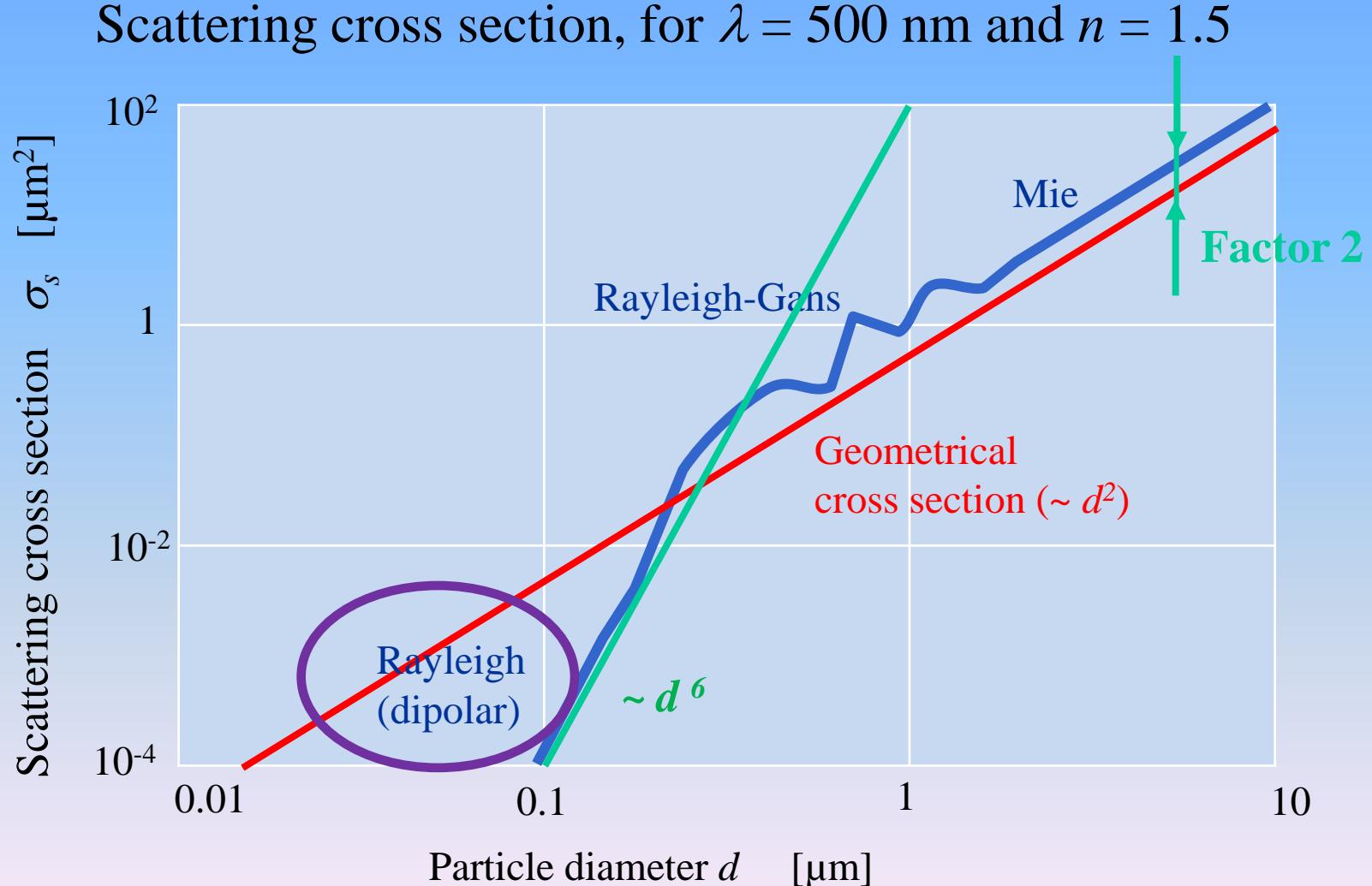
$$I(\vec{r}, t) \propto \langle \vec{E}_I^*(\vec{r}, 0) \bullet \vec{E}_I(\vec{r}, t) \rangle \equiv \lim_{T \rightarrow \infty} \frac{1}{2\pi} \int_{-T}^{+T} d\tau \vec{E}_I^*(\vec{r}, \tau) \bullet \vec{E}_I(\vec{r}, \tau + t)$$

Intensity  $\sim$  (Field Strength)<sup>2</sup>

$$\begin{aligned} &\sim k^4 \sim \lambda^{-4} \\ &\sim r^{-2} \\ &\sim \varepsilon_1^2 \\ &\sim \text{volume}^2 \end{aligned}$$

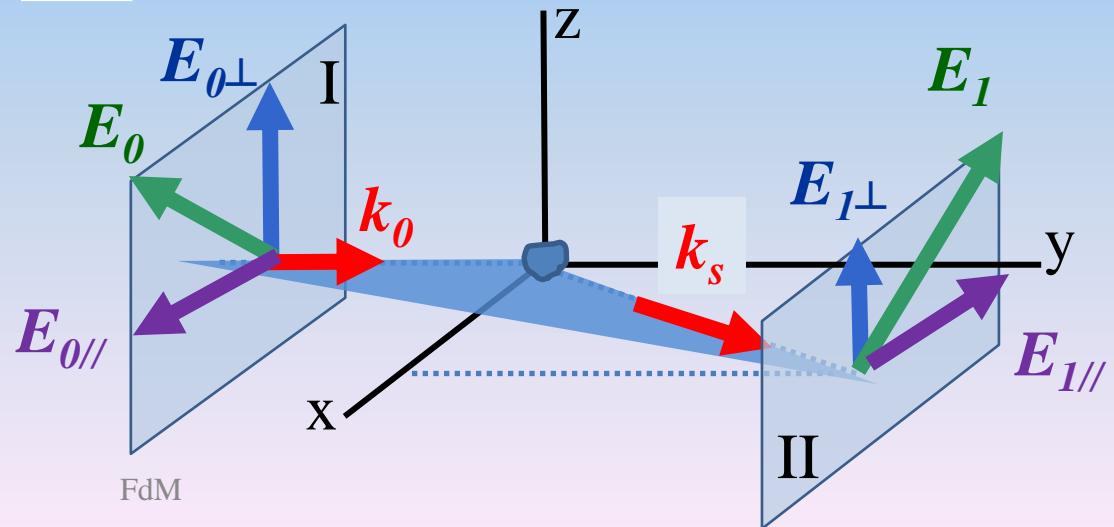
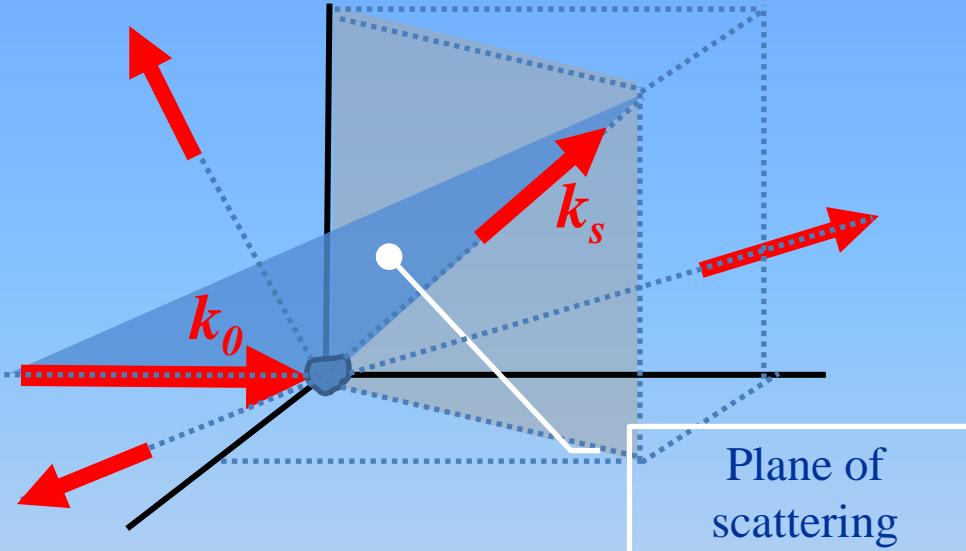
NB. If  $\varepsilon$  = tensor function of coordinates,  
then polarization direction will differ.

# Optical properties: scattering



# Dipole (Rayleigh) Scattering (1)

EM  
D  
RG  
M  
HG  
I  
PF  
G  
B  
P  
F



Wavevectors:

- Incident field:  $k_0$
- Scattered field:  $k_s$

Define **plane of scattering**  
using  $k_0$  and  $k_s$

Define **coordinate axes**:

x, y, z

Plane I , II  $\perp k_0 , k_s$  resp.

Electric field:

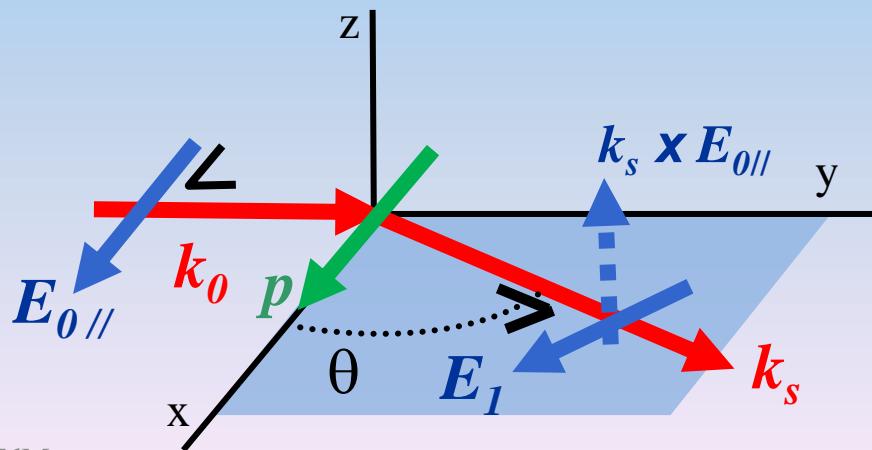
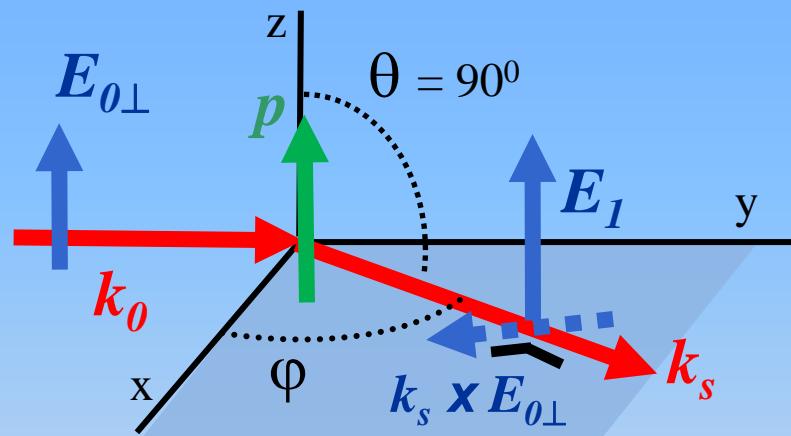
- Incident:  $E_0$
- Scattered:  $E_1$  (or  $E_s$ )

$E$ -field has components  
 $E_\perp$  and  $E_{//}$   
w.r.t. this scattering plane.

# Dipole (Rayleigh) Scattering (2)

EM  
D  
RG  
M  
HG  
I  
PF  
G  
B  
P  
F

$$\mathbf{E}_1 \parallel [\mathbf{k}_s \times \mathbf{k}_s \times \mathbf{E}_0]$$



Dipole  $\mathbf{p}$  induced by  $E$ -field  $\mathbf{E}_0$

$$\mathbf{p} = \alpha \mathbf{E}_0 \quad \mathbf{E}_1 \perp \mathbf{k}_s$$

$\alpha \sim$  relative dielectric constant

$E$ -field has components  $\mathbf{E}_\perp$  and  $\mathbf{E}_{\parallel}$  w.r.t. the scattering plane.

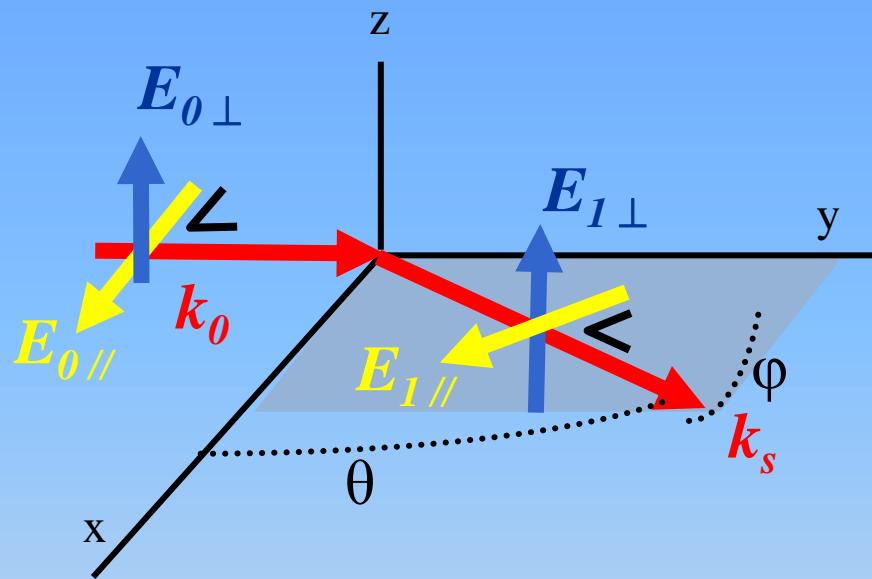
$$\begin{bmatrix} \mathbf{E}_{1\perp} \\ \mathbf{E}_{1\parallel} \end{bmatrix} \sim \frac{\alpha k_s^2}{4\pi\epsilon_0 r} \begin{bmatrix} 1 \\ \sin \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{0\perp} \\ \mathbf{E}_{0\parallel} \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{I}_{\perp} \\ \mathbf{I}_{\parallel} \end{bmatrix} \sim \frac{\alpha^2 k_s^4}{r^2} \begin{bmatrix} 1 \\ \sin^2 \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{0\perp}^2 \\ \mathbf{E}_{0\parallel}^2 \end{bmatrix}$$

Derivation in Appendix

# Dipole (Rayleigh) Scattering (3)

EM  
D  
RG  
M  
HG  
I  
PF  
G  
B  
P  
F



NB. Instead of  $\theta$ ,  
angle  $\varphi$  is used,  
 $\varphi = 90^\circ - \theta$   
 $\rightarrow \sin \theta = \cos \varphi$

Polar plot of  
Intensity:



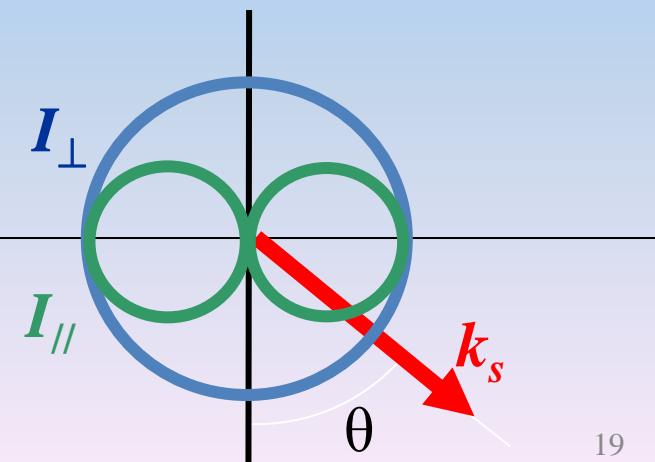
$$\begin{bmatrix} E_{I\perp} \\ E_{I//} \end{bmatrix} \sim \frac{\alpha k_s^2}{4\pi\epsilon_0 r} \begin{bmatrix} 1 \\ \sin \theta \end{bmatrix} \begin{bmatrix} E_{0\perp} \\ E_{0//} \end{bmatrix}$$

Lorentz:  
Spheres (radius  $a$ ; volume  $V$ ):

$$\alpha = \frac{\epsilon_r - 1}{\epsilon_r + 2} \frac{3V}{4\pi} = \frac{\epsilon_r - 1}{\epsilon_r + 2} a^3$$

$$\epsilon_r = n^2$$

$\epsilon_r$  = relative dielectric constant  
 $n$  = refractive index.



# Dipole (Rayleigh) Scattering (4)

EM  
D  
RG  
M  
HG  
I  
PF  
G  
B  
P  
F

Dipolar Scattering  
for 1 scatterer:

$$\begin{bmatrix} \mathbf{E}_{I\perp} \\ \mathbf{E}_{I//} \end{bmatrix} \propto \frac{\alpha k_s^2}{4\pi\epsilon_0 r} \begin{bmatrix} 1 \\ \sin \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{o\perp} \\ \mathbf{E}_{o//} \end{bmatrix}$$

If  $n$  scatterers per  $\text{m}^3$  (each radius  $a$ ):

$$\begin{bmatrix} \mathbf{E}_{I\perp} \\ \mathbf{E}_{I//} \end{bmatrix} \propto nV \frac{\alpha k_s^2}{4\pi\epsilon_0 r} \begin{bmatrix} 1 \\ \sin \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{o\perp} \\ \mathbf{E}_{o//} \end{bmatrix}; \text{ with } V = \frac{4}{3}\pi a^3$$

$$\begin{bmatrix} I_{\perp} \\ I_{//} \end{bmatrix} \propto n^2 a^6 \frac{\alpha^2 k_s^4}{r^2} \begin{bmatrix} 1 \\ \sin^2 \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{o\perp}^2 \\ \mathbf{E}_{o//}^2 \end{bmatrix}$$

“Natural” light :  
(randomly polarized)  
 $I_{nat} = \frac{1}{2} [I_{//} + I_{\perp}] \sim \frac{1}{2} [1 + \sin^2 \theta]$

Intensity is  
proportional to:

- $\alpha^2$  ;  $\alpha$  = dipole response on  $\mathbf{E}_o$ -field:  $\mathbf{p} = \alpha \mathbf{E}_o$
- $a^6$  ;  $a$  = particle radius
- $V^2$  ;  $V$  = volume
- $k_s^4 \sim \lambda^{-4}$  ;  $\lambda$  = wavelength
- $r^{-2}$  ;  $r$  = detector distance (spherical wave)

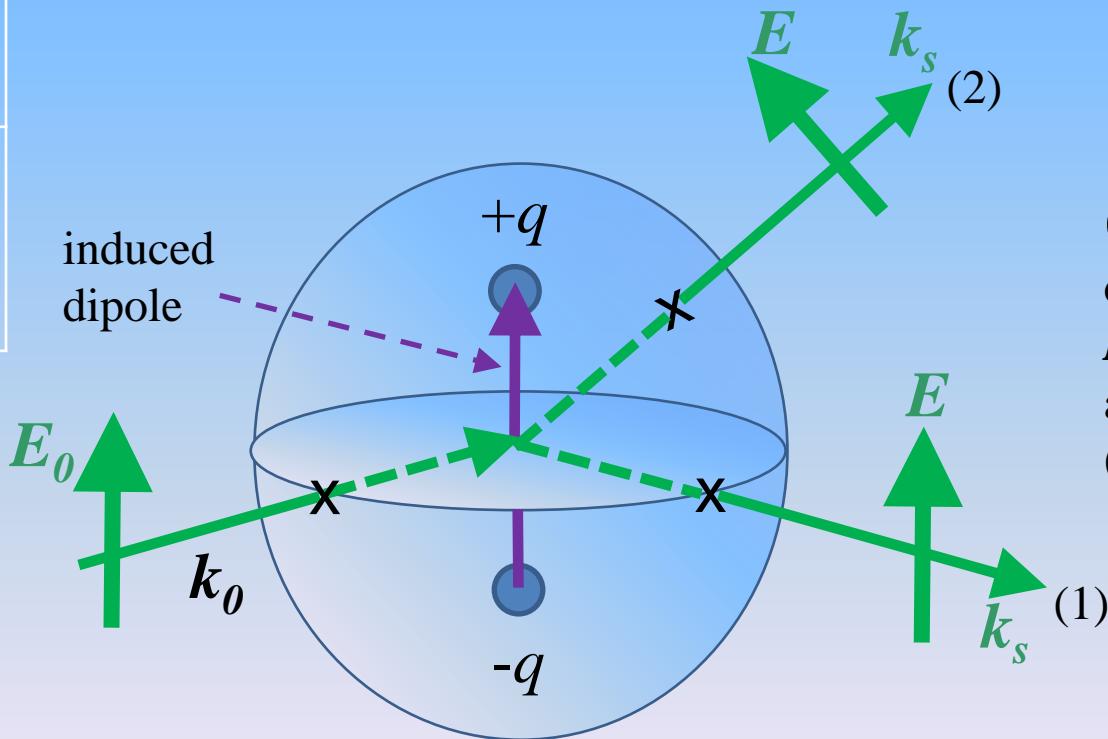
# Dipole (Rayleigh) Scattering (5)

EM  
**D**  
RG  
M

HG  
I  
PF  
G  
B  
P  
F

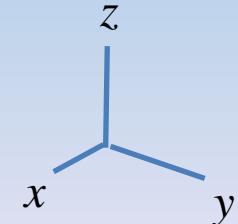
Dipolar Scattering  
for 1 scatterer:  
 $n$  scatterers / m<sup>3</sup>

$$\begin{bmatrix} \mathbf{E}_{1\perp} \\ \mathbf{E}_{1//} \end{bmatrix} \propto nV \frac{\alpha k_s^2}{4\pi\epsilon_0 r} \begin{bmatrix} 1 \\ \sin \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{0\perp} \\ \mathbf{E}_{0//} \end{bmatrix}; \text{ with } V = \frac{4}{3}\pi a^3$$



(1):  $\theta = 90^\circ : \mathbf{E} // \mathbf{E}_0 :$   
no depolarization

(2):  $\theta \neq 90^\circ :$   
depolarization present,  
 $\mathbf{E}$  has  $z$ -component  $\perp xy$ -plane  
and component  $// xy$ -plane  
( $\sim \sin \varphi$ ).

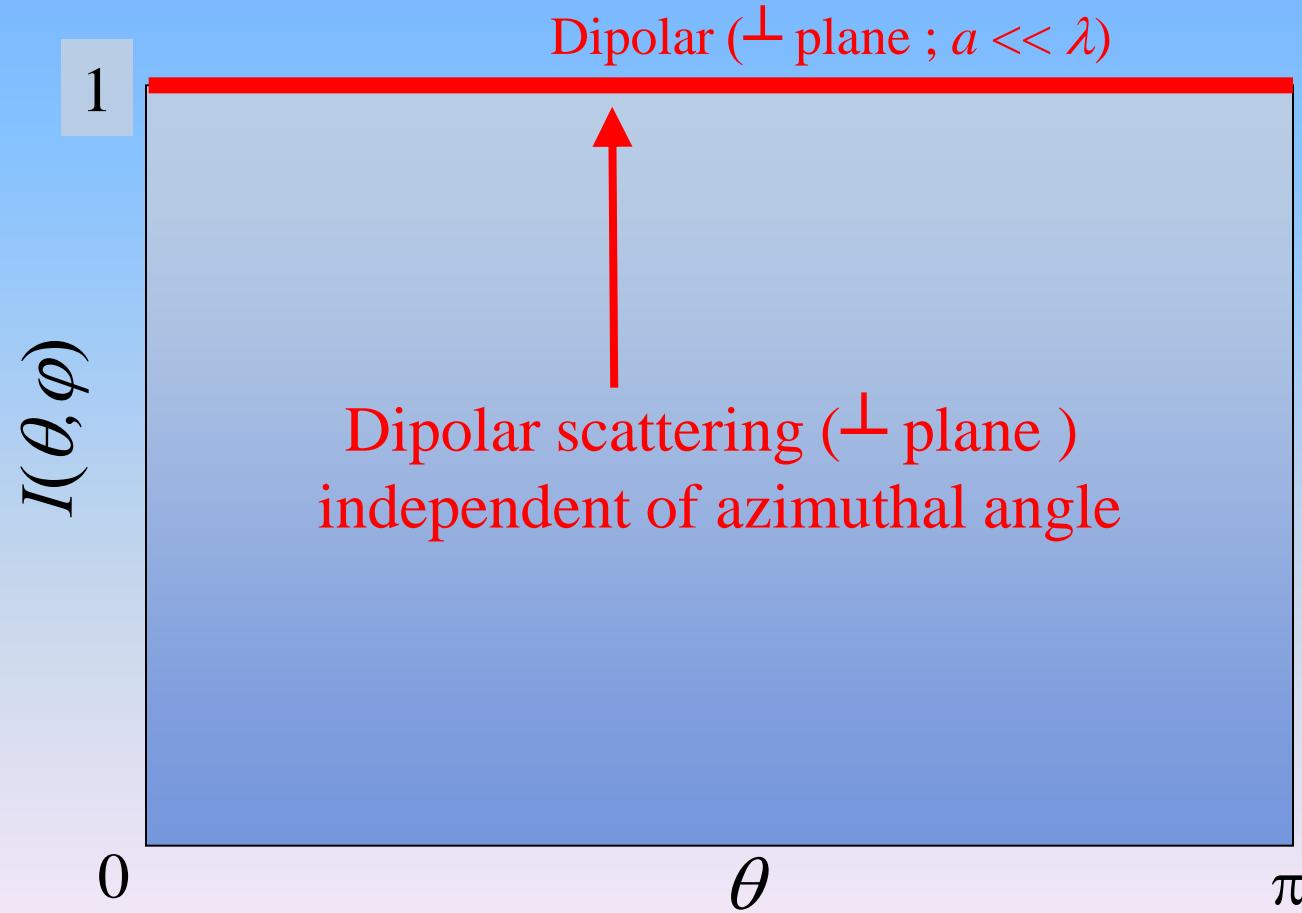


# Dipole (Rayleigh) Scattering (6)

EM  
**D**  
RG  
M  
HG  
I  
PF  
G  
B  
P  
F

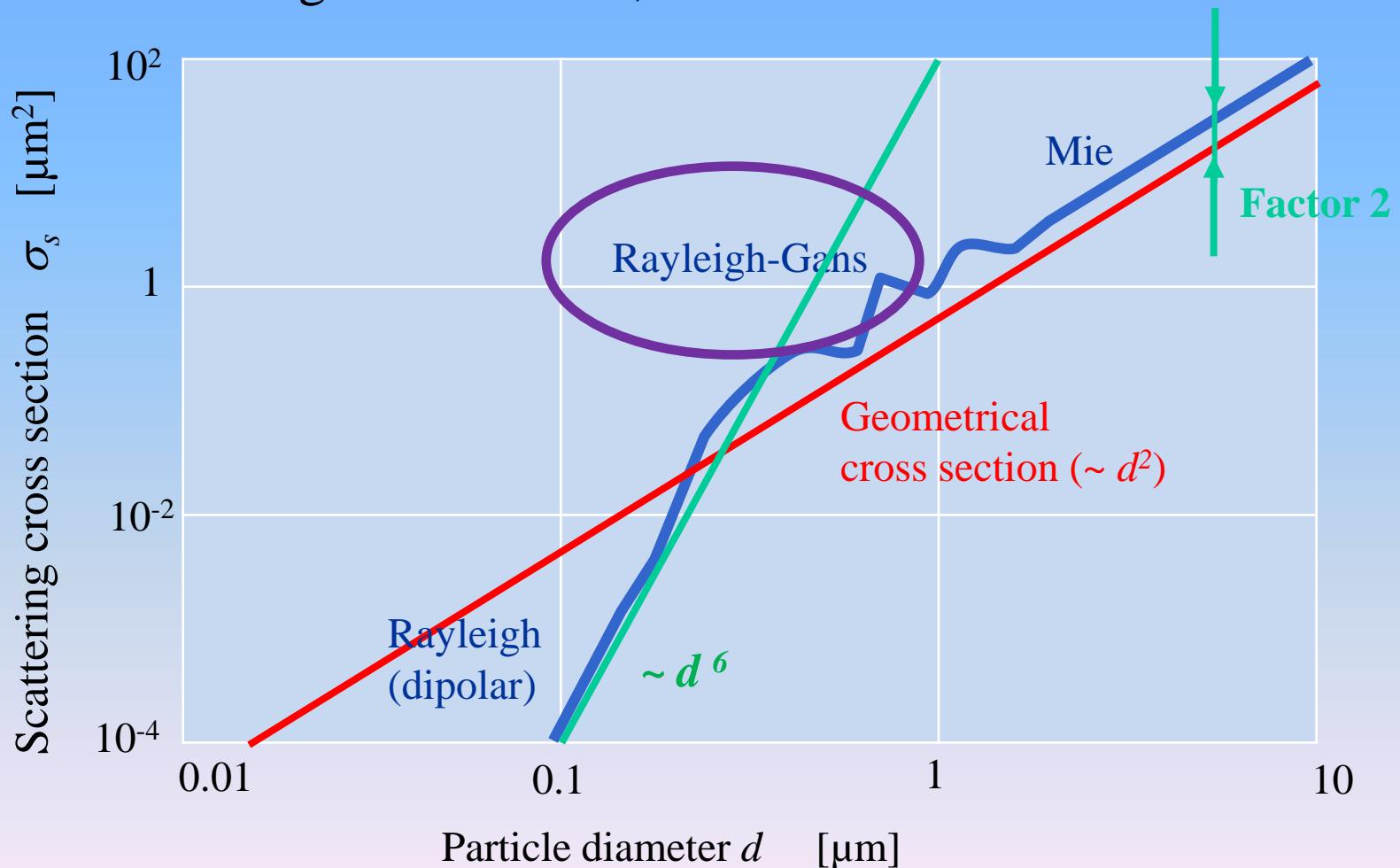
In-plane Scattering Intensity  $I(\theta, \phi)$   
(vertical polarization)

$a = \text{particle radius}$



# Optical properties: scattering

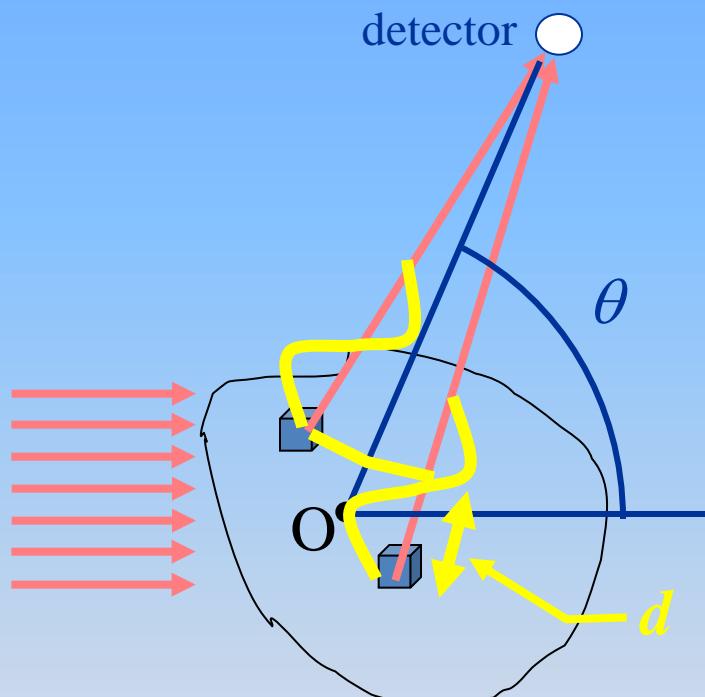
Scattering cross section, for  $\lambda = 500 \text{ nm}$  and  $n = 1.5$



# Rayleigh-Gans scattering (1)

Particles with radius  $a$ , not  $\ll \lambda$  : *Rayleigh-Gans*

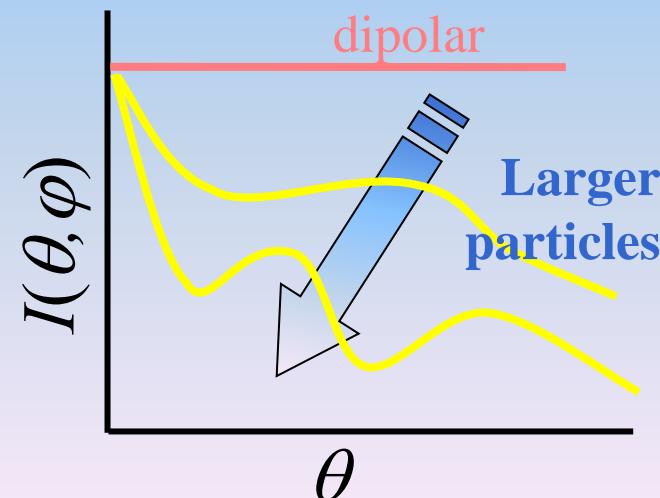
EM
D
<b>RG</b>
M
HG
I
PF
G
B
P
F



*Rayleigh-Gans* is  
approximative treatment

Scattering from different parts may have different phases and will interfere at detector.

Destructive interference possible (e.g. if  $d = \frac{1}{2} \lambda$ )  
dependent upon angle  $\theta$  and upon particle shape.



# Rayleigh-Gans scattering (2)

EM  
D  
**RG**  
M

HG  
I  
PF

G  
B  
P  
F

Rayleigh-Gans scattering:

accounts for phase differences  
when particles grow larger:

If  $n$  scatterers per  $\text{m}^3$ :

$$\begin{bmatrix} d\mathbf{E}_{I\perp} \\ d\mathbf{E}_{I//} \end{bmatrix} \propto n \frac{\alpha k_s^2}{4\pi\epsilon_0 r} \begin{bmatrix} 1 \\ \sin \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{0\perp} \\ \mathbf{E}_{0//} \end{bmatrix} e^{i\partial} dV$$

$\partial$  accounts for phase differences;

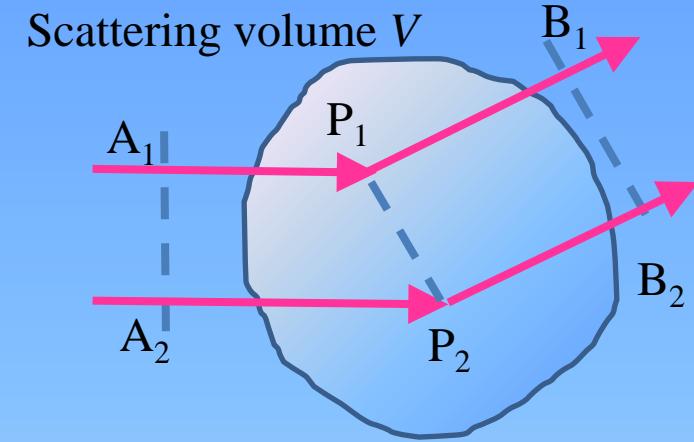
$$\begin{bmatrix} \mathbf{E}_{I\perp} \\ \mathbf{E}_{I//} \end{bmatrix} \propto nV \frac{\alpha k_s^2}{4\pi\epsilon_0 r} \begin{bmatrix} 1 \\ \sin \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{0\perp} \\ \mathbf{E}_{0//} \end{bmatrix} . R(\theta, \varphi)$$

Final result depends on  $R$ -function.

e.g. Phase difference between  
2 wave fronts: A and B :

Result for “natural” incident light:  $I_{nat} = \frac{1}{2} [I_{//} + I_{\perp}]$  ;  $a$  = particle radius:

$$I_{nat} \propto n^2 V^2 \frac{\alpha^2 k_s^4}{(4\pi\epsilon_0 r)^2} \frac{1 + \sin^2 \theta}{2} E_0^2 |R(\theta, \varphi)|^2 ; V^2 \propto a^6$$



with  $R(\theta, \varphi) = \frac{1}{V} \iiint_V e^{i\partial} dV$

$$\varphi = 2\pi \frac{(B_1 P_1 + P_1 A_1) - (B_2 P_2 + P_2 A_2)}{\lambda} ; \lambda = \frac{2\pi}{k_s}$$

# Rayleigh-Gans scattering (3)

EM  
D  
**RG**  
M

HG  
I  
PF

G  
B  
P  
F

## Rayleigh-Gans scattering:

accounts for phase differences between paths from different spots in the scattering medium, when particles grow larger

**Phase function:**

$$R(\theta, \varphi) = \frac{1}{V} \iiint_V e^{i\hat{\sigma}} dV$$

### Examples:

1. solid homogeneous sphere:  
( $J$  = Bessel function)

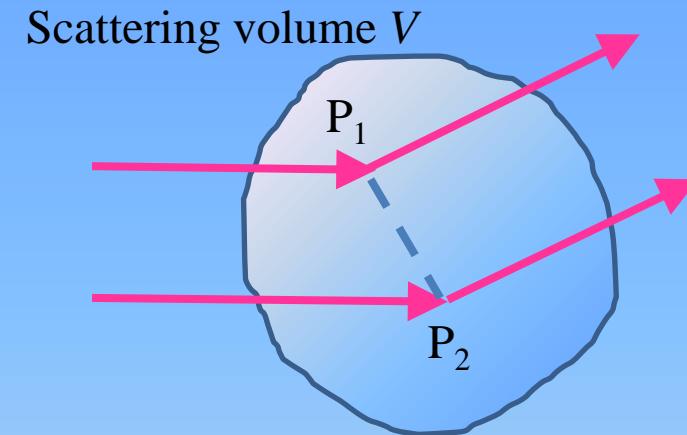
$$R(\theta, \varphi) = \sqrt{\frac{9\pi}{2u^3}} \cdot J_{3/2}(u) ; \quad u = 2ka \sin\left(\frac{1}{2}\theta\right)$$

2. inhomogeneous sphere :  $\varepsilon = f(r)$ :

$$R(\theta, \varphi) = \frac{1}{\varepsilon_c} \int_0^\infty 4\pi r^2 \varepsilon(r) \frac{\sin v}{v} dr ; \quad v = 2kr \sin\left(\frac{1}{2}\theta\right) ; \quad \varepsilon_c = \int_0^\infty 4\pi r^2 \varepsilon(r) dr$$

3. cylinder (circular, length  $l$ , radius  $a$ ); disk and rod, and other shapes:  
see Van de Hulst: “Light scattering by small particles”

4. for (tissue) particles with random orientations: use 1 or 2 as approximation .

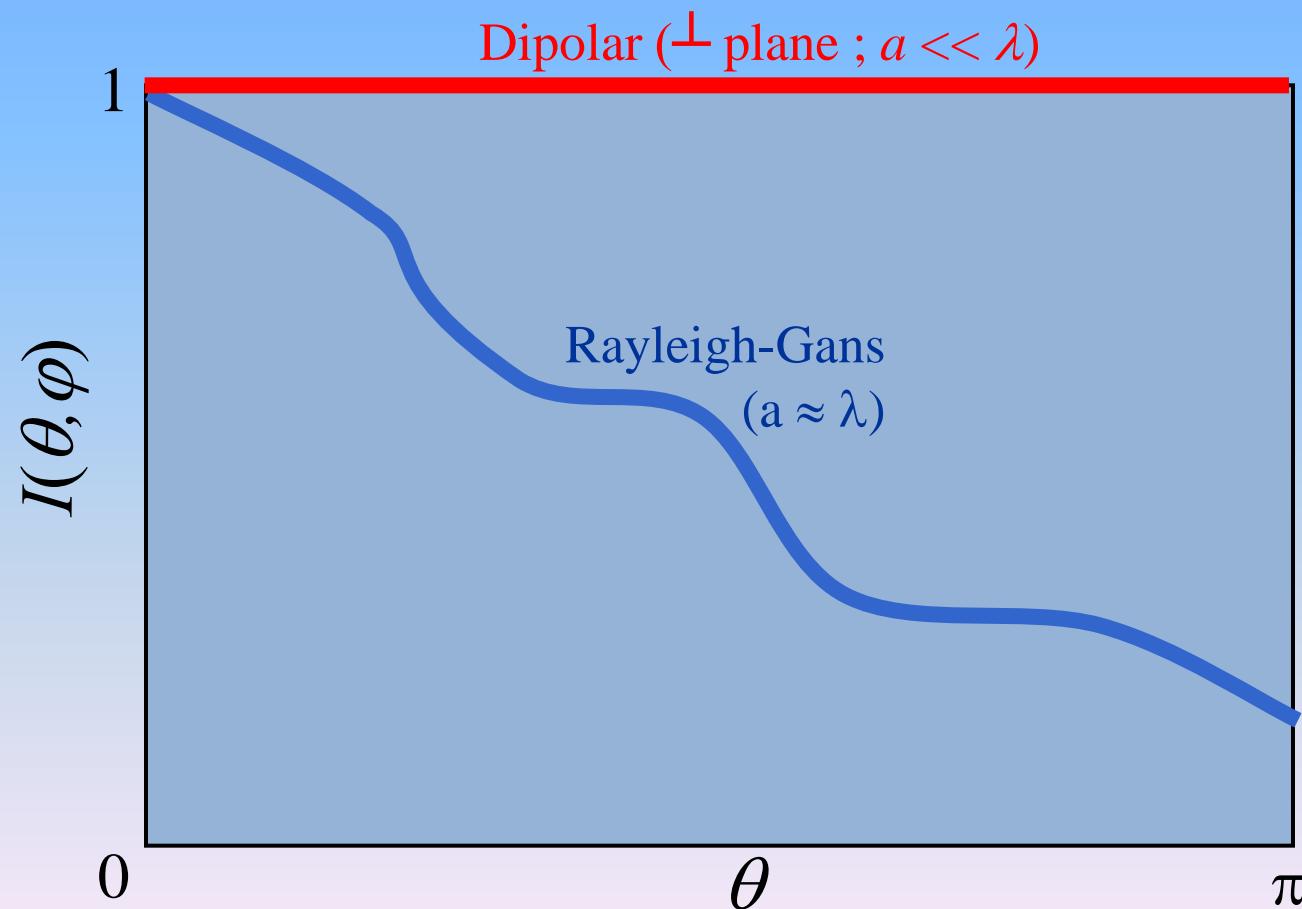


# Rayleigh-Gans scattering (4)

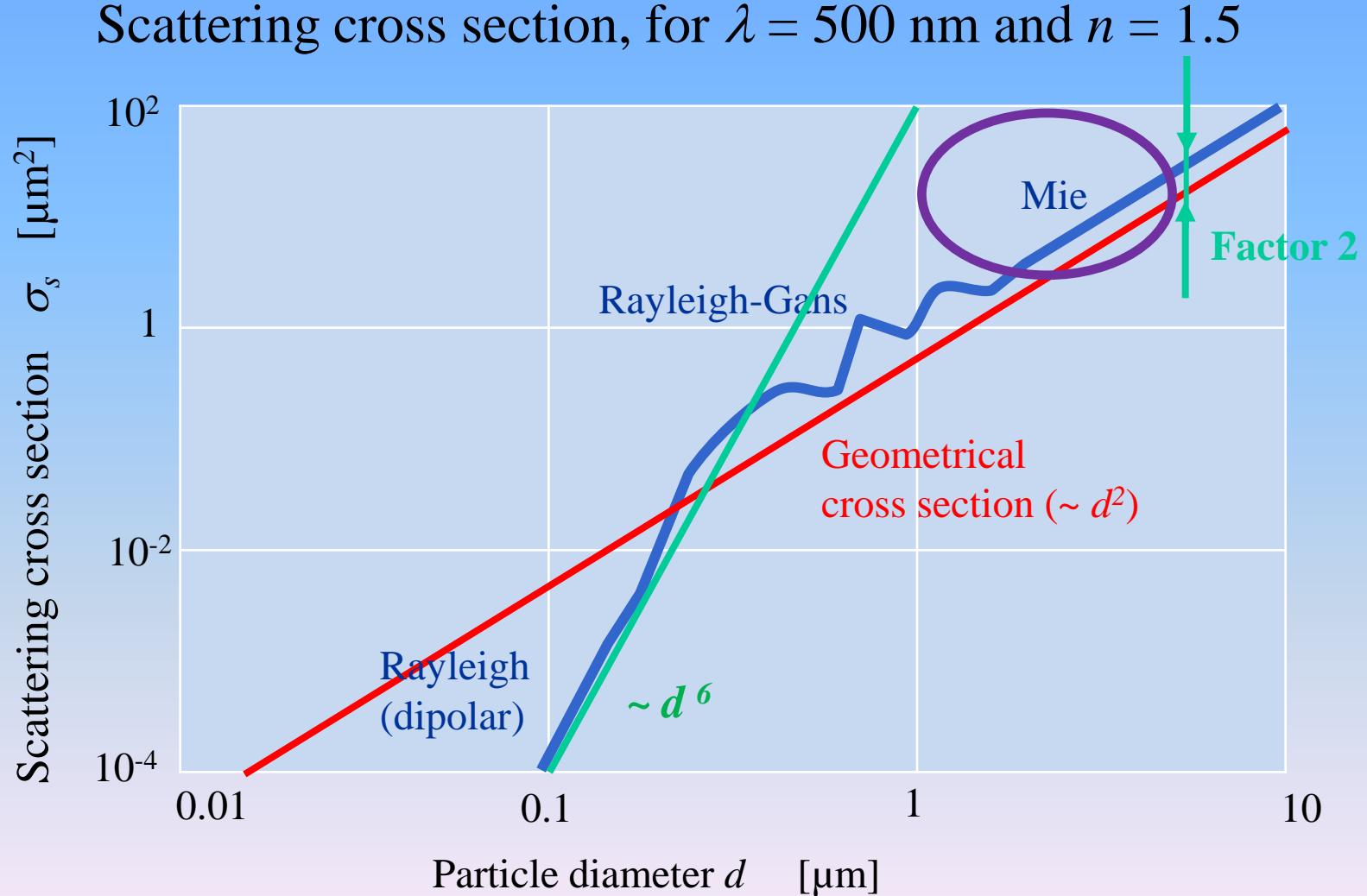
EM  
D  
**RG**  
M  
HG  
I  
PF  
G  
B  
P  
F

In-plane Scattering Intensity  $I(\theta, \varphi)$   
(vertical polarization)

$a = \text{particle radius}$



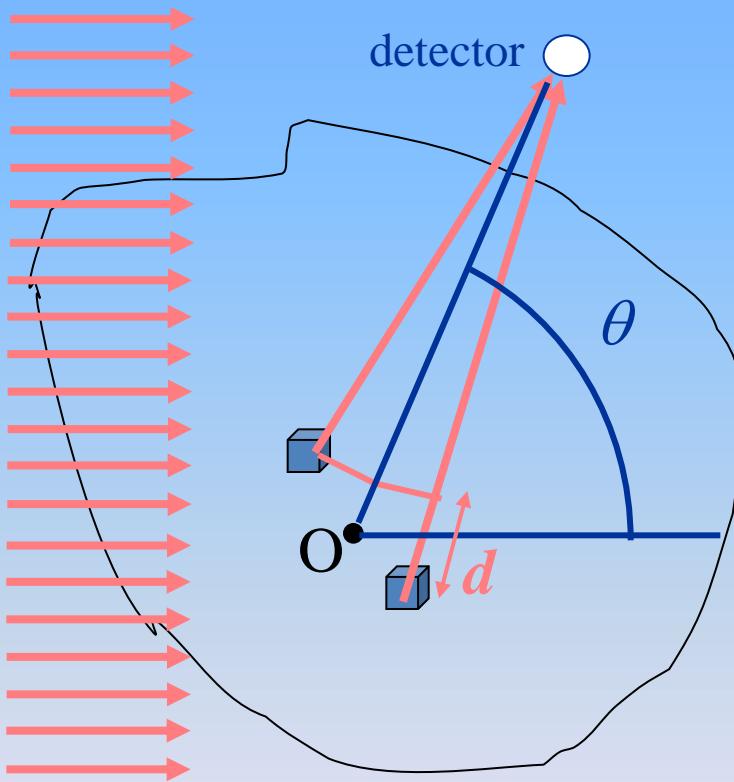
# Optical properties: scattering



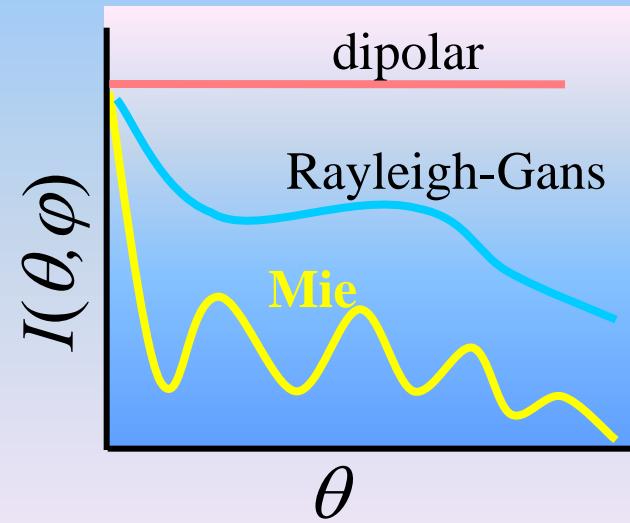
# Formalism of Mie-scattering (1)

EM
D
RG
<b>M</b>
HG
I
PF
G
B
P
F

Large particles:  $a \gg \lambda$  : (*Rigorous*) **Mie-scattering**



Scattering from different parts will interfere at detector.  
**Destructive interference** will be dependent upon angle  $\theta$  and upon particle shape.



Mie derived a rigorous treatment from Maxwell's equations; see below

# Formalism of Mie-scattering (2)

EM  
D  
RG  
**M**

HG  
I  
PF

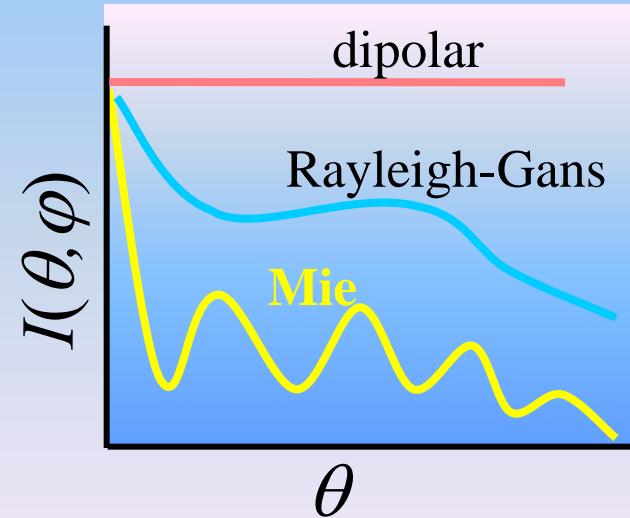
G  
B  
P  
F

Large particles:  $a \gg \lambda$  : (*Rigorous*) **Mie-scattering**

*Mie* derived a rigorous treatment from  
Maxwell's equations;

For the derivation and resulting expressions  
for the field components  $E_\theta$  and  $E_\phi$  see:

H.C. van de Hulst,  
“Light scattering by small particles”,  
Sect. 9.2-3.

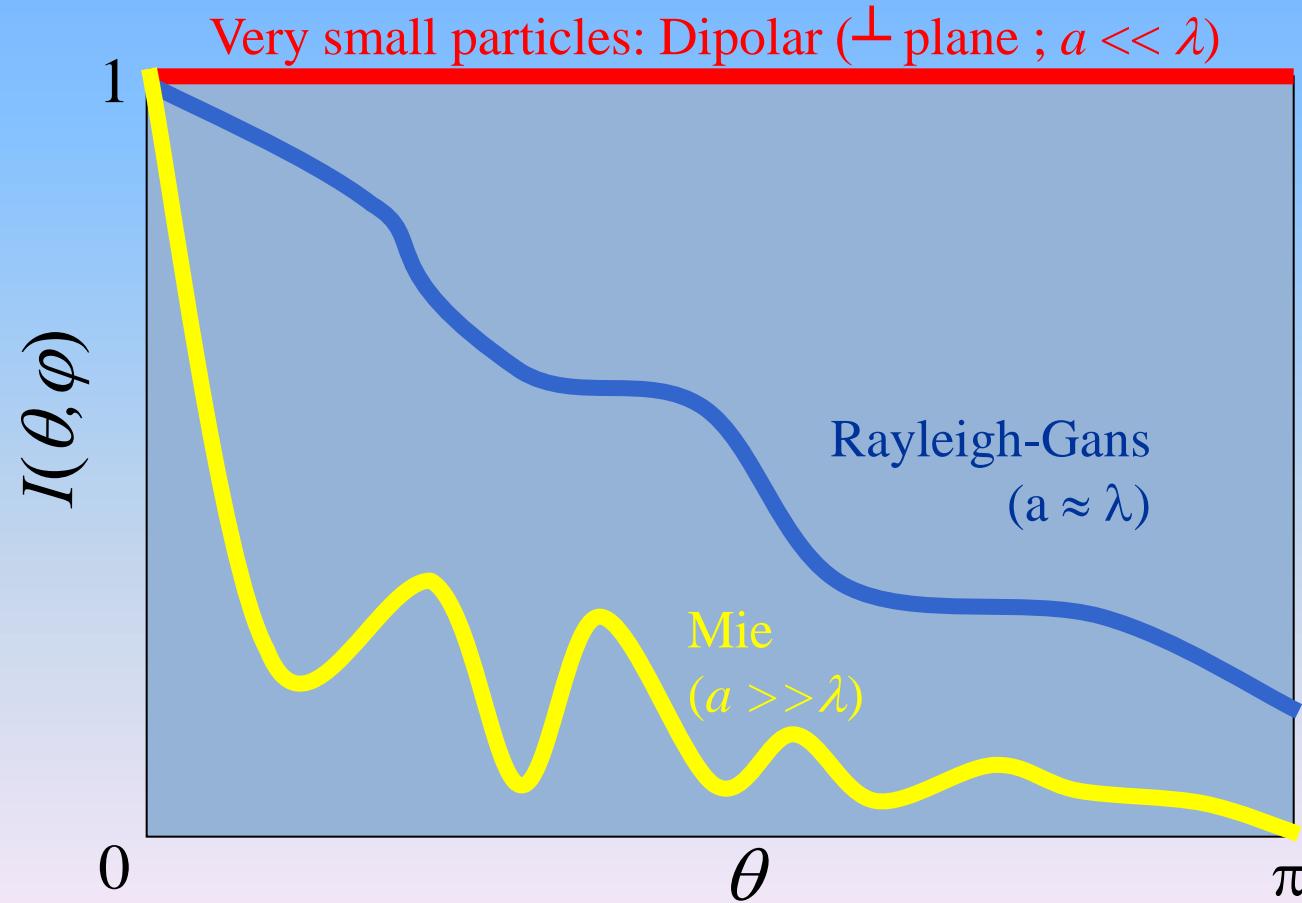


# Formalism of Mie-scattering (3)

EM
D
RG
M
HG
I
PF
G
B
P
F

In-plane Scattering Intensity  $I(\theta, \varphi)$   
 (vertical polarization)

$a = \text{particle radius}$



# Other scattering functions (1)

 EM  
D  
RG  
M

 HG  
I  
PF

 G  
B  
P  
F

- from astronomy:
  - Henyey-Greenstein: (radius  $a > \approx 10 \lambda$ )

$$p(\theta, \varphi) = \frac{1}{4\pi} \frac{1-g^2}{[1+g^2 - 2g \cdot \cos \theta]^{3/2}} \quad \text{with} \quad g = \langle \cos \theta \rangle$$

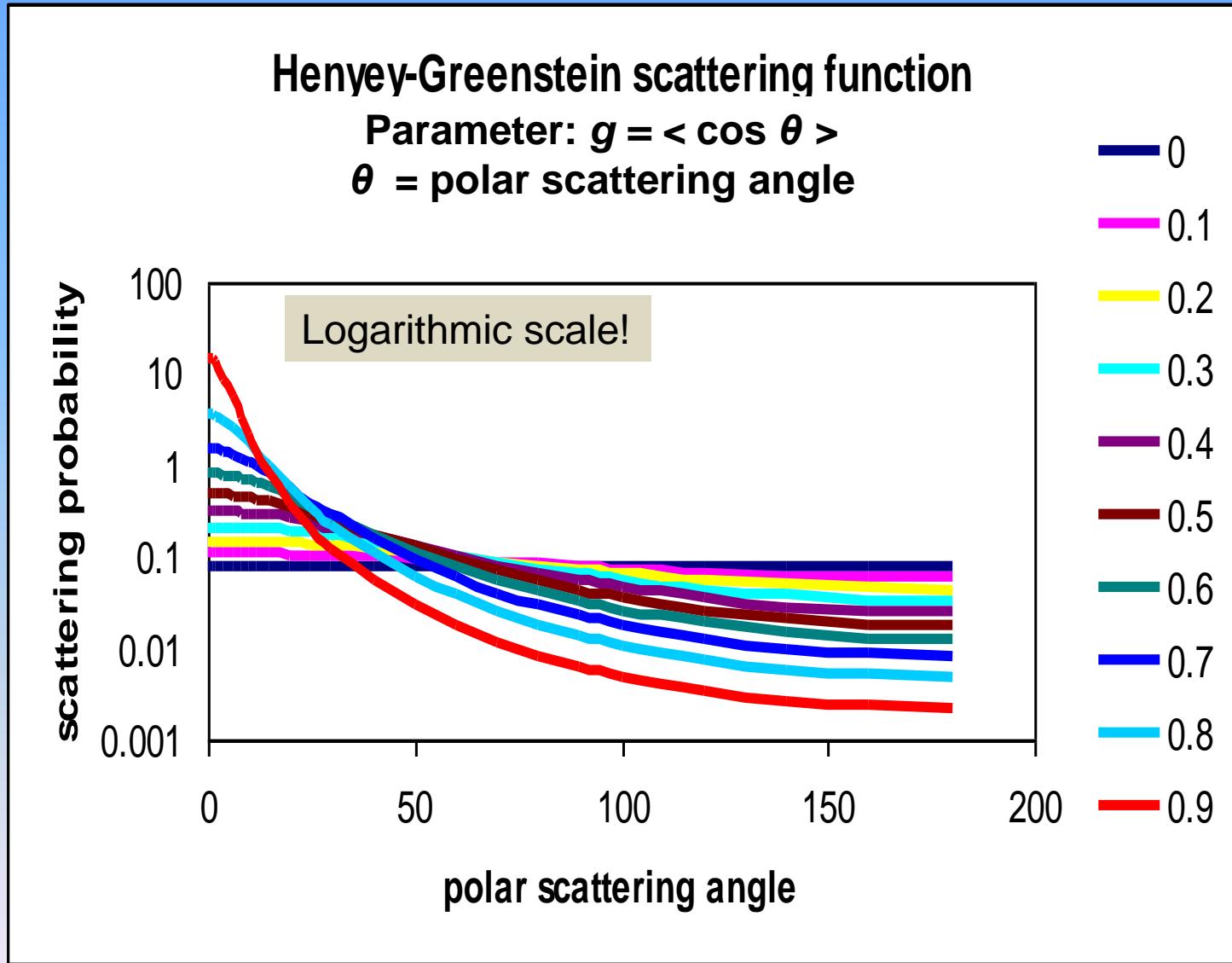
- Gegenbauer
- Isotropic:
- Peaked-forward (*e.g.* Gaussian shape):

$$p(\theta, \varphi) = \frac{1}{4\pi}$$

$$p(\theta, \varphi) = \frac{1}{4\pi} \exp(-\theta^2 / \theta_0^2)$$

# Other scattering functions (2)

EM  
D  
RG  
M  
**HG**  
I  
PF  
G  
B  
P  
F



# Other scattering models

EM  
D  
RG  
M

HG  
I  
PF

G  
B  
P  
F

Other scattering models, all based on the Diffusion Equation (from Transport Equation):

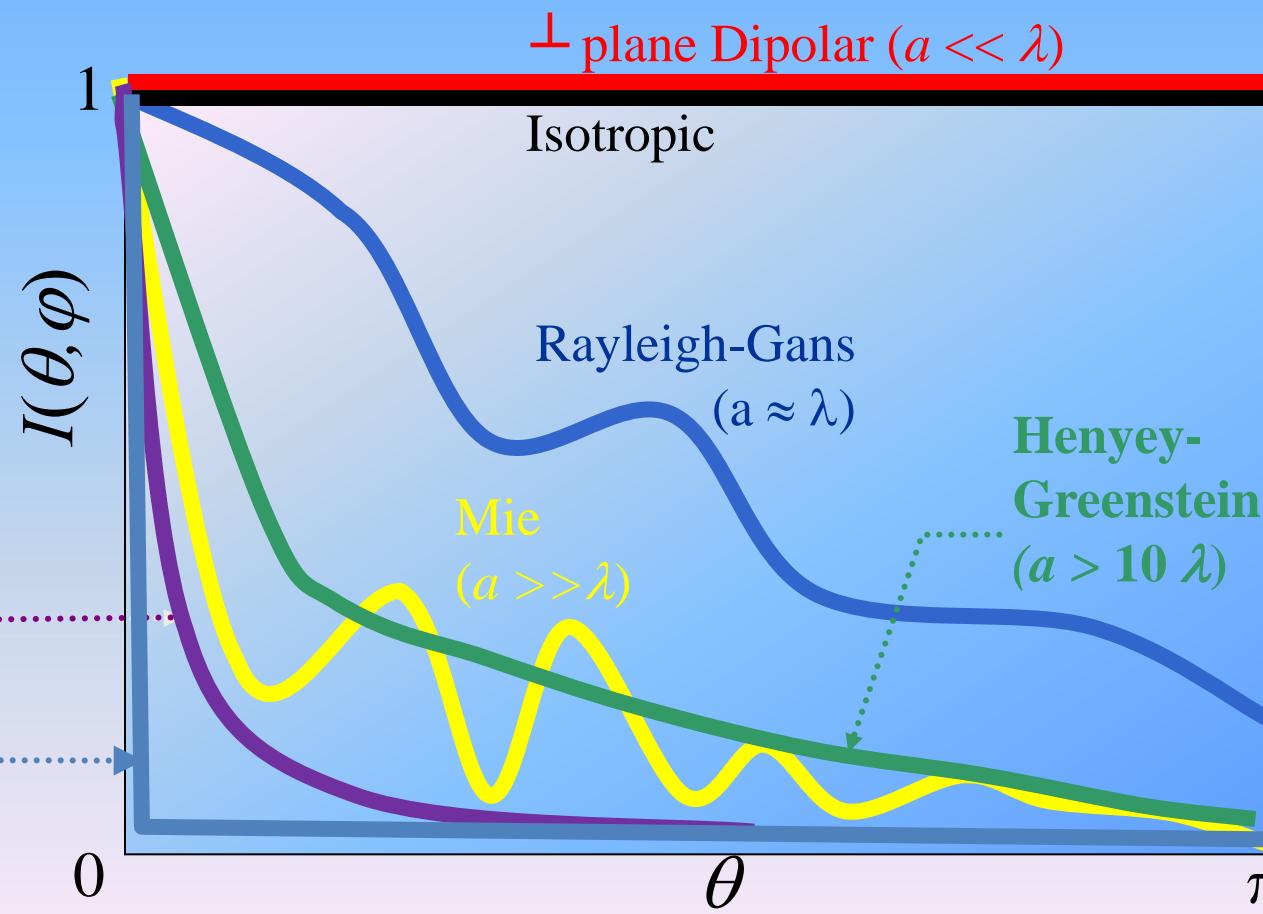
- G. Groenhuis, Ferwerda, Ten Bosch
  - Scattering function: isotropic + peaked forward
  - Source: pencil beam attenuating in tissue
- B. Bonner, Nossal *et al.*
  - 3D-grid of discrete scattering points
  - Probabilistic approach
- P. Patterson, Chance, Wilson
  - Virtual point source for 1<sup>st</sup> scatter event at depth  $z_0 = 1/\mu_s'$ .
- F. Farrell, Patterson, Wilson
  - Attenuating pencil beam, creating line of point sources.
  - Each point source creates "image source" above tissue surface (accounts for refr. index mismatch)

# Overview of scattering functions

EM  
D  
RG  
M  
HG  
I  
PF  
G  
B  
P  
F

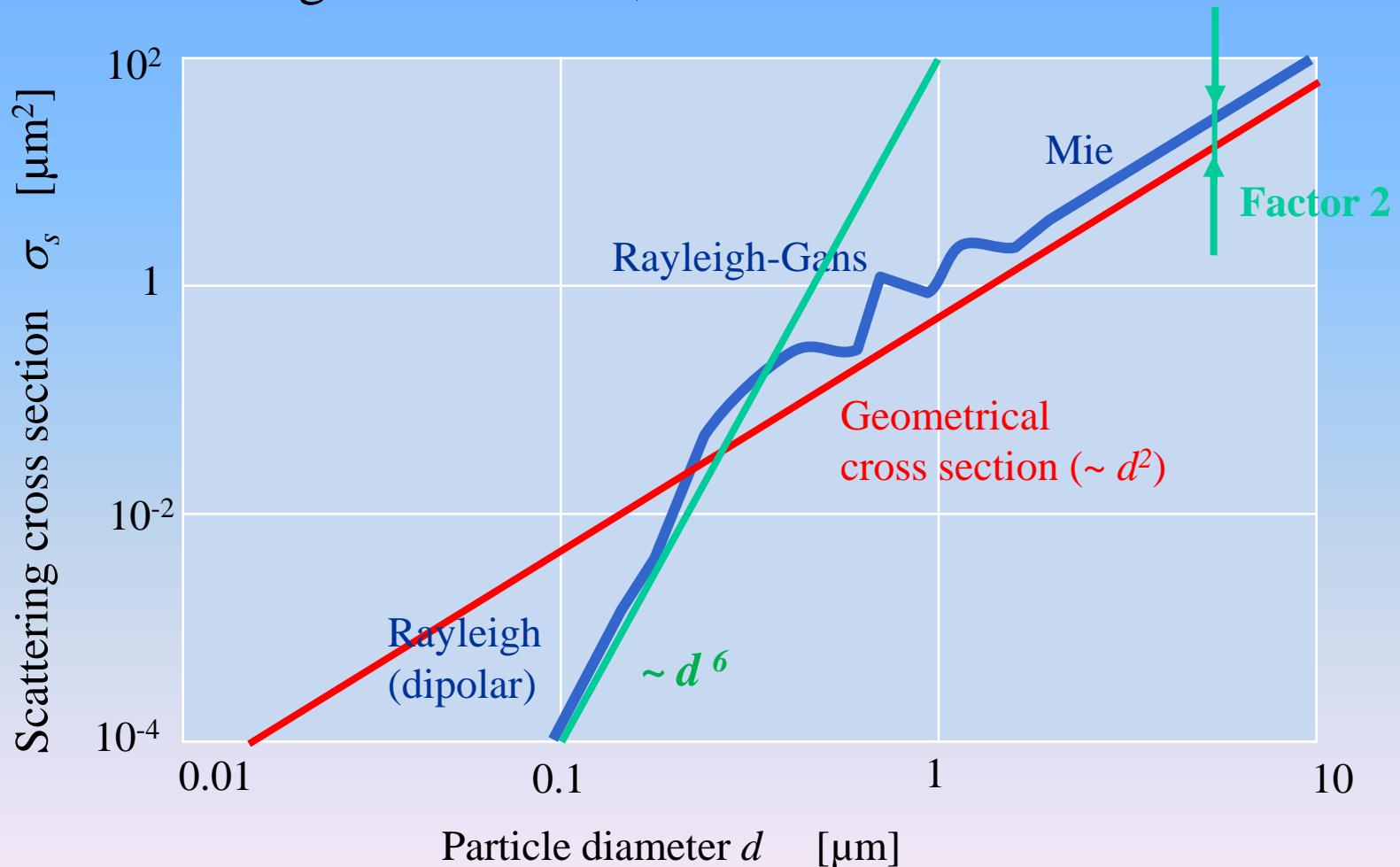
Scattering Intensity  $I(\theta, \varphi)$

$a$  = particle radius



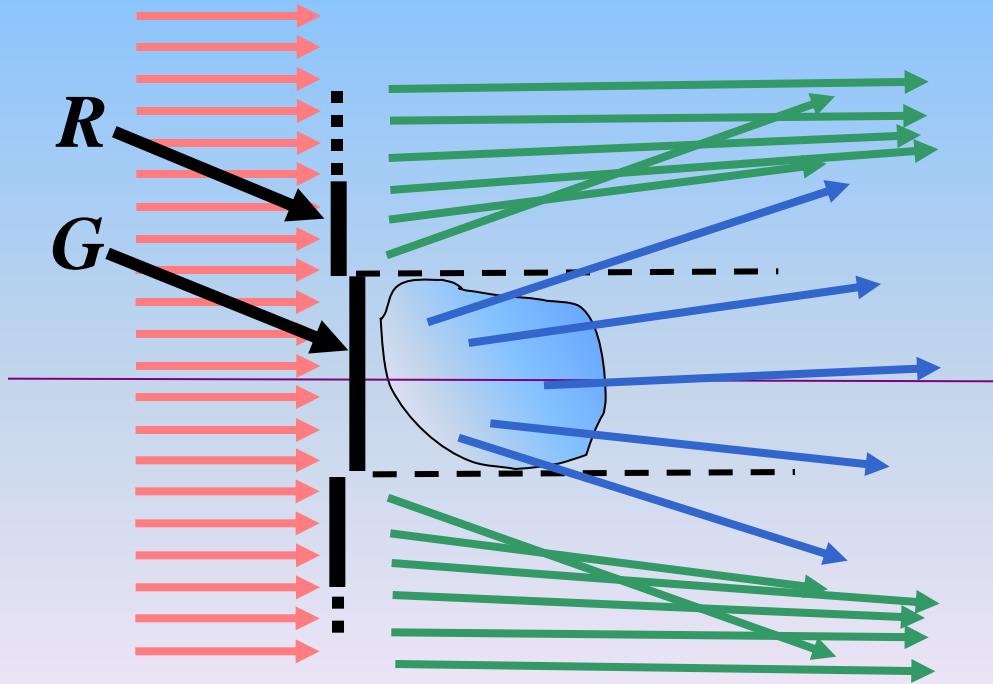
# Optical properties: scattering

Scattering cross section, for  $\lambda = 500 \text{ nm}$  and  $n = 1.5$



# Scattering by very large particles

Scattering by very large particles:  
 Scattering cross section =  $2 \times$  geometrical cross section.  
 Why ?

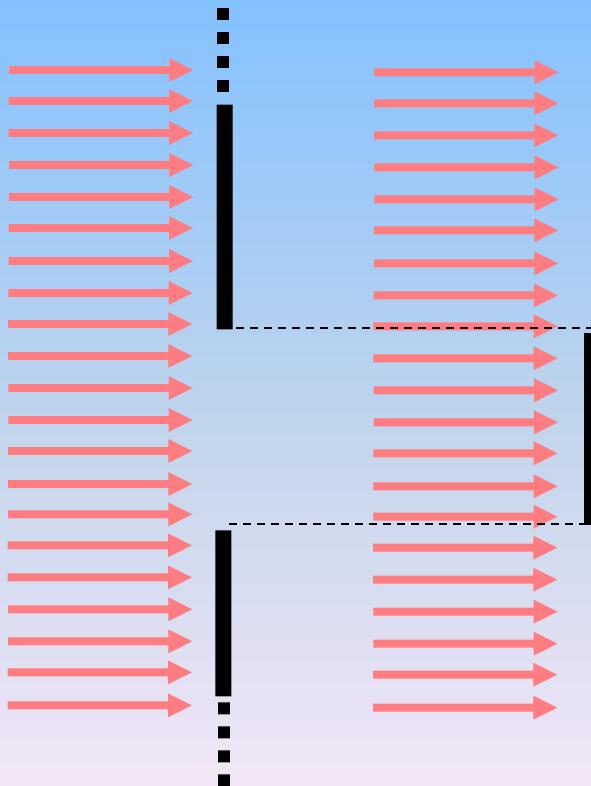


- Scattering from inside particle will take away light due to geometrical cross section  $G$
  - Diffraction around particle will take away light in a ring  $R$  equal to geometrical cross section  $G$
- “Extinction Paradox”**

# Very large particles: Extinction Paradox

Extinction Paradox:

Diffraction through hole = diffraction around obstruction,  
if hole and obstruction have identical shadow



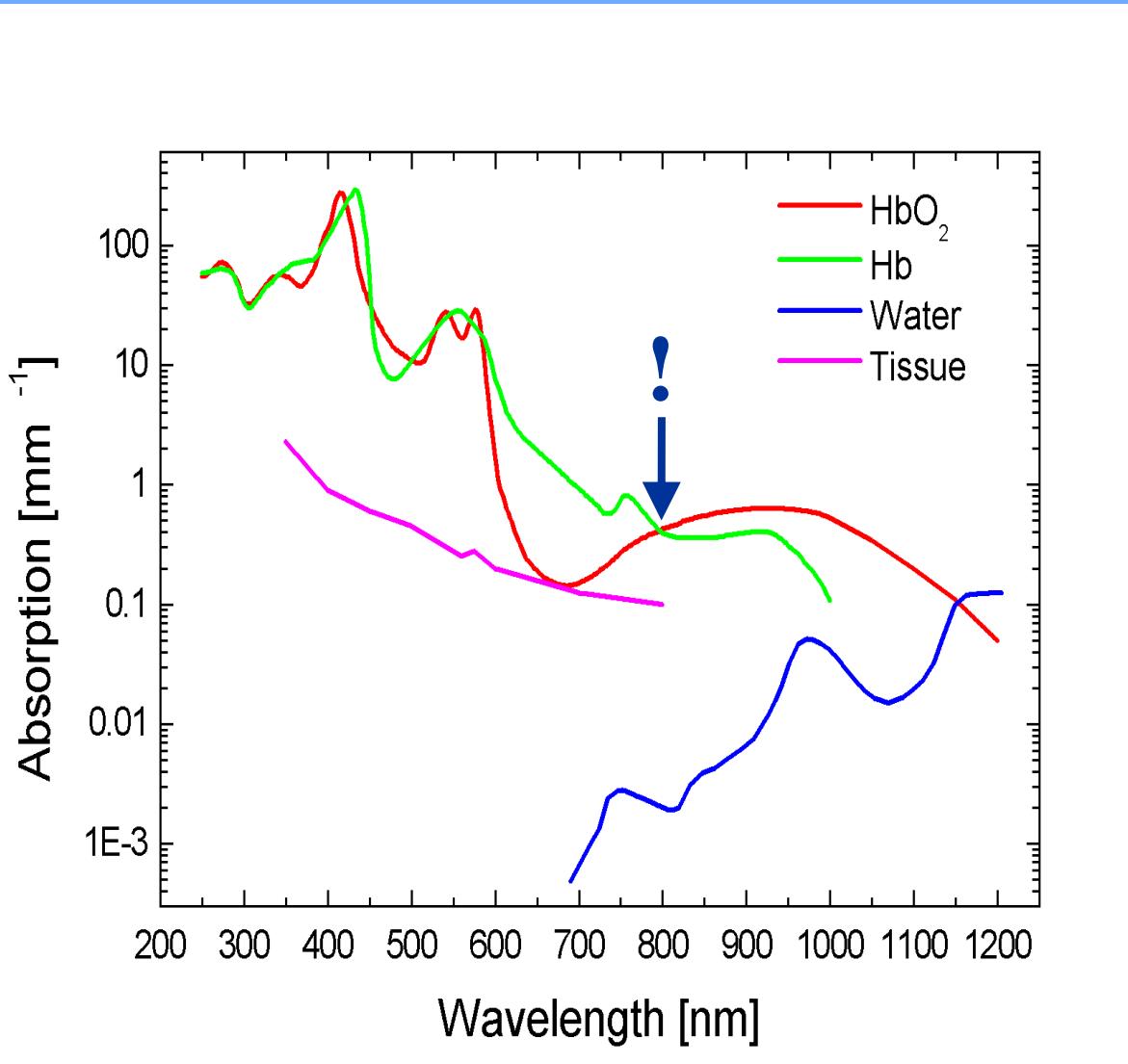
Original field +  
disturbance field behind:

- hole:  $E_{dist}$
- obstruction:  $E_0 - E_{dist}$

Intensity of disturbance field  
(= diffraction):

- hole:  $I \sim E_{dist}^2$
- obstruction:  $I \sim (-E_{dist})^2$

# Optical properties of tissue and blood



(Reduced) Scattering coefficient:  $\mu_s'$

$\lambda = 580 \text{ nm}:$

Dermis:  $3 \text{ mm}^{-1}$

Blood:  $1 \dots$

- $\bullet \lambda = 850 \text{ nm}:$

Dermis:  $1 \dots$

Blood:  $0.5 \dots$

$! =$  Oxygen saturation measurements

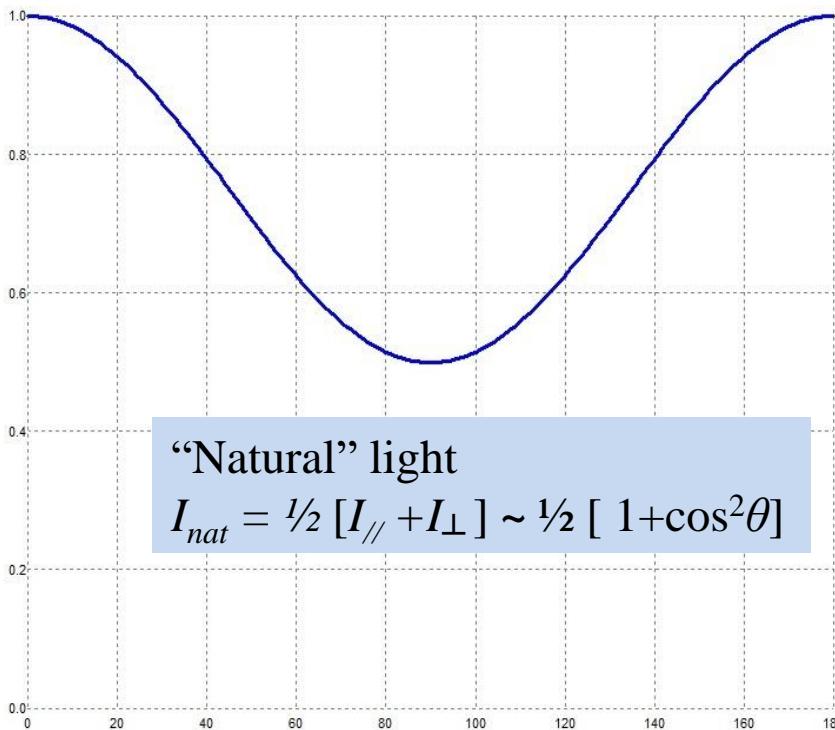
based on differences in absorption for

$\lambda >$  and  $< 800 \text{ nm}$

# Examples of scattering functions

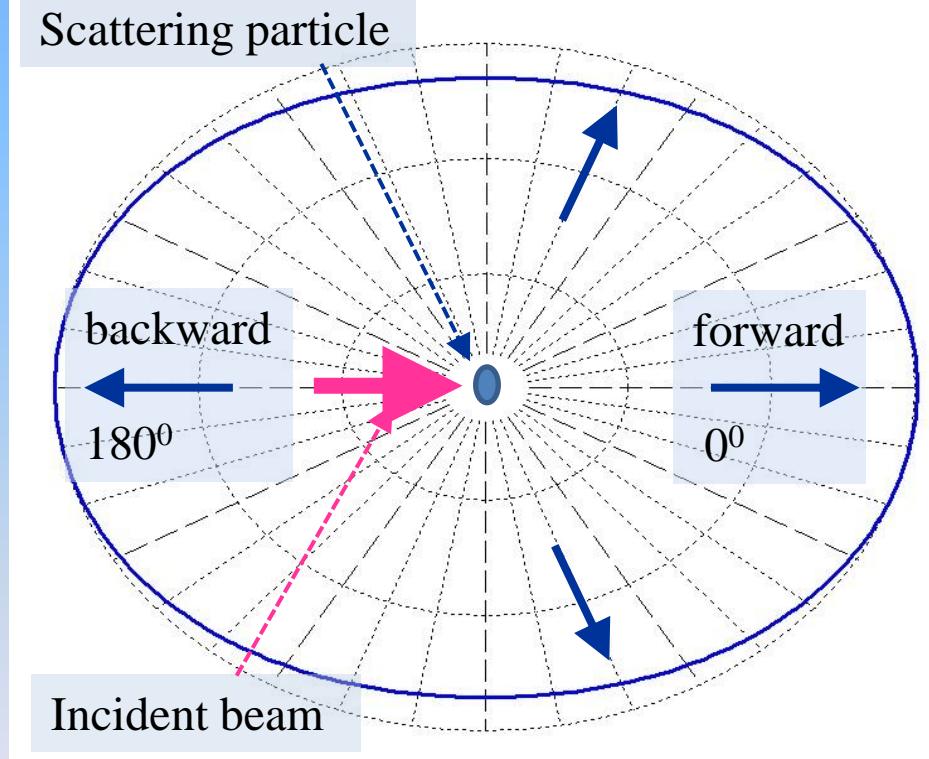
## Dipolar scattering (in-plane and out-of-plane components summed)

MIE-File: D:\FRITS\MC\Mie\Unknown.MIE  
 Scattering function = f(theta) | (theta = polar scattering angle)  
 Nr.angles = 181 | Max. = 4.27985E+03 | Linear plot; blue: >0; green: <0



Linear plot: linear scale:  
 X:  $0 .. 180^\circ$ ; Y:  $0 .. 1$

MIE-File: D:\FRITS\MC\Mie\Unknown.MIE  
 Scattering function = f(theta) | (theta = polar scattering angle)  
 Nr.angles = 181 | Max. = 4.27985E+03 | 10-Log. plot; blue: >0; green: <0

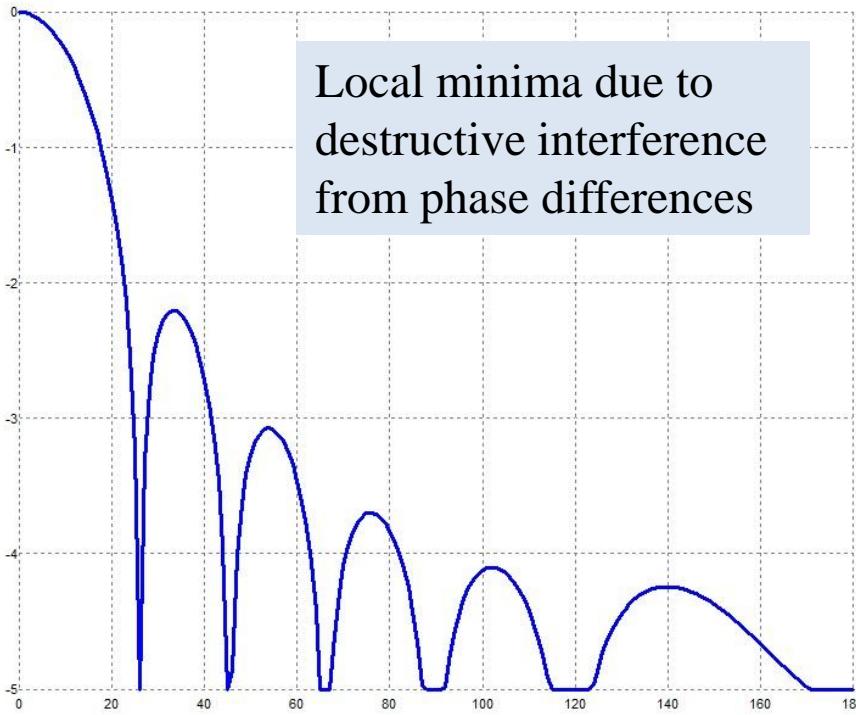


Polar plot: log. scale: 3 decades

# Examples of scattering functions

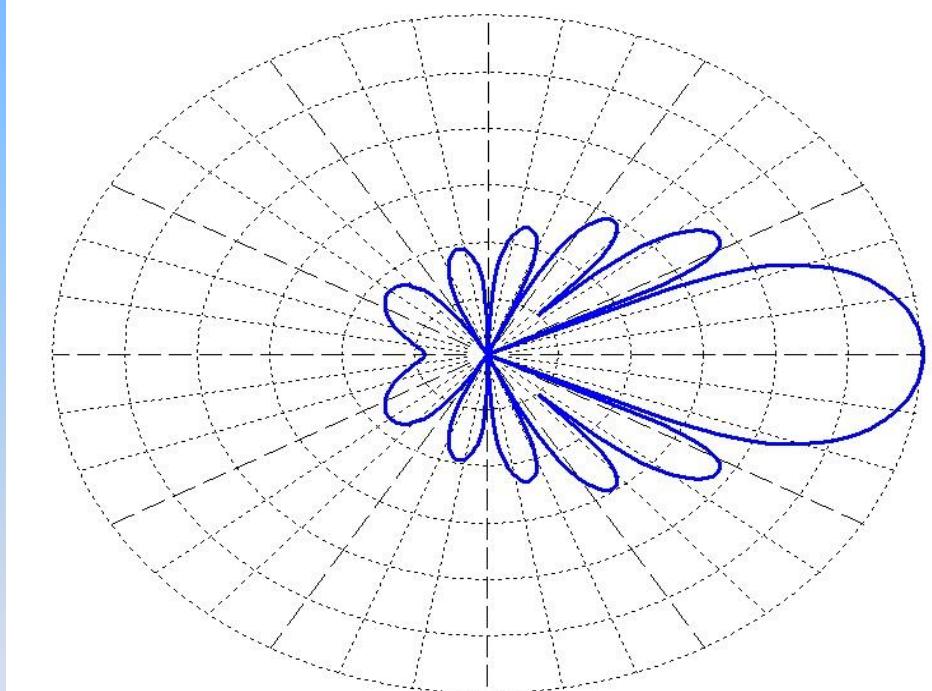
## Rayleigh - Gans scattering

MIE-File: D:\FRITS\MC\mie\Unknown.MIE  
 Scattering function = f(theta) | (theta = polar scattering angle)  
 Nr.angles = 181 | Max. = 4.44445E+03 | 10-Log. plot; blue: >0; green: <0



Linear plot: log scale:  
 X: 0 .. 180<sup>0</sup>; Y: 5 decades: 1 .. 10<sup>-5</sup>

MIE-File: D:\FRITS\MC\mie\Unknown.MIE  
 Scattering function = f(theta) | (theta = polar scattering angle)  
 Nr.angles = 181 | Max. = 4.44445E+03 | 10-Log. plot; blue: >0; green: <0

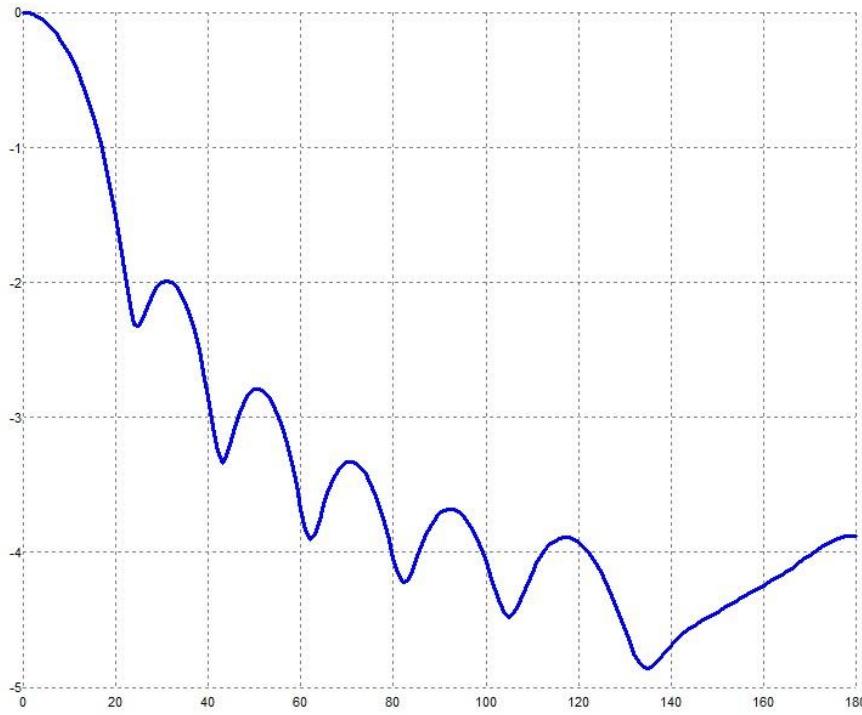


Polar plot: log. scale: 5 decades

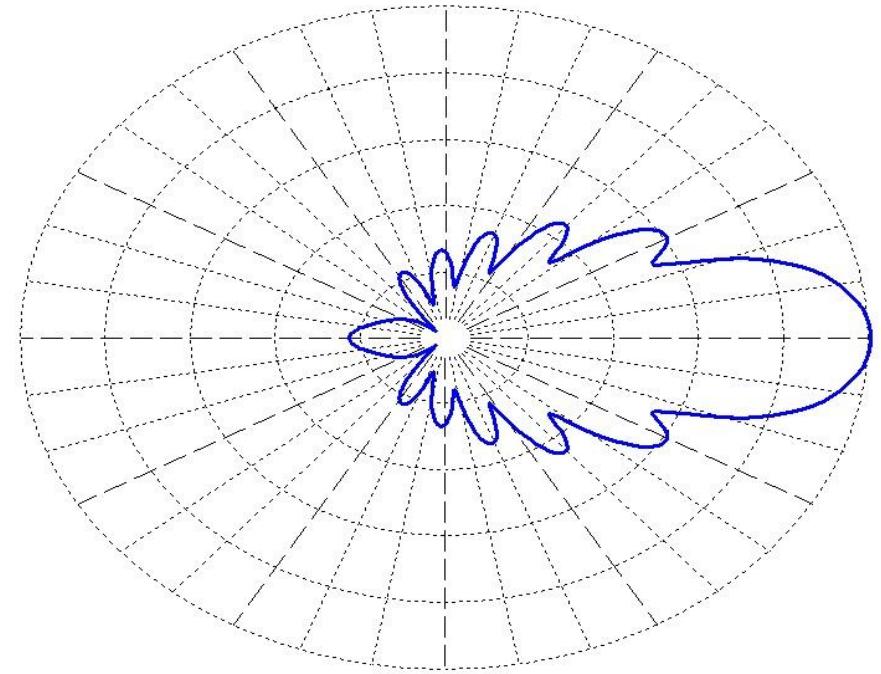
# Examples of scattering functions

## Mie scattering

MIE-File: D:\FRITSMCMie\Unknown.MIE  
 Scattering function = f(theta) | (theta = polar scattering angle)  
 Nr.angles = 181 | Max. = 4.09657E+03 | 10-Log. plot; blue: >0; green: <0



MIE-File: D:\FRITSMCMie\Unknown.MIE  
 Scattering function = f(theta) | (theta = polar scattering angle)  
 Nr.angles = 181 | Max. = 4.09657E+03 | 10-Log. plot; blue: >0; green: <0



Linear plot: log scale:

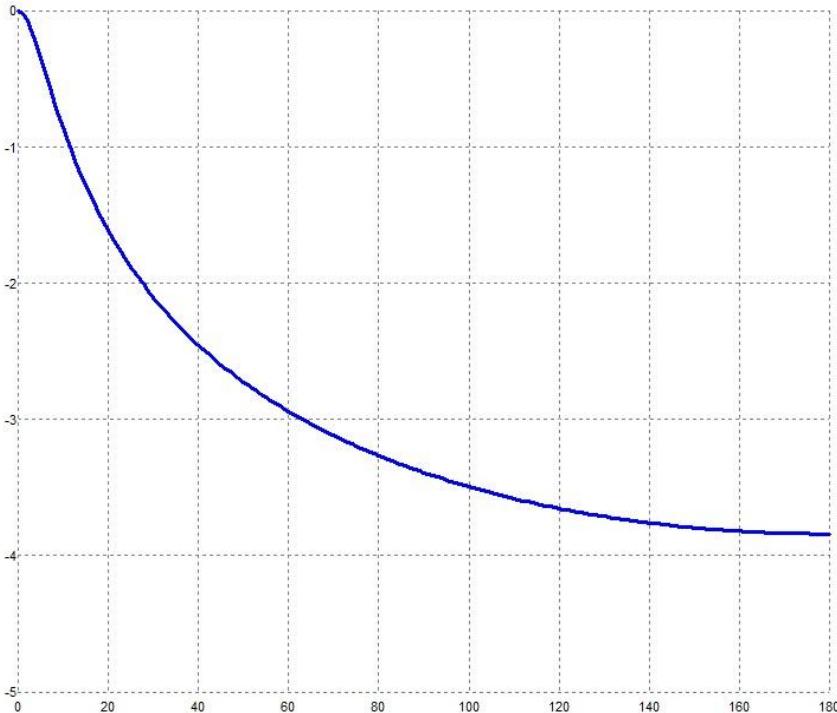
X: 0 ..  $180^\circ$ ; Y: 5 decades: 1 ..  $10^{-5}$

Polar plot: log. scale: 5 decades

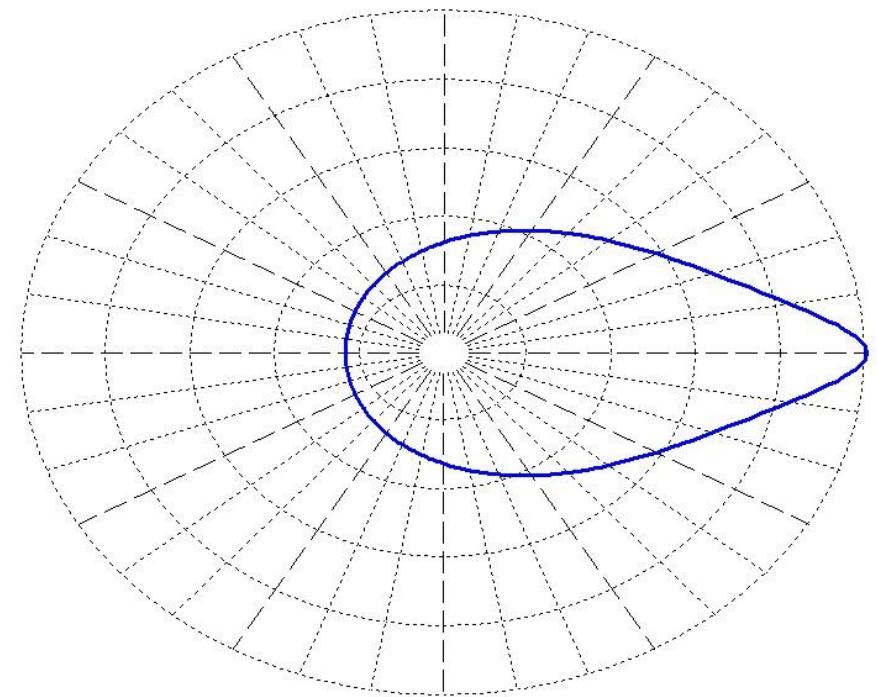
# Examples of scattering functions

## Henyey-Greenstein scattering

MIE-File: D:\FRITS\MC\mie\Unknown.MIE  
Scattering function = f(theta) | (theta = polar scattering angle)  
Nr.angles = 181 | Max. = 8.14145E+03 | 10-Log. plot; blue: >0; green: <0



MIE-File: D:\FRITS\MC\mie\Unknown.MIE  
Scattering function = f(theta) | (theta = polar scattering angle)  
Nr.angles = 181 | Max. = 8.14145E+03 | 10-Log. plot; blue: >0; green: <0



Linear plot: log scale:  
X: 0 .. 180<sup>0</sup>; Y: 5 decades: 1 .. 10<sup>-5</sup>

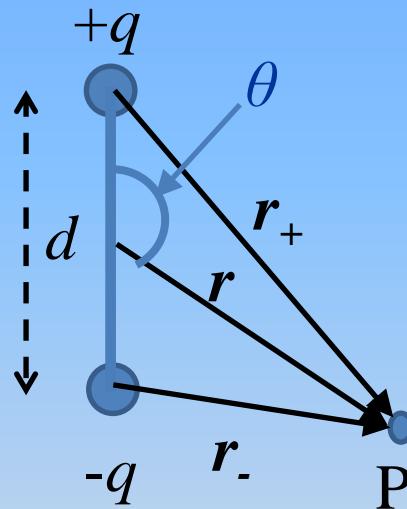
Polar plot: log. scale: 5 decades

# Appendices

Appendices:

- 
- A. Derivation of the dipole radiation formula
  - B. Derivation of the general scattering equation.

# Appendix A: dipolar scattering



Dipole: dipole moment  $p = qd$

Oscillating dipole:  $d(t) = d_0 \cdot \cos \omega t$

$$p(t) = p_0 \cdot \cos \omega t ; p_0 = qd_0$$

(time-dependent part only)

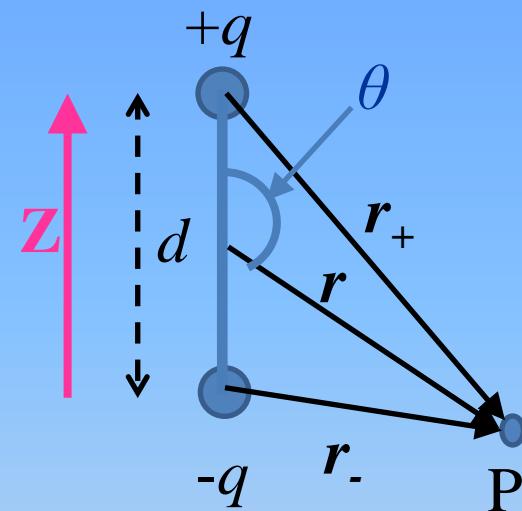
We have to calculate  
the  $E$ -field  
in point P:

$$\vec{E} = -\nabla V - \frac{\partial \vec{A}}{\partial t}$$

$V$  = electric (scalar) potential

$A$  = magnetic (vector) potential

# Appendix A: dipolar scattering



$z$  = coordinate along Z-axis;  
assume  $E_0$ -field // Z-axis

$F_e$  = electric force

$m$  = mass

$\eta$  = damping factor

$\omega_r$  = resonance frequency

Dipole: dipole moment  $p = qd$

Oscillating dipole:  $d(t) = d_0 \cdot \cos \omega t$  ;  $p_0 = qd_0$   
(time-dependent part only)

Dipole, induced by  $E$ -field:  
classical harmonic oscillator :

$$\frac{d^2 z}{dt^2} + \eta \frac{dz}{dt} + \omega_r^2 z = \frac{F_e}{m} = \frac{qE_0}{m} e^{i\omega t}$$

Solution:

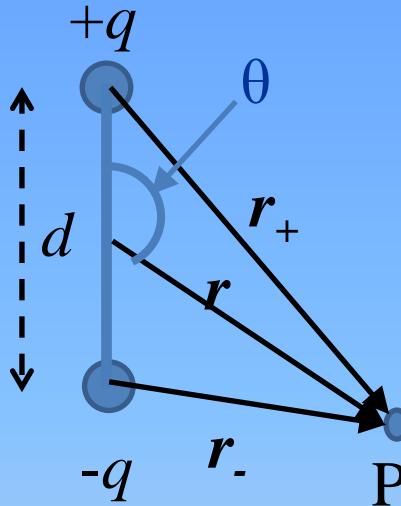
$$d(t) = 2z(t) = \frac{2qE_0}{m} \frac{e^{i\omega t}}{\omega_r^2 - \omega^2 + i\eta\omega}$$

Electron free resonance frequency  $\omega_r$   
 $>>$  induced frequency  $\omega$   
 (otherwise: if  $\omega_r \ll \omega$  : “Thomson scattering”)

Induced  
dipole  
moment:

$$p(t) = p_0 \cos \omega t ; p_0 = \frac{2q^2 E_0}{m \cdot \omega_r^2}$$

# Appendix A: dipolar scattering



Dipole: dipole moment  $p = qd$

Oscillating dipole:  $p(t) = p_0 \cos \omega t ; \quad p_0 = q.d_0$

Now calculate the  $E$ -field:

$$\vec{E} = -\nabla V - \frac{\partial \vec{A}}{\partial t}$$

We start with  $V$ ; later  $A$

**Potential function** of two charges (+ and -)

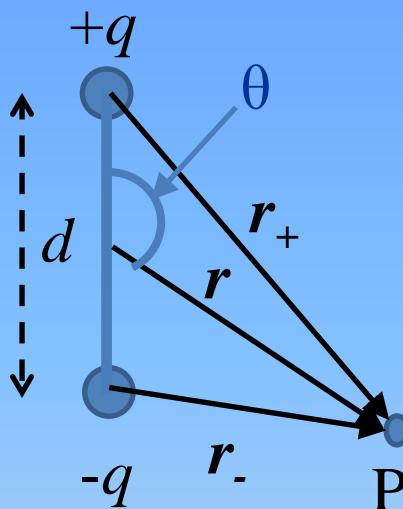
$$V(\vec{r}, \theta, t) = \frac{1}{4\pi\epsilon_0} \left[ \frac{q \cos\{\omega(t - r_+/c)\}}{r_+} - \frac{q \cos\{\omega(t - r_-/c)\}}{r_-} \right]$$

with  $q = \frac{p_0}{d_0}$

and  $r_{\pm} = \sqrt{r^2 \mp rd \cdot \cos \theta + (d/2)^2}$

**Retarded time:** ( $t' = t - r_{\pm}/c$  ;  $c$  = light velocity),  
accounts for flight time and phase differences between paths.

# Appendix A: dipolar scattering



$$V(\vec{r}, \theta, t) = \frac{q}{4\pi\epsilon_0} \left[ \frac{\cos\{\omega(t - r_+/c)\}}{r_+} - \frac{\cos\{\omega(t - r_-/c)\}}{r_-} \right]$$

with  $q = \frac{p_0}{d_0}$  and  $r_{\pm} = \sqrt{r^2 \mp rd \cdot \cos \theta + (d/2)^2}$

Use **far-field approximation** ( $d \ll r$ ; expansion to 1st order):

$$r_{\pm} \approx r \left( 1 \mp \frac{d}{2r} \cos \theta + \left\{ \frac{d}{2r} \right\}^2 + \dots \right) \Rightarrow \frac{1}{r_{\pm}} \approx \frac{1}{r} \left( 1 \pm \frac{d}{2r} \cos \theta \right)$$

Use **small-dipole approximation** ( $d \ll \lambda = 2\pi c/\omega \rightarrow \omega d/c \ll 1$ ; use  $\cos(A \pm B)$ ):

$$\cos(A \pm B) = \cos A \cdot \cos B \mp \sin A \cdot \sin B \rightarrow 1 \cdot \cos B \mp A \cdot \sin B \text{ if } A \rightarrow 0$$

$$\cos[\omega(t - \frac{r_{\pm}}{c})] \approx \cos \left[ \omega(t - \frac{r}{c}) \pm \frac{\omega d}{2c} \cos \theta \right] \approx 1 \cdot \cos[\omega(t - \frac{r}{c})] \mp \frac{\omega d}{2c} \cdot \cos \theta \sin[\omega(t - \frac{r}{c})].$$

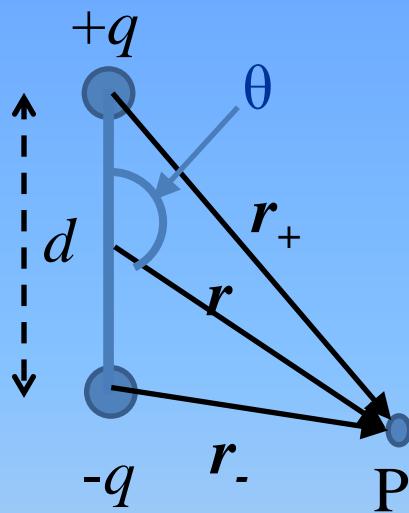
$$V(\vec{r}, \theta, t) = \frac{p_0 \cos \theta}{4\pi\epsilon_0 r} \left[ -\frac{\omega}{c} \sin\{\omega(t - \frac{r}{c})\} + \frac{1}{r} \cos\{\omega(t - \frac{r}{c})\} \right]$$

Use **small-wavelength approximation**  
( $r \gg \lambda = 2\pi c/\omega$ ):

FdM

$$V(\vec{r}, \theta, t) = \frac{p_0 \cos \theta}{4\pi\epsilon_0 r} \left[ -\frac{\omega}{c} \sin\{\omega(t - \frac{r}{c})\} \right]$$

# Appendix A: dipolar scattering



Dipole: dipole moment  $p = qd$

Oscillating dipole.  $p(t) = p_0 \cos(\omega t)$  ;  $p_0 = q_0 \cdot d$

Retarded potential: ( $c$  = light velocity)

Calculation of  $V$ :

$$V(\vec{r}, \theta, t) = \frac{1}{4\pi\epsilon_0} \left[ \frac{q \cos\{\omega(t - r_+ / c)\}}{r_+} - \frac{q \cos\{\omega(t - r_- / c)\}}{r_-} \right]$$

with  $r_{\pm} = \sqrt{r^2 \mp rd \cdot \cos \theta + (d/2)^2}$

$$V(\vec{r}, \theta, t) = \frac{p_0 \cos \theta}{4\pi\epsilon_0 r} \left[ -\frac{\omega}{c} \sin\{\omega(t - \frac{r}{c})\} + \frac{1}{r} \cos\{\omega(t - \frac{r}{c})\} \right]$$

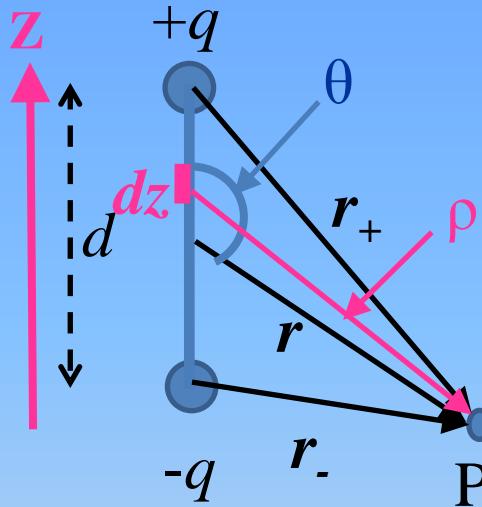
Result for potential  
 $V: \sim 1/r :$

$$V(\vec{r}, \theta, t) = \frac{p_0 \cos \theta}{4\pi\epsilon_0 r} \left[ -\frac{\omega}{c} \sin\{\omega(t - \frac{r}{c})\} \right]$$

Result for Electrostatic  
 limit:  $\sim 1/r^2 :$

$$\omega \rightarrow 0 : V(\vec{r}, \theta, t) \rightarrow \frac{p_0 \cos \theta}{4\pi\epsilon_0 r^2}$$

# Appendix A: dipolar scattering

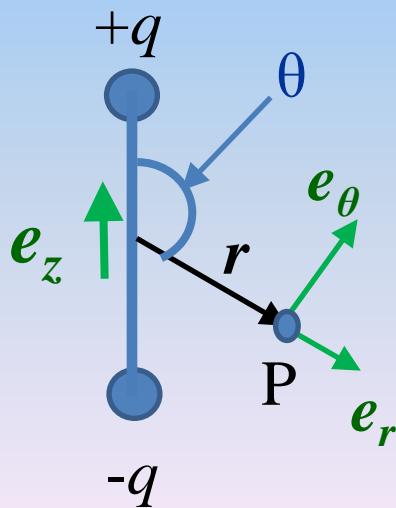


$E$ -field:  $\vec{E} = -\nabla V - \frac{\partial \vec{A}}{\partial t}$

Now calculate the  $A$ -field (vector potential):

$$\vec{A} = \frac{\mu_0}{4\pi} \int \frac{\vec{I}}{r} dl = \frac{\mu_0}{4\pi} \int_{-d_0/2}^{d_0/2} \frac{-q\omega \sin[\omega(t - \rho/c)]}{r} \vec{e}_z dz$$

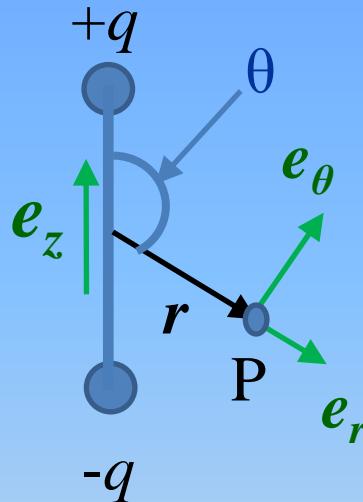
with  $\vec{I} = \frac{dq}{dt} \vec{e}_z = -q\omega \sin(\omega t) \vec{e}_z$  ;  $q = \frac{p_0}{d_0}$  and  $\rho = f(z)$



We want the result at large distances,  
so we use as an approximation:  
replace the integrand by its value at center O,  
multiply with  $2 \cdot d_0/2 = d_0$  and take  $d_0 q = p_0$ .

$$\vec{A}(\vec{r}, t) = -\frac{\mu_0 p_0 \omega}{4\pi r} \sin\left\{\omega\left(t - \frac{r}{c}\right)\right\} \vec{e}_z$$

# Appendix A: dipolar scattering



$$V(\vec{r}, \theta, t) = -\frac{p_0 \cos \theta}{4\pi \epsilon_0 r} \frac{\omega}{c} \sin\left\{\omega(t - \frac{r}{c})\right\}$$

$$\vec{A}(\vec{r}, t) = -\frac{\mu_0 p_0 \omega}{4\pi r} \sin\left\{\omega(t - \frac{r}{c})\right\} \vec{e}_z$$

Now calculate the  $\vec{E}$ -field:

$$\vec{E} = -\nabla V - \frac{\partial \vec{A}}{\partial t}$$

$$\text{with } \nabla V = \frac{\partial V}{\partial r} \vec{e}_r + \frac{1}{r} \frac{\partial V}{\partial \theta} \vec{e}_\theta$$

and  $\vec{e}_z = \cos \theta \vec{e}_r - \sin \theta \vec{e}_\theta$

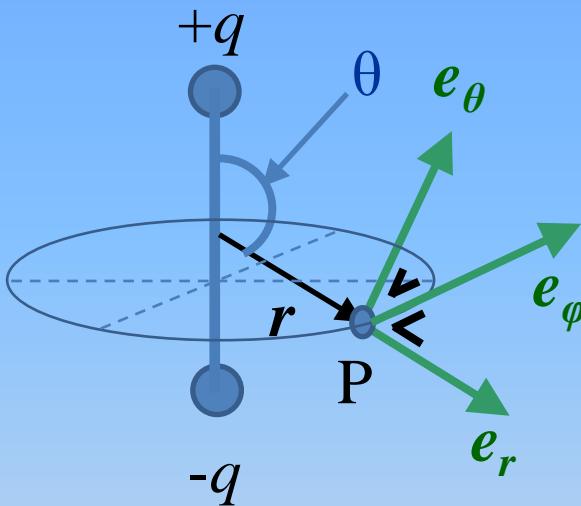
Final result:

$$\vec{E} = -\frac{\mu_0 p_0 \omega^2}{4\pi} \frac{\sin \theta}{r} \cos\left[\omega\left(t - \frac{r}{c}\right)\right] \vec{e}_\theta$$

$E$ -field:  $\sim E_0$  (incident field)  
 $\sim \omega^2$  ( $\rightarrow$  intensity  $\sim \omega^4$ )  
 $\sim r^{-1}$  ( $\rightarrow$  intensity  $\sim r^{-2}$ )  
 $\theta$ -component only!  
 retarded time.

**NB.**  $V$ -field renders  $r$ -component only!  
 $A$ -field renders both  $r$  and  $\theta$ -components;  
 and in resulting  $E$ -field both  $r$ -components  
 cancel;  
 $\theta$ -component remains only!

# Appendix A: dipolar scattering



If  $\vec{X} \parallel \vec{e}_z$ :  $\nabla \times \vec{X} =$

$$= \frac{1}{r} \left[ \frac{\partial}{\partial r} (r X_\theta) - \frac{\partial X_r}{\partial \theta} \right] \vec{e}_\phi$$

using  $\vec{e}_z = \cos \theta \vec{e}_r - \sin \theta \vec{e}_\theta$

What is emitted energy?

Radiated power [W/m<sup>2</sup>] :

Poynting vector  $\vec{S}$  :

$$\vec{S} = \frac{1}{\mu_0} \vec{E} \times \vec{B}$$

$$\vec{E} = -\frac{\mu_0 p_0 \omega^2}{4\pi} \frac{\sin \theta}{r} \cos \left[ \omega \left\{ t - \frac{r}{c} \right\} \right] \vec{e}_\theta$$

$$p_0 = \frac{2q^2 E_0}{m \omega_r^2}$$

Analogously:

$$\vec{B} = \nabla \times \vec{A} = -\frac{\mu_0 p_0 \omega^2}{4\pi c} \frac{\sin \theta}{r} \cos \left[ \omega \left\{ t - \frac{r}{c} \right\} \right] \vec{e}_\phi$$

with  $\vec{A}(\vec{r}, t) = -\frac{\mu_0 p_0 \omega}{4\pi r} \sin \left\{ \omega \left( t - \frac{r}{c} \right) \right\} \vec{e}_z$

$\vec{B} \parallel \vec{e}_\phi$ : in **tangential** direction  $\rightarrow$  Ampère's Law.

$$\vec{S} = \frac{1}{\mu_0} \vec{E} \times \vec{B} = \frac{\mu_0 p_0^2 \omega^4}{32\pi^2 c} \frac{\sin^2 \theta}{r^2} \vec{e}_r$$

NB.  $S$  in **radial** direction!

# Appendix A: dipolar scattering

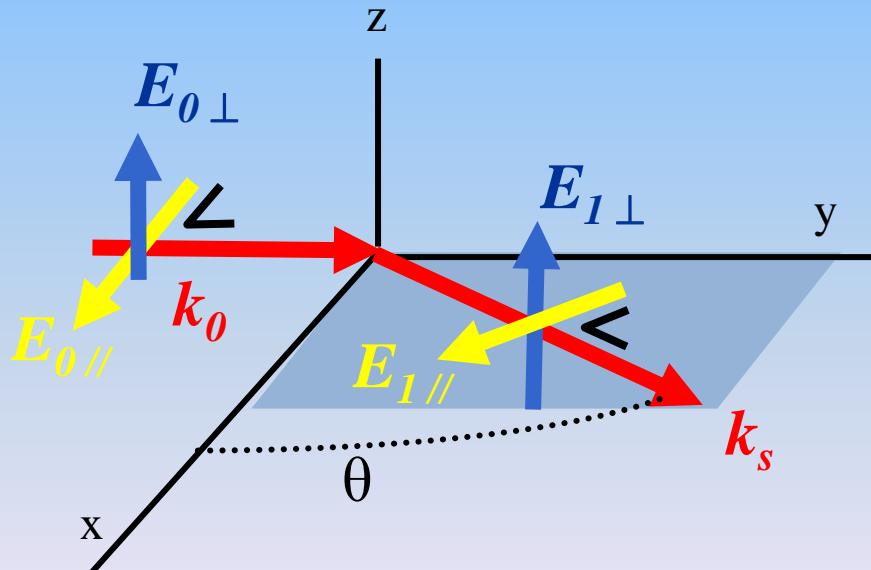
Final result  
for 1 dipole:

$$\vec{E} = \frac{\mu_0 p_0 \omega^2}{4\pi} \frac{\sin \theta}{r} \cos\left[\omega\left\{t - \frac{r}{c}\right\}\right] \hat{e}_\theta$$

$$p_0 = \frac{2q^2 E_0}{m \cdot \omega_r^2}$$

with  $k = \frac{\omega}{c}$  and  $\epsilon_0 \mu_0 = c^{-2}$  :  $\vec{E} = \frac{p_0 k^2}{4\pi \epsilon_0} \frac{\sin \theta}{r} \cos\left[\omega\left\{t - \frac{r}{c}\right\}\right] \hat{e}_\theta$

For  $\perp$  component:  $\sin \theta = 1$



Expression for dipoles in part I:  
(amplitude)

$$\begin{bmatrix} \mathbf{E}_{1\perp} \\ \mathbf{E}_{1/\parallel} \end{bmatrix} \propto \frac{\alpha k_s^2}{4\pi \epsilon_0 r} \begin{bmatrix} 1 \\ \sin \theta \end{bmatrix} \begin{bmatrix} \mathbf{E}_{0\perp} \\ \mathbf{E}_{0/\parallel} \end{bmatrix}$$

Correspondence if set:  $p_0 = \alpha E_0$

# Appendices

Appendices:

- A. Derivation of the dipole radiation formula
- B. Derivation of the general scattering equation

## Appendix B: scattering field

Electromagnetic Theory from Maxwell's Equations     $\rho = 0 ; j = 0$

$$\nabla \bullet \vec{D} = 0 \quad ; \quad \nabla \bullet \vec{B} = 0 \quad ; \quad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad ; \quad \nabla \times \vec{B} = \mu_0 \frac{\partial \vec{D}}{\partial t}$$

Wave Equation:

$$\nabla \times \nabla \times \vec{E} = -\mu_0 \frac{\partial^2 \vec{D}}{\partial t^2}$$

$\nabla \times \vec{E}$  = "rotation", "curl"

Assume: scattering field is small compared with incident field

$$\vec{D} = \epsilon \cdot \vec{E}, \quad \text{with} \quad \vec{E} = \vec{E}_0 + \vec{E}_1$$

$$\epsilon = \epsilon_0 + \epsilon_1 ;$$

All  $D$ 's,  $E$ 's and  $\epsilon$ 's  
are  $f(r, t)$

$$\epsilon_1 = \epsilon_0(\epsilon_r - 1)$$

Assume:  $\epsilon_1 \ll \epsilon_0$  and  $E_1 \ll E_0$  ;    **1<sup>st</sup> order approximation:**  
0<sup>th</sup> and 1<sup>st</sup> order terms only:

$$\vec{D}_0 = \epsilon_0 \cdot \vec{E}_0$$

$$\vec{D}_1 = \epsilon_0 \cdot \vec{E}_1 + \epsilon_1 \cdot \vec{E}_0$$

## Appendix B: scattering field

Wave  
Equation:

$$\nabla \times \nabla \times \vec{E} = -\mu_0 \frac{\partial^2 \vec{D}}{\partial t^2}$$

All  $D$ 's,  $E$ 's and  $\epsilon$ 's  
are  $f(r,t)$

$$\vec{D}_0 = \epsilon_0 \cdot \vec{E}_0$$

$$\vec{D}_1 = \epsilon_0 \cdot \vec{E}_1 + \epsilon_1 \cdot \vec{E}_0$$

$$\epsilon_1 = (\epsilon_r - 1) \epsilon_0$$

0th order :  $\nabla \times \nabla \times \vec{E}_0 = -\nabla^2 \vec{E}_0 + \nabla(\nabla \bullet \vec{E}_0) = -\epsilon_0 \mu_0 \frac{\partial^2 \vec{E}_0}{\partial t^2}$

$$\nabla \bullet \vec{E}_0 = 0 : \quad \nabla^2 \vec{E}_0 = \epsilon_0 \mu_0 \frac{\partial^2 \vec{E}_0}{\partial t^2}$$

Solution: incident field from light source:      harmonic wave:

$$\vec{E}_0(\vec{r},t) = \vec{E}_{0m} \exp[i(\vec{k}_0 \bullet \vec{r} - \omega_0 t)] \quad k = 2\pi/\lambda ; \quad \omega = 2\pi f$$

1st order :  $\nabla^2 \vec{D}_1 - \epsilon_0 \mu_0 \frac{\partial^2 \vec{D}_1}{\partial t^2} = -\nabla \times \nabla \times (\epsilon_1 \vec{E}_0)$

## Appendix B: scattering field

1st order :  $\nabla^2 \vec{D}_1 - \varepsilon_0 \mu_0 \frac{\partial^2 \vec{D}_1}{\partial t^2} = -\nabla \times \nabla \times (\varepsilon_1 \vec{E}_0)$

$\varepsilon_1$ ,  $\vec{E}_0$  and  $\vec{E}_1$  are  $f(\mathbf{r}, t)$ ;  
 $\varepsilon_0$  = constant

Derivation 1<sup>st</sup> order:  $\nabla^2 \vec{D}_1 = \nabla^2 (\varepsilon_0 \vec{E}_1 + \varepsilon_1 \vec{E}_0) =$

$$= -\nabla \times \nabla \times (\varepsilon_0 \vec{E}_1) - \nabla \times \nabla \times (\varepsilon_1 \vec{E}_0) + \nabla (\nabla \bullet (\varepsilon_0 \vec{E}_1)) + \nabla (\nabla \bullet (\varepsilon_1 \vec{E}_0)) =$$

use :  $\nabla \bullet \vec{D}_1 = \nabla \bullet (\varepsilon_0 \vec{E}_1 + \varepsilon_1 \vec{E}_0) = 0$

$$= -\varepsilon_0 \nabla \times \nabla \times \vec{E}_1 - \nabla \times \nabla \times (\varepsilon_1 \vec{E}_0) =$$

$$= +\varepsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} (\varepsilon_0 \vec{E}_1) - \nabla \times \nabla \times (\varepsilon_1 \vec{E}_0) = \quad (\text{since } \nabla \bullet \vec{E}_1 = 0)$$

And so:

$$\nabla^2 \vec{D}_1 = \varepsilon_0 \mu_0 \frac{\partial^2}{\partial t^2} \vec{D}_1 - \nabla \times \nabla \times (\varepsilon_1 \vec{E}_0)$$

At the detector:  
no incident field present!

There:

$$\vec{D}_1 = \varepsilon_0 \vec{E}_1 + \varepsilon_1 \vec{E}_0 \rightarrow \varepsilon_0 \vec{E}_1$$

# Appendix B: scattering field

Wave Equation:

$$\nabla \times \nabla \times \vec{E} = -\mu_0 \frac{\partial^2 \vec{D}}{\partial t^2}$$

$$\vec{D}_0 = \epsilon_0 \cdot \vec{E}_0 \quad ; \quad \epsilon_0, \epsilon_1, \vec{D} \text{ and } \vec{E} \text{ are } f(\vec{r}, t)$$

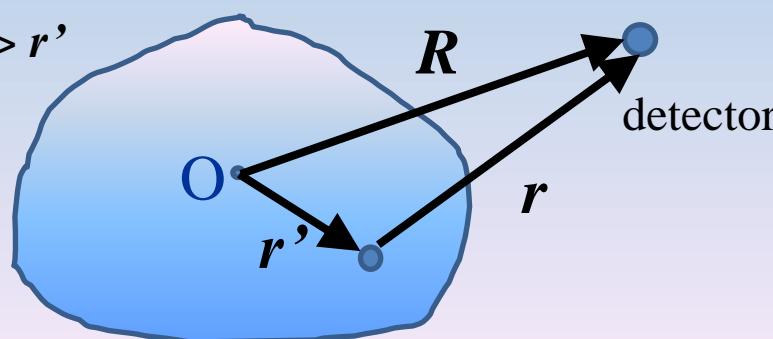
$$\vec{D}_1 = \epsilon_0 \vec{E}_1 + \epsilon_1 \vec{E}_0$$

1st order :  $\nabla^2 \vec{D}_1 - \epsilon_0 \mu_0 \frac{\partial^2 \vec{D}_1}{\partial t^2} = -\nabla \times \nabla \times (\epsilon_1 \vec{E}_0)$

Define  $\vec{Z}$  using :  $\vec{D}_1 = \nabla \times \nabla \times \vec{Z}$

$$\nabla^2 \vec{Z} - \epsilon_0 \mu_0 \frac{\partial^2 \vec{Z}}{\partial t^2} = -\epsilon_1 \vec{E}_0$$

Scattering volume:  
 $R \gg r'$



Solution using  
Green's  
functions:

$$\vec{Z}(\vec{R}, t) = \frac{1}{4\pi} \iiint d^3 \vec{r}' \frac{\epsilon_1 \vec{E}_0(\vec{r}', t')}{|\vec{R} - \vec{r}'|}$$

$t'$  = retarded time:  $t' = t - |\vec{R} - \vec{r}|/c$   
 $c$  = light velocity:  $c = 1 / \sqrt{(\epsilon_0 \mu_0)}$   
 $t'$  accounts for flight time to detector

(Solution explained later)

## Appendix B: scattering field

$\vec{Z}$  is defined using :  
 $\vec{D}_1 = \nabla \times \nabla \times \vec{Z}$

Solution using  
Green's  
functions:

with :  $\vec{E}_0(\vec{r}', t') = \vec{E}_{0m} \exp[i(\vec{k}_{\vec{r}} \bullet \vec{r}' - \omega_0 t')]$

$$\vec{D}_1 = \frac{1}{4\pi} \iiint d^3\vec{r}' \cdot \nabla \times \nabla \times \frac{\varepsilon_1 \vec{E}_0(\vec{r}', t')}{|\vec{R} - \vec{r}'|}$$

using :  $\iiint d^3\vec{r}' \cdot \nabla \times \nabla \times f(e^{i\vec{k} \bullet \vec{r}'}, \vec{r}') = \iiint d^3\vec{r}' \cdot \vec{k} \times \vec{k} \times f(e^{i\vec{k} \bullet \vec{r}'}, \vec{r}')$

(after volume integration,  $\vec{k}$  is the only coordinate-dependent variable;  
 $\vec{k} = f(x, y, z)$  ;  $\vec{r}' = f(x', y', z')$  ; integration and differentiation can be swapped)

$$\vec{Z}(\vec{R}, t) = \frac{1}{4\pi} \iiint d^3\vec{r}' \frac{\varepsilon_1 \vec{E}_0(\vec{r}', t')}{|\vec{R} - \vec{r}'|}$$

At detector no incoming field present:

$$\vec{D}_1 = \varepsilon_0 \vec{E}_1 + \varepsilon_1 \vec{E}_0 \rightarrow \varepsilon_0 \vec{E}_1$$

$f$  denotes  
any  
function  
of the  
arguments

$$\varepsilon_0 \vec{E}_1 = \frac{1}{4\pi} \iiint d^3\vec{r}' \cdot \vec{k} \times \vec{k} \times \frac{\varepsilon_1 \vec{E}_0(\vec{r}', t')}{|\vec{R} - \vec{r}'|}$$

- retarded time : accounts for flight time from scattering volume to detector
- $(\vec{k} \times \vec{k} \times ..)$  operator : accounts for polarization directions of  $\vec{E}_1$  from  $\vec{E}_0$ .
- $|\vec{R} - \vec{r}'|$  in denominator: spherical wave; intensity ( $\sim |\vec{E}_1|^2$ ) is  $\sim 1/R^2$ .

# Appendix B: scattering field

Solution using Green's functions:

$$\vec{\mathbf{Z}}(\vec{\mathbf{R}}, t) = \frac{1}{4\pi} \iiint d^3 \vec{\mathbf{r}}' \frac{\varepsilon_1 \vec{\mathbf{E}}_0(\vec{\mathbf{r}}', t')}{|\vec{\mathbf{R}} - \vec{\mathbf{r}}'|}$$

$\vec{\mathbf{Z}}$  defined with :  
 $\varepsilon_0 \vec{\mathbf{E}}_I = \nabla \times \nabla \times \vec{\mathbf{Z}}$

Derivation of this solution using **Green's functions**:

Solution obtained from: .

$$\nabla^2 \vec{\mathbf{Z}} - \varepsilon_0 \mu_0 \frac{\partial^2 \vec{\mathbf{Z}}}{\partial t^2} = -\varepsilon_1 \vec{\mathbf{E}}_0$$

$$\text{with : } \vec{\mathbf{E}}_0(\vec{\mathbf{r}}', t') = \vec{\mathbf{E}}_{0m} \exp[i(\vec{k}_{\vec{r}} \bullet \vec{\mathbf{r}}' - \omega_0 t')]$$

This is an equation of the form:

$$\nabla^2 \Phi - \varepsilon_0 \mu_0 \frac{\partial^2 \Phi}{\partial t^2} = -A$$

use  $\Phi = \Psi(x, y, z) e^{i\omega t}$  ;  $c^2 = 1/(\varepsilon_0 \mu_0)$  and  $k = \omega/c$

Now do the derivation to time:

$$\nabla^2 \Psi + k^2 \Psi = -A' ; \text{ with } A' = A e^{i\omega t}$$

Solution using Green's theorem:  
 (with surface  $S$  encloses volume  $V$ ):

$$\iiint_V [\Psi_2 \cdot \nabla^2 \Psi_1 - \Psi_1 \nabla^2 \Psi_2] dV = \iint_S \left[ \Psi_2 \cdot \frac{\partial \Psi_1}{\partial n} - \Psi_1 \cdot \frac{\partial \Psi_2}{\partial n} \right] dS$$

# Appendix B: scattering field

Solution using  
**Green's Theorem:**  
 Surface  $S$  encloses  
 volume  $V$

$$\nabla^2 \Psi + k^2 \Psi = -A' ; \text{ with } A' = A e^{i\omega t'}$$

$$\iiint_V [\Psi_2 \cdot \nabla^2 \Psi_1 - \Psi_1 \nabla^2 \Psi_2] dV = \oint_S \left[ \Psi_2 \cdot \frac{\partial \Psi_1}{\partial n} - \Psi_1 \cdot \frac{\partial \Psi_2}{\partial n} \right] dS \quad (1)$$

**Green's Theorem follows from  
 Gauss Law:**

$$\iiint_V \nabla \bullet \vec{X} dV = \oint_S \vec{X} \bullet \vec{n} dS$$

upon substituting:  $\vec{X} = \psi \nabla \varphi ; \vec{X} \bullet \vec{n} = \psi \frac{\partial \varphi}{\partial n} ; \nabla \bullet \vec{X} = \nabla \psi \cdot \nabla \varphi + \psi \nabla^2 \varphi$

Now substitute:  $\vec{X} = \Psi_2 \cdot \nabla \Psi_1 - \Psi_1 \cdot \nabla \Psi_2$

set  $\Psi_1 = \Psi$  and try  $\Psi_2 = \frac{e^{-ikr}}{r}$  (spherical wave:  $\nabla^2 \Psi_2 + k^2 \Psi_2 = 0 \rightarrow \nabla^2 \Psi_2 = -k^2 \Psi_2$ )

Left side of (1):  $\iiint_V \left[ \frac{e^{-ikr}}{r} (-k^2 \Psi - A') + k^2 \Psi \frac{e^{-ikr}}{r} \right] dV = \iiint_V \left[ -A' \frac{e^{-ikr}}{r} \right] dV$

## Appendix B: scattering field

Solution using  
Green's theorem:  
Surface  $S$  encloses  
volume  $V$

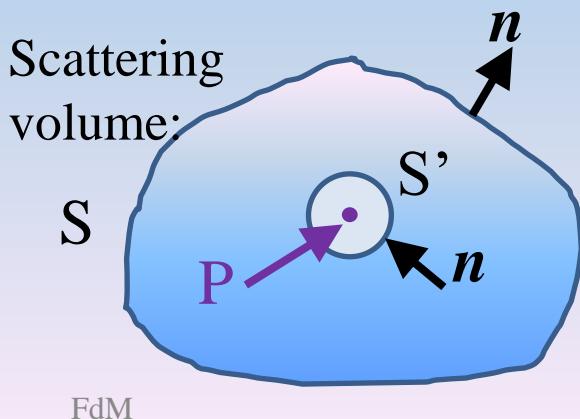
$$\nabla^2 \Psi + k^2 \Psi = -A' e^{i\omega t} ; \text{ with } A' = A e^{-i\omega t}$$

$$\iiint_V [\Psi_2 \cdot \nabla^2 \Psi_1 - \Psi_1 \nabla^2 \Psi_2] dV = \iint_S \left[ \Psi_2 \cdot \frac{\partial \Psi_1}{\partial n} - \Psi_1 \cdot \frac{\partial \Psi_2}{\partial n} \right] dS \quad (1)$$

We did :  $\Psi_1 = \Psi$  and  $\Psi_2 = \frac{e^{-ikr}}{r}$  (spherical wave:  $\nabla^2 \Psi_2 + k^2 \Psi_2 = 0$ )

Left side of (1) :  $\iiint_V \left[ \frac{e^{-ikr}}{r} (-k^2 \Psi - A') + k^2 \Psi \frac{e^{-ikr}}{r} \right] dV = \iiint_V \left[ -A' \frac{e^{-ikr}}{r} \right] dV$

Now: Right side of (1):



P = detection point, to be excluded from *volume* integration

Take spherical volume  $S'$  around P and let  $S'$  shrink to zero

$$\iint_S \rightarrow \iint_S + \iint_{S'}$$

and with  $S: \frac{\partial}{\partial n} = \frac{\partial}{\partial r}$  ;  $S': \frac{\partial}{\partial n} = -\frac{\partial}{\partial r}$

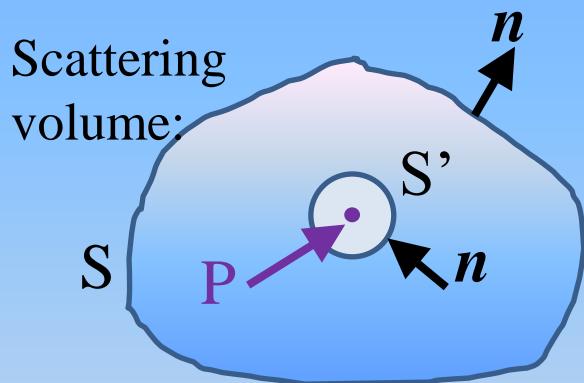
$$\iint_{S'} = \iint_{S'} \left[ \frac{e^{-ikr}}{r} \cdot \frac{-\partial \Psi}{\partial r} - \Psi \left( \frac{e^{-ikr}}{r^2} + \cdot \frac{i k e^{-ikr}}{r} \right) \right] dS$$

## Appendix B: scattering field

$$\text{Left side of (1)}: \iiint_V \left[ \frac{e^{-ikr}}{r} (-k^2 \Psi - A') + k^2 \Psi \frac{e^{-ikr}}{r} \right] dV = \iiint_V \left[ -A' \frac{e^{-ikr}}{r} \right] dV$$

Right side of (1):

P = detection point, to be excluded from *volume* integration



Take spherical volume  $S'$  around P and let  $S'$  shrink to zero.

$$S: \frac{\partial}{\partial n} = \frac{\partial}{\partial r};$$

$$S': \frac{\partial}{\partial n} = -\frac{\partial}{\partial r}$$

$$\iint_{S'} = \iint_{S'} \left[ \frac{e^{-ikr}}{r} \cdot \frac{-\partial \Psi}{\partial r} - \Psi \left( \frac{e^{-ikr}}{r^2} + \frac{i k e^{-ikr}}{r} \right) \right] dS$$

On  $S'$ :  $dS = r^2 d\Omega$  ( $d\Omega$  is integration element over solid angle)

Integration over  $S'$ , followed by limit  $r \rightarrow 0$ :

$$\iint_{S'} = \iint_{\Omega} \left[ \frac{e^{-ikr}}{r} \cdot \frac{-\partial \Psi}{\partial r} - \Psi \left( \frac{e^{-ikr}}{r^2} + \frac{i k e^{-ikr}}{r} \right) \right] r^2 d\Omega$$

$$\rightarrow 4\pi \cdot \Psi_P$$

Left and right sides:

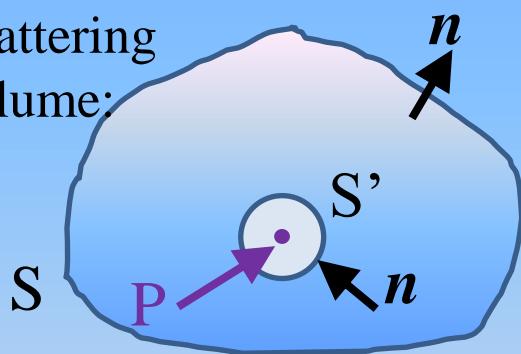
$$\Psi_P = \frac{1}{4\pi} \iint_S \left[ \frac{e^{-ikr}}{r} \cdot \frac{\partial \Psi}{\partial n} - \Psi e^{-ikr} \frac{\partial}{\partial n} \left( \frac{1}{r} \right) + \frac{i k e^{-ikr}}{r} \Psi \frac{\partial r}{\partial n} \right] dS + \iiint_V \frac{A' e^{-ikr}}{4\pi r} dV$$

# Appendix B: scattering field

Result:

$$\Psi_P = \frac{1}{4\pi} \oint_S \left[ \frac{e^{-ikr}}{r} \cdot \frac{\partial \Psi}{\partial n} - \Psi e^{-ikr} \frac{\partial}{\partial n} \left( \frac{1}{r} \right) + \frac{ike^{-ikr}}{r} \Psi \frac{\partial r}{\partial n} \right] dS + \iiint_V \frac{A' e^{-ikr}}{4\pi r} dV$$

Scattering volume:



Suppose  $S$  is very large ( $\gg$  scattering volume)

and  $A'$  is limited in space (finite scattering volume) →

Contribution of  $S$  will be = 0 (due to time retardation).

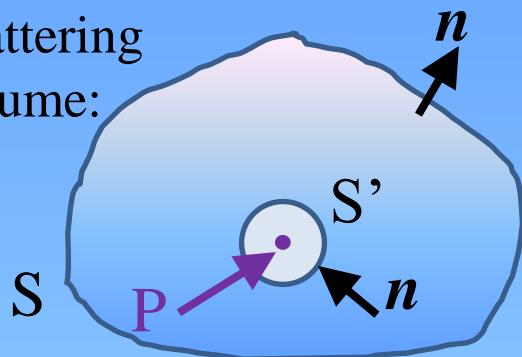
Final result:

$$\Psi_P = \iiint_V \frac{A' e^{-ikr}}{4\pi r} dV$$

Now go back to:  $\epsilon_0 E_I$  and  $Z$

# Appendix B: scattering field

Scattering volume:



$$\Psi_P = \iiint_V \frac{A' e^{-ikr}}{4\pi r} dV$$

We now have solved:  
using  $\Phi = \Psi(xyz).e^{i\omega t}$

$$\nabla^2 \Phi - \epsilon_0 \mu_0 \frac{\partial^2 \Phi}{\partial t^2} = -A'$$

$\mathbf{Z}$  was represented by  $\Phi$   
and  $\mathbf{E}_0$  by  $A' = A \cdot \exp(-i\omega t')$

$$\nabla^2 \vec{\mathbf{Z}} - \epsilon_0 \mu_0 \frac{\partial^2 \vec{\mathbf{Z}}}{\partial t^2} = -\epsilon_1 \vec{\mathbf{E}}_0$$

with :  $\vec{\mathbf{E}}_0(\vec{r}', t') = \vec{\mathbf{E}}_{0m} \exp[i(\vec{k}_{\vec{r}} \bullet \vec{r}' - \omega_0 t')]$  :  $t'$  = retarded time

Now include time retardation:

$$\vec{\mathbf{Z}}(\vec{R}, t) = \frac{1}{4\pi} \iiint d^3 \vec{r}' \frac{\epsilon_1 \vec{\mathbf{E}}_0(\vec{r}', t')}{|\vec{R} - \vec{r}'|}$$

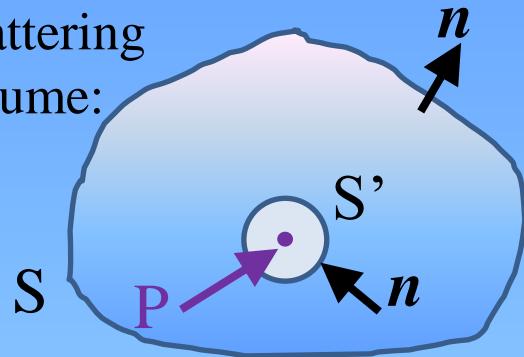
$\vec{\mathbf{Z}}$  was defined with :  
 $\vec{\mathbf{D}}_I (= \epsilon_0 \vec{\mathbf{E}}_1) = \nabla \times \nabla \times \vec{\mathbf{Z}}$

Final result:

$$\vec{\mathbf{E}}_1 = \frac{1}{4\pi \epsilon_0} \iiint d^3 \vec{r}' \cdot \vec{k} \times \vec{k} \times \frac{\epsilon_1 \vec{\mathbf{E}}_0(\vec{r}', t')}{|\vec{R} - \vec{r}'|}$$

# Appendix B: scattering field

Scattering volume:



Final result:

$$\vec{E}_I = \frac{1}{4\pi\epsilon_0} \iiint d^3\vec{r}' \cdot \vec{k} \times \vec{k} \times \frac{\epsilon_1 \vec{E}_0(\vec{r}', t')}{|\vec{R} - \vec{r}'|}$$

Mie (and others) have calculated this integral expression for various geometries and dielectric constant distributions.

In case the incident light has a beam shape with symmetry around the symmetry axis of the beam, an approach with Bessel/Legendre functions is feasible. but this goes beyond the goal of this presentation.

End of this presentation

Thank you for your attention