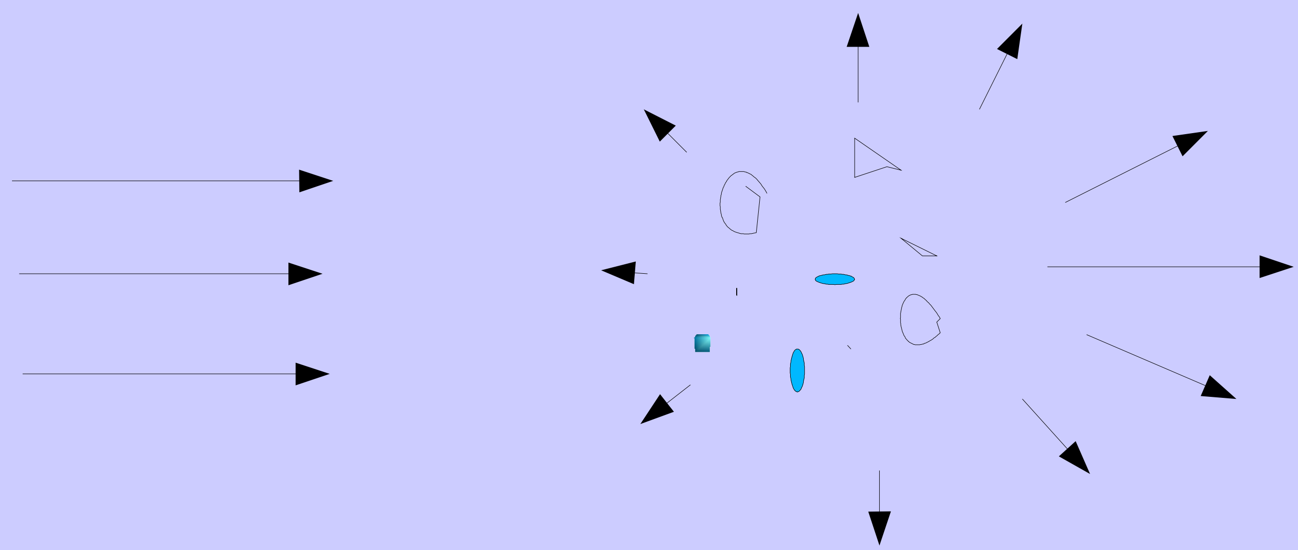
Light Scattering by Dust: Theoretical Approaches

S K Sharma
S N Bose National Centre for Basic Sciences
Block JD, Sector III, Salt Lake
Kolkata 700098

Scope of the Talk

- The light scattering technique is used in many disciplines of science and engineering as a diagnostic tool.

- We look at some aspects of elastic scattering of light by a collection of particles which have relevance to the understanding of light scattering by dust. It will be assumed in all future discussions that the collection is random and tenuous. Scattering process is depicted below:



Approaches to Solution

- DIRECT METHOD: In this approach a model for the scattering problem is assumed. Parameters of the model are varied to achieve best fit to the observed quantities. This is the approach is almost invariably used to characterize dust particles.

- INVERSE METHOD: This approach attempts is to characterize the scatterers by a suitable analysis of the scattered fields.

- In either case, one needs the knowledge of theories which describe the scattering by an isolated single scatterers.

- We begin with a survey of solutions to the problem of scattering of light by an isolated particle. We return to ensemble later and discuss two important quantities which contain information on scatterers: extinction spectrum and phase function..

Single Particle: Exact Solutions

- ANALYTIC METHODS: Mie theory and its extensions have been used to obtain exact analytic solutions for scattering of light by: Homogeneous and Concentric Spheres, Magnetic (Kerker et al. JOSA 73 (1983) 765) and Chiral Spheres (Bohren and Huffman 1983), Homogeneous and Concentric Infinitely Long Cylinders, Homogeneous and Concentric Spheroids and Ellipsoids etc.

- NUMERICALMETHODS: 1. T-matrix or Extended Boundary Condition Method (ECBM) is one of the first tools developed to treat more irregularly shaped particles. Disadvantages are convergence for certain shapes and difficulty in dealing with particle heterogeneities.

- 2. Discrete Dipole Approximation (DDA) has been extensively used for Dust. Disadvantage: algorithms are computationally intensive in both time and memory and convergence problems may occur for large refractive indices.

- 3. Finite Difference Time Domain Method (FDTD) has been extensively used in other fields. It appears to be slower than the DDA but is more stable for large refractive indices.

Single Particle:Exact Solutions

- A comparison of computational demands of various numerical techniques has been performed by Wriedt and Comberg, JQSRT 60 (1998) 411-423 for a cube on a IBM RISC/6000-595-workstation.

- A review of numerical methods used in elastic light scattering theories can be found in (i) Wriedt Part. Part Syst. Charact, 15 (1998) 67-74 (ii) Light scattering by Non-Spherical Particles, Ed. M I Mishchenko, J W Hovenier and L D Travis , Academic Press (2000)(iii) Scattering, Absorption and Emission of Light by Small Particles, M I Mishchenko, L D Travis and A Lacis , Cambridge University Press (2002).

- Some useful sites for light scattering informations and computer programs are: 1. NASA (M Mishchenko); 2. University of Bremen (T Wriedt) 3. St. Petersburg State University (N V Voshcinnikov); 4. University of Amsterdam (A Hoekstra); 5. DDA (P Flatau); 6. B T Draine (optical properties)

Single Particle: Approximate Solutions

- For large particles of irregular shapes it is often advantageous to use approximate methods, particularly for those who believe that it is better to use approximate theory for right particle rather than right theory for wrong particle.

  APPROXIMATION METHODS~~~~~~~~~VALIDITY DOMAINS
- Rayleigh   x<<1; |mx|<<1
- Rayleigh-Gans |m-1|<<1; x|m-1}<1
- S-approximation |m-1|<<1; x>1
- Anomalous Diffraction and Eikonal |m-1}<<1
- Diffraction   x>>1; Im m large
- WKB Approximation   x>>1, |m-1|x>>1
- GO Approximation   same
- The EA in conjunction with GO has been used in the analysis of large interplanetary dust particles.
- A comparison of many of these methods can be found in "Light Scattering by Optically Soft Particles: Theory and Applications" by S K Sharma and D J Somerford, Springer-Praxis Books (2006).

Dust Particle Shape Models 1

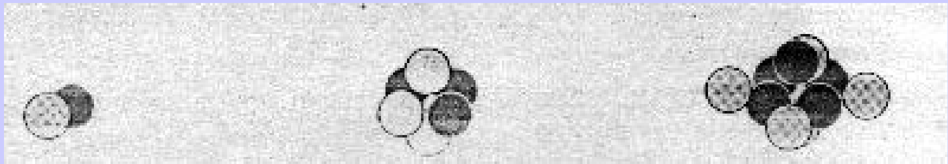
- The shape of interstellar grains remains uncertain. Even the simple homogeneous sphere model is consistent with observed interstellar extinction, observed infrared emission and X-ray scattering. Thus, Bare grains of spherical and spheroidal particles are being used. The Mie theory and T-matrix can be applied to such shapes.

- Composite or Heterogeneous Particles: Effective medium theories (EMTs) have been used. Applicability: A general conclusion is that for Rayleigh particles the volume fraction of embedded particles should not exceed 40-60 percent. For non-Rayleigh Particles it should not exceed 10%.

- A layered sphere model (carbon, silicate and vacuum in equal volume factions) was examined by Voshchinnikov et al (Astron Astrophys 2003) in the context of interstellar dust. It was found that EMT rules have acceptable accuracy for whole range of particles sizes provided the porosity does not exceed about 50%.

Dust Particle Shape Models 2

- Aggregates: Borghese et al. (Scattering from Model Nonspherical Particles (2002) Springer) considered aggregates of spheres of silicates, amorphous carbon and vacuum occupying equal volumes and compared exact results with calculations of Voshchinnikov. Results show several differences in behaviour of the cluster cross-section with respect to results of multilayered spheres.

- 

  The extinction from a dispersion of clusters was noted to be strikingly different from a dispersion of equal volume spheres.

- Wright has examined scattering by fractal shapes generated by the clustering process using DDA (Wright E L in Interstellar Dust, IAU Symposium No. 135 (1989) 337). Clusters with upto about 300 spherical particles were examined.

Dust Particle Shape Models 3

- Chiapetta (1981) has modeled roughness by assuming that

$$m(r) - 1 \propto (m-1)/[1 + e^{k(b-a)}]$$

Physically this means that refractive index decreases continuously in the region close to the surface. The EA was used for forward scattering and for backward scattering geometrical optics was used. The predictions of this model have been found to be in good agreement with the microwave analogue scattering measurements of Zerull et al. (1977) for irregular compact and fluffy particles for scattered intensity as well as polarization.

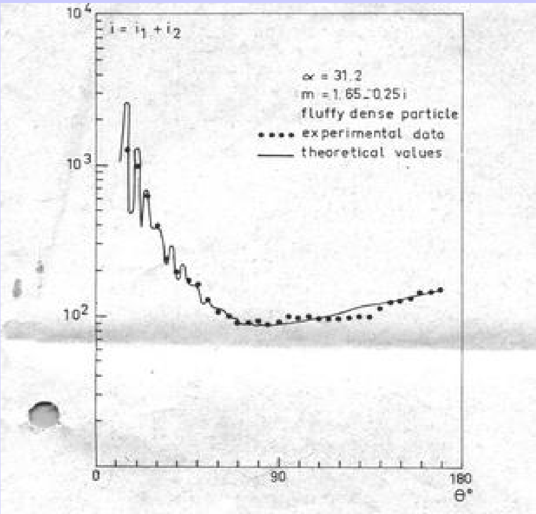


Fig. 1. Scattering function i for a fluffy dense particle (α = 31.2, m = 1.65 − 0.25i)

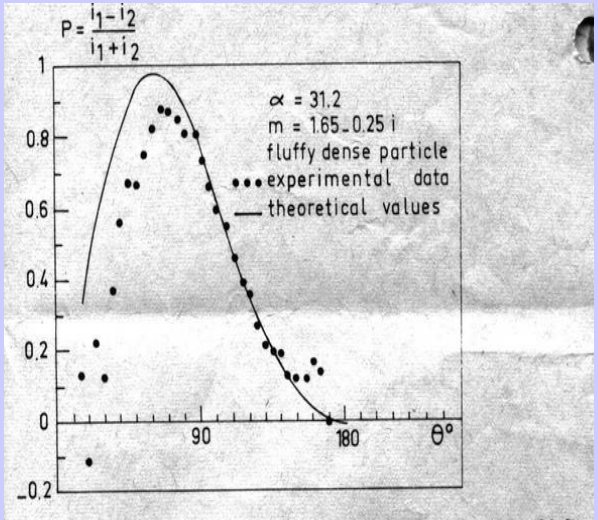


Fig. 8. Polarization P for a fluffy dense particle (α = 31.2, m = 1.65 − 0.25i)

Dust Particle Shape Models 4

- Bourrely et. al (1986) modeled roughness using a fractal description. They introduced deviations from a perfect sphere by adding smaller and smaller circles. There basic finding was that for large soft particles the roughness should result in rise in backscattering.

- They used in there calculations the EA. However, T-matrix can be used for exact calculations as these particles were considered spherically symmetric.

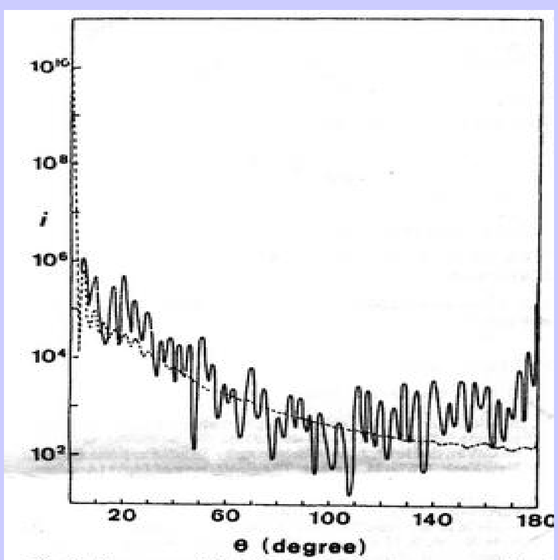


Fig. 7. The same as Fig. 6. Solid curve, surface corresponding tc Fig. 4; dashed curve, perfect sphere.

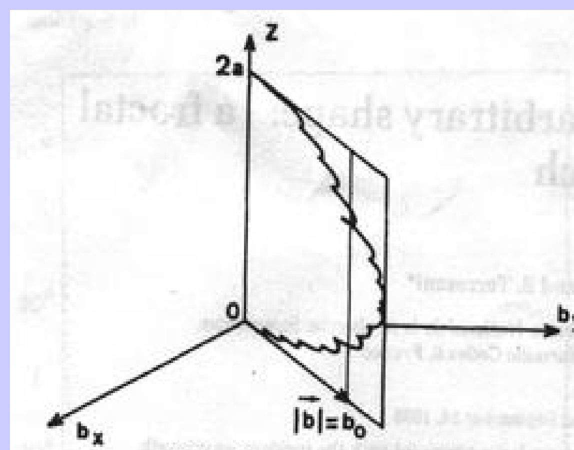


Fig. 1. Geometry of the problem.

In cylindrical coordinates, putting $\mathbf{r} = \mathbf{b} + \mathbf{e}_z \cdot z$, where $\mathbf{b}$ i the impact parameter, the scattering amplitude reads as

$$\rho = (\pi\, l / \lambda)\,(m - 1)$$

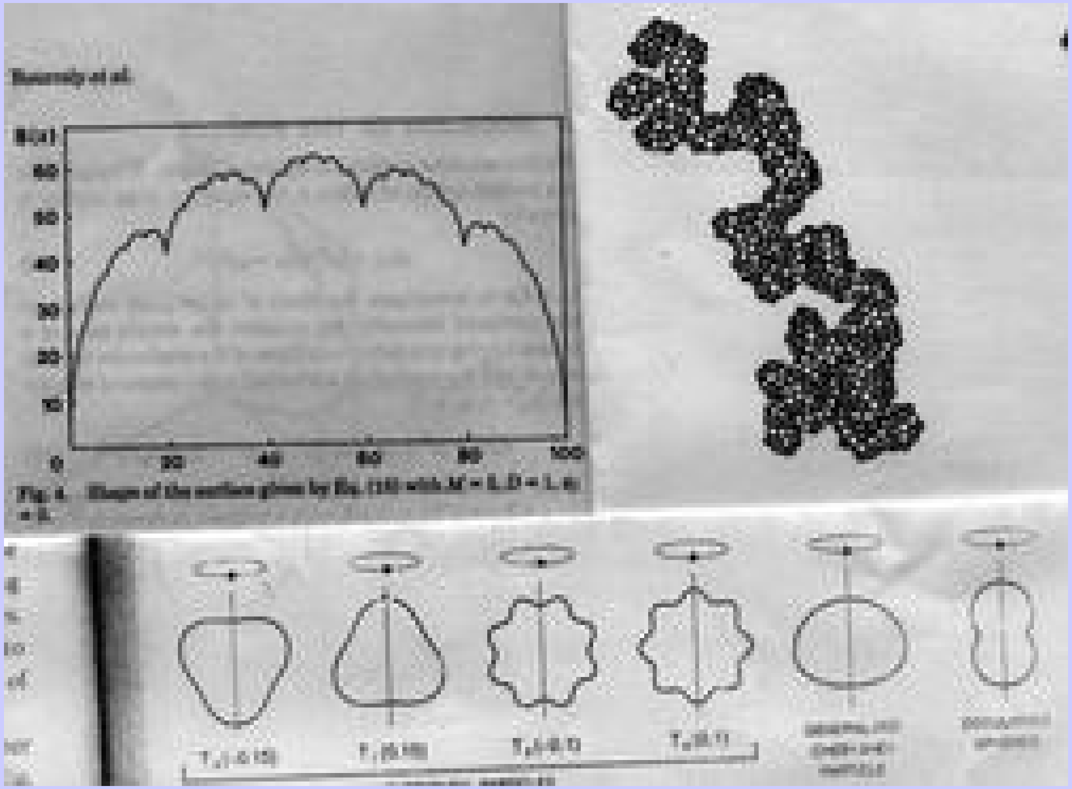
Dust Particle Shape Models 5

- Chebyshev Particles: These are obtained by continuously deforming a sphere by means of a Chebyshev polynomial of degree n (Wiscombe and Mugani 1986). Their shape is given by

$$r(\cos\theta) = R[1 + \zeta T_n(\cos n\theta)], \qquad |\zeta| < 1$$

where R is the radius of the unperturbed sphere, ζ is the deformation parameter and $T_n = \cos n\theta$ is the Chebyshev polynomial of degree n.

Rough Particles

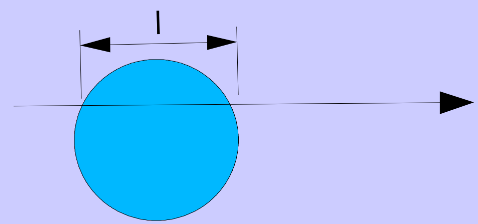


Anomalous Diffraction Approximation

- For large particles, the approximations become important. Anomalous diffraction or the eikonal approximation is one such method. $|m-1| \ll 1$

$$Q_{ext} = (2/P)\,\Re \iint dP\,[1 - e^{ikl\,(m-1)}]$$

$$Q_a = (1/P) \iint dP\,[1 - e^{-kln}]$$



Note the simplicity of expressions. Further, dividing the projected area into equal area elements and counting the geometric lengths, a probability function p(l)dl can be defined that gives the probability of length between l and l+dl. With this interpretation one can write:

$$Q_e = 2\,\Re \int [1 - e^{ikl\,(m-1)}]\,p(l)\,dl\,, \qquad Q_a = \int [1 - e^{-kln}]\,p(l)\,dl$$

Above expressions are essentially independent of size of the particle. Thus, in problems involving polydisperse particles computer resources required are much much less.

Inverse Scattering

- The idea here is to deduce size distribution from the extinction spectrum. For a given size parameter $x = ka = 2\pi a/\lambda$, and refractive index m :

$$K_{ext} = 2\pi N \int Q_{ext}(m, x)\, a^2 f(a)\, da$$

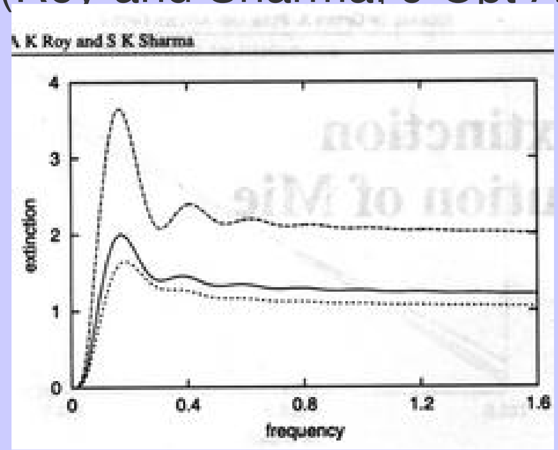
One way to invert this equation is to choose and try appropriate $f(a)$. But this does not guarantee a Unique solution. For example, there are at least fifteen dust models that differ in composition and size distribution but simultaneously satisfy the local extinction, infrared emission and abundances constraints. Second way is to use approximate expressions for extinction efficiency. For example, if we use

$$Q_{ext}(ADA) = 2\left(1 + \frac{2}{\rho^2}\right) + 2\left(2\frac{\pi}{\rho}\right)^{1/2} J_{-3/2}(\rho) \qquad \rho = (\pi d/\lambda)(m-1)$$

for a Mie particle in the equation for K_{ext} it is possible to invert it analytically. It is also possible to use the mean value theorem of the integral calculus and determine the key parameters of the distribution and then construct the distribution (Roy and Sharma, Appl. Opt. 1997) .

Inverse Scattering

- We have recently considered the inversion without employing any approximation. For the case of monomodal distribution of Mie particles, we have demonstrated that an extinction spectrum, in general, has some easily identifiable regions where the extinction-frequency relationship can be approximated by simple formulae involving the first four moments. EXAMPLE: Linear Growth can be expressed as (Roy and Sharma, J Opt A: Pure and App Opt. 7 (2005) 675)



$$K_{ext} = 2\pi N [A\nu - B]$$

Naïvely, such a form is possible only if

$$Q_{ext} \sim l_1 (\nu a) - l_2$$

and thus,

$$K_{ext} = 2\pi N [l_1 \nu \overline{a^3} - l_2 \overline{a^2}]$$

l_1, l_2 depend only on m and may be determined using any standard distribution.

QUESTION: Can the same analysis be redesigned for application to the well known extinction curve for interstellar dust? There are two differences here from our earlier analysis. 1. We now have mltimodal distributions and 2. The refractive index varies with wavelength.

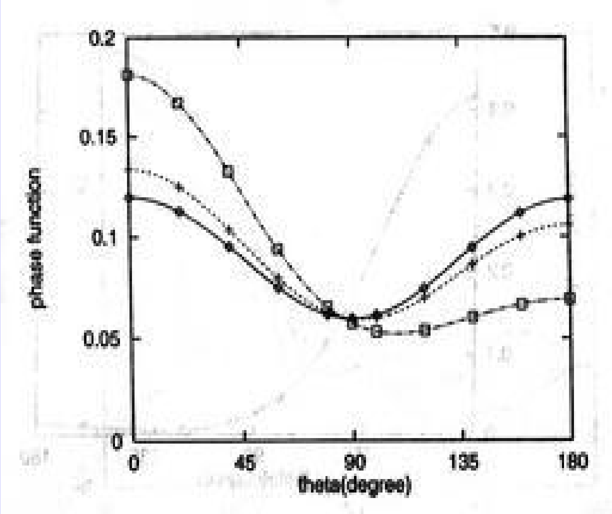
Parametric Phase Function

- One of the Importance of phase function is in the solution of radiative transfer equation. Henyey Greenstein phase function and modifications.

- In an earlier work (Sharma , Roy and Somerford JQSRT 60 (1998) 1001), we showed that the phase function for the scattering by a small particle can be expressed as :

$$P(\theta) = a_0 + a_1 \cos\theta + a_2 \cos^2\theta + a_3 \cos^3\theta + a_4 \cos^4\theta ,$$

where $a_{0,} a_{1,} a_{2,} a_{3,} a_4$ can be expressed in terms of $P(0), P(\pi/2), P(\pi)$ and slope of the phase function at $\pi/2$ or the asymmetry parameter g.



$$x < 2 ; \quad g < 0.6$$

For a maximum particle size in dust to be 0.2 micron, the maximum size parameter at wavelength 6000 A is about $x = 1$

Parametric Phase Function

- Possible use of this phase function for radiative transfer calculations was discussed by us (Sharma, Shah and Somerford, J Opt (India) 28 (1999) 123). However, we did not made any specific dust calculations. Phase functions calculated by Draine (2003) for Milky way dust clearly show the desirability of use of this phase function.

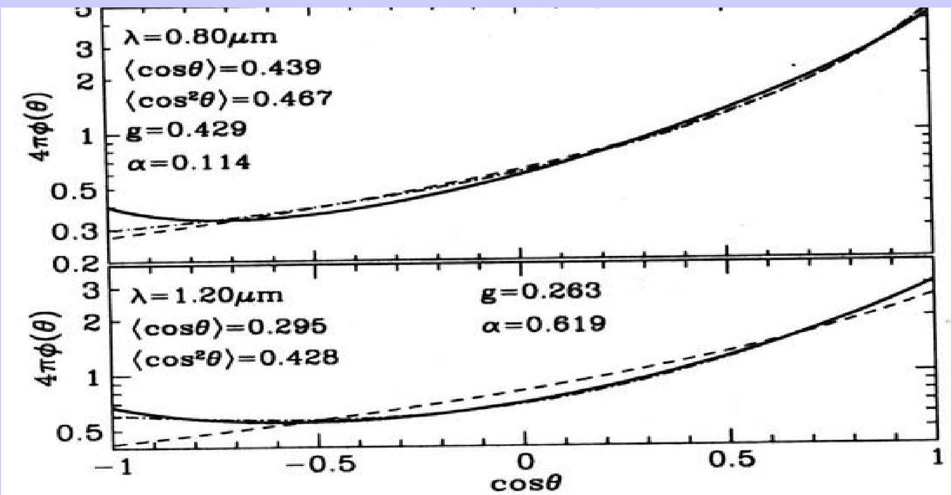


FIG. 6.—Scattering phase function for the WD01 Milky Way dust model at three wavelengths (*solid lines*) compared with the Henyey-Greenstein phase function ϕ_0 and our new phase function $\phi_{\alpha\leq1}$. For $\lambda = 0.4\ \mu m$ a nine-term Legendre polynomial representation is also shown.

Parametric Phase Function

- Another possible use of this phase function could be to obtain size distribution in the ensemble. For this purpose what we have do is that we parametrize

$$P(0) = \alpha + \beta x + \gamma x^2 + \delta x^3 + \epsilon x^4$$

Similarly we also parametrize phase function at other angles and write

$$P(\theta) = A_0 + A_1 x + A_2 x^2 + A_3 x^3 + A_4 x^4$$

where A_0, A_1, A_2, A_3, A_4 are independent of x. For` a distribution of particle sizes, one can therefore write:

$$\phi(\theta) = C_0 + C_1 \bar{x} + C_2 \overline{x^2} + C_3 \overline{x^3} + C_4 \overline{x^4} \qquad \overline{x^n} = \int x^n f(x)\, dx$$

Employing this equation, it is straightforward to calculate moments of the distribution and hence the distribution itself.

Summary

- The presentation I have made can be summed up as follows:
- 1. We made a survey of Exact and Approximate methods for light scattering by a single isolated particle suitable for shapes used in dust modelling.
- 2. We outlined some theoretical extinction and phase function analyses in a general set up. These with appropriate situation specific details can be used to good effect in the context of dust.