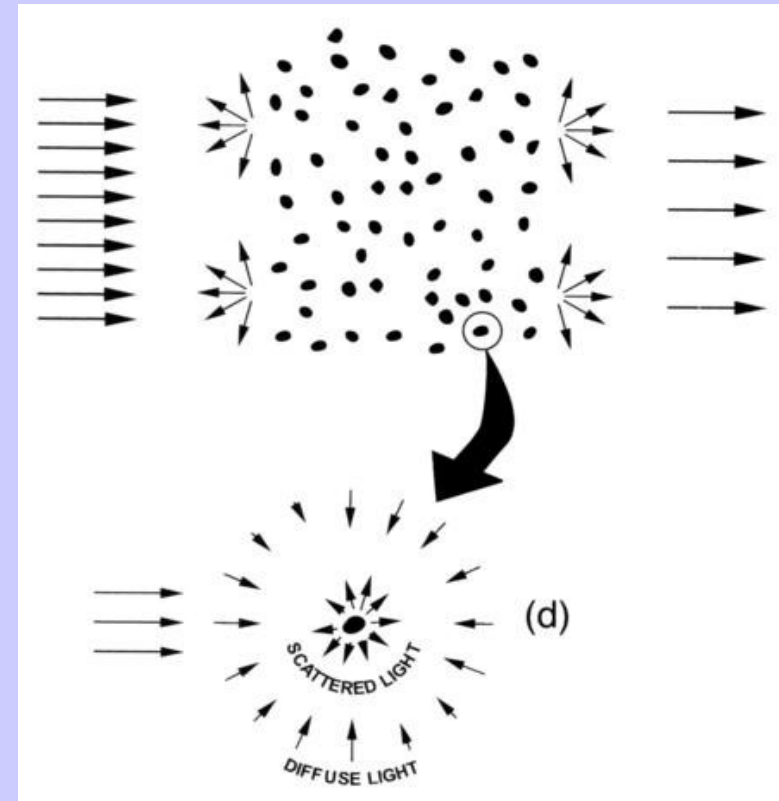
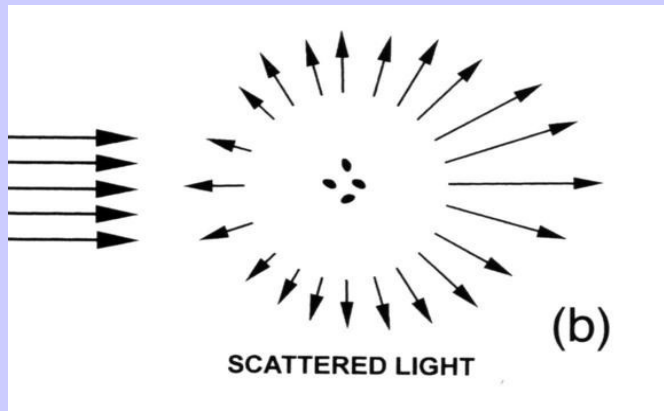
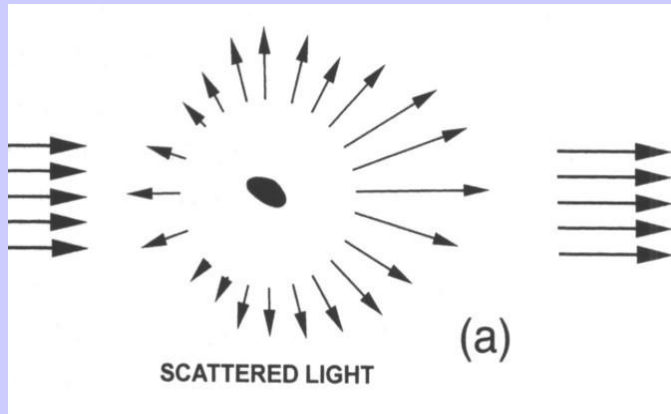


# ***Analytic formulas for frequency and size dependence of absorption and scattering efficiencies of PAHs***

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# *Introduction to general scattering problems of interest*



While dealing with astrophysical situations, one is often interested in (b). Here from the extinction (scattering+absorption) one attempts to infer properties of dust particles.

# *Extinction spectrum*

The extinction spectrum, which is essentially a measure of radiation removed from the incident beam by absorption and scattering, by such a collection can be employed to characterize the scatterers. Expressed mathematically, the extinction from a dilute collection of particles is,

$$K_{ext}(m, \nu, a_0, a_m) = \pi N \int_{a_0}^{a_m} Q_{ext}(m, ka) a^2 f(a) da$$

where  $N$  is the number of particles,  $Q_{ext}$  is the extinction efficiency of a single scatterer of radius  $a$  and refractive index  $m$  when the light of wavenumber  $k$  is incident on the particle. The probability of obtaining a particle in the size range  $a$  and  $a+da$  is  $f(a)da$ .

# *Extinction efficiencies of a homogeneous sphere*

For the simplest shape ( homogeneous spheres), the extinction from a single isolated particle can be expressed as:

$$Q_{ext} = \sum_n (2n+1)(a_n + b_n)$$

$$a_n = \frac{\psi_n'(y)\psi_n(x) - m\psi_n(xy)\psi_n'(x)}{\psi_n'(y)\zeta_n(x) - m\psi_n(y)\zeta_n'(x)}, b_n = \frac{m\psi_n'(y)\psi_n(x) - \psi_n(y)\psi_n'(x)}{m\psi_n'(y)\zeta_n(x) - \psi_n(y)\zeta_n'(x)}$$

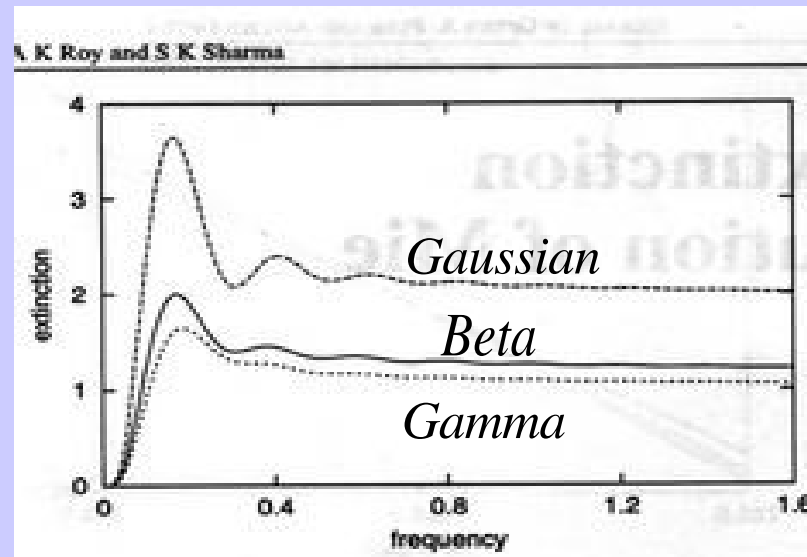
$$x = \frac{\pi d}{\lambda} = ka, y = mx$$

Clearly, even for this simplest shape, complexity of solutions does not allow any physical insight into the solution of the problem for a collection of particles.

This prompted us to look for simple analytic formulas for the extinction spectrum which give more physical insight and provide a quick and efficient method for computation of extinction spectrum.

# *Inverse Scattering (Spheres)*

Figure below shows typical shape of extinction spectra for three distinct classes of monomodal distributions of Mie particles.



It was demonstrated that, in general, the spectra have some easily identifiable regions where the extinction-frequency relationship can be approximated by simple formulas involving the first four moments.

( A K Roy and S K Sharma, A simple analysis of of extinction spectrum of a size distribution of Mie particles, J Opt 7A (2005) 675)

# Formulas for extinction by graphite and silicate grains

Logical Question : What if the refractive index of scatterer varies with wavelength ?

We studied the extinction spectrum produced by silicate and graphite grains described in the MRN model.

$$f(a) \propto a^{-3.5} \quad a_0 \leq a \leq a_m$$

A careful study of  $K_{ext}$  reveal that it can have the general form

$$K_{ext} \propto N a_0^{5/2} [\phi(a_0, \nu) + \psi(a_m, \nu)]$$

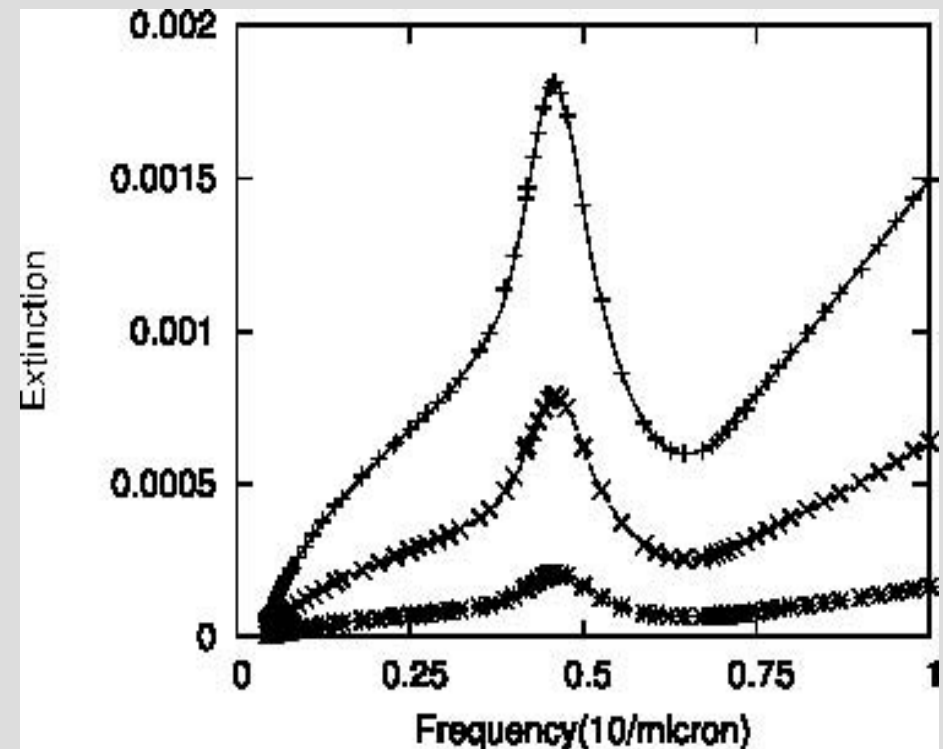
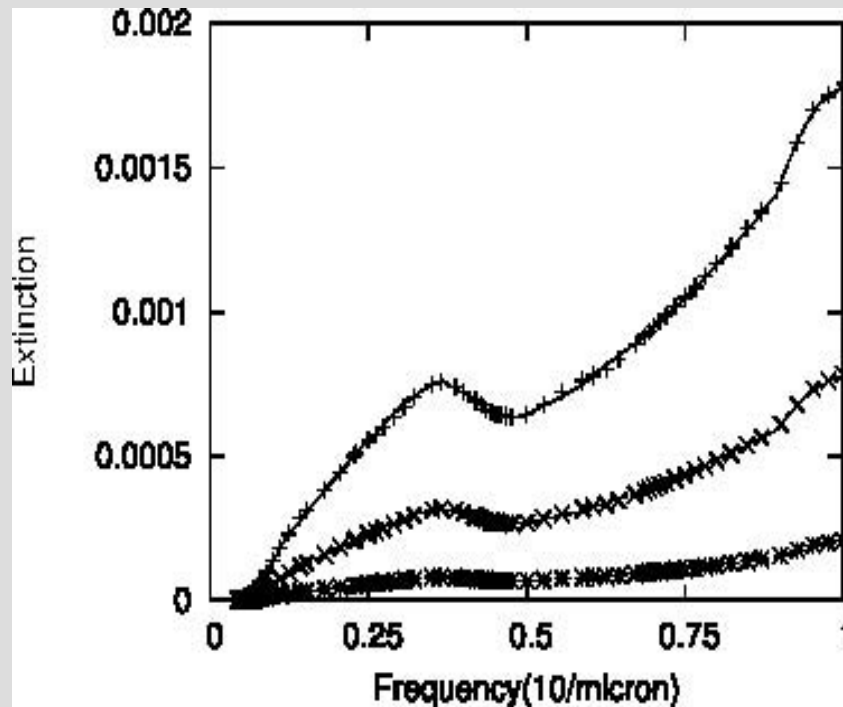
The functions  $\phi$  and  $\psi$  have forms which change in various frequency sub-intervals (1000 – 22,500 Å). Validity range

$$0.002 \leq a_0 \leq 0.005, \quad 0.15 \leq a_m \leq 0.25 \quad \mu m \quad (\text{graphite})$$

$$0.004 \leq a_0 \leq 0.006, \quad 0.2 \leq a_m \leq 0.4 \quad \mu m \quad (\text{silicate})$$

AKR, SKS and RG JQSRT 110 (2009) 1733; 111 (2010) 795

# Inversion from extinction spectrum: Interstellar dust



Graphite parallel max radius,      Graphite parallel max rad=0.25 micron  
Min radius =0.005 (upper),      =0.0035 (middle), =0.002 (lower)  
Max error < 3 percent

# Extinction by polycyclic aromatic hydrocarbons: PAHs

It is now recognized that carbonaceous component has a sub-component of “very small grains” whose optical properties are different from that of graphite. These are the so called PAHs.

On the basis of some laboratories studies and astronomical observations, Li and Draine (ApJ 554 (2001) 778) computed absorption and scattering efficiencies of PAHs of sizes 3.5-100 Å.

In reality, however, the PAHs in the size range 5-50 Å have been taken as major contributors as far as the extinction is concerned. Thus, for the present, we have restricted ourselves to this range.

The problem here is to parametrize the absorption and scattering efficiencies of PAHs and not their extinction coefficient. Note the difference from silicate and graphite parametrization

# Absorption efficiencies of PAHs

For absorption, the wavelength range was divided in five regions.

- 1. Far ultraviolet 1000-1800 Angstrom
- 2. Ultraviolet 1800-4000 Angstrom
- 3. Visible 4000-8000 Angstrom
- 4. Infrared-I 8000-12,500 Angstrom
- 5. Infrared-II 12,500-22,500 Angstrom

Barring region 4, one formula was possible in entire 5-50 A size range. Infrared-I required two formulas 5-10 and 10-50 Angstrom.

# Absorption efficiencies of PAHs

As the effective size of PAHs is small in comparison to the wavelength, the formulas for the absorption efficiency, obtained here are generally of the form

$$Q_a = x (A + Bx^2 + Cx^3 + \dots)$$

This is in agreement with the power series expansion in size parameter of Mie results. A typical formula is ( $1800 \leq \lambda \leq 5000 \text{ \AA}$ )

$$Q_a = x \left[ \frac{1.19}{\nu} - 3.99 \left| 1.0 - \frac{0.462}{\nu} \right| + \frac{1}{0.74 \nu + 83 \nu \left( 1 - \frac{0.46}{\nu} \right)^2} \right] \equiv x \phi(\nu)$$

In the region 4 (Infrared-I), the molecular structure of PAHs become vital for the absorption and hence absorption efficiency does not seem to follow the above expression.

# Absorption formulas of Li and Draine

For  $\lambda \geq 3000 \text{ \AA}$  ,

$$Q_a = \frac{a}{\pi} (1286)^2 \left[ 34.58 * 10^{-18-3.431/x} \text{cutoff}(\lambda, \lambda_c) + \sum_{j=3}^{14} S_j(\lambda) \right]$$

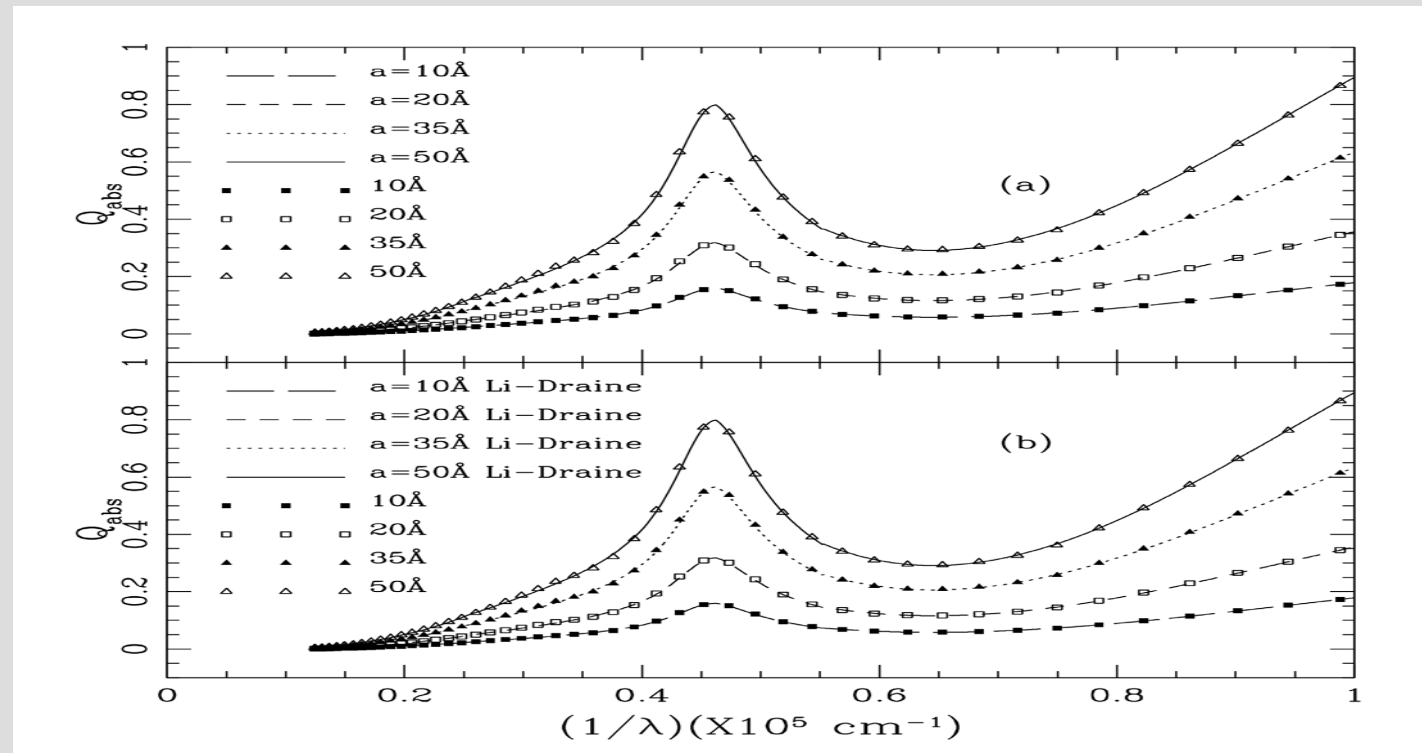
with  $x = 1/\lambda$  . The formula is modeled around many appropriate Drude absorption profiles

$$S_j(\lambda) = \frac{2}{\pi} \frac{\gamma_j \lambda_j \sigma_{n,j}}{(\lambda/\lambda_j - \lambda_j/\lambda)^2 + \gamma_j^2}; \quad \sigma_{n,j} = \frac{\pi}{2} S_j(\lambda_j) \gamma_j \lambda_j^{-1}.$$

$$\text{cutoff}(\lambda, \lambda_c) = \frac{1}{\pi} \arctan \left[ \frac{10^3 (y-1)^3}{y} \right] + 0.5, \quad y = \lambda_c / \lambda$$

where the cutoff wavelength depends on the PAH radius in a complex manner.

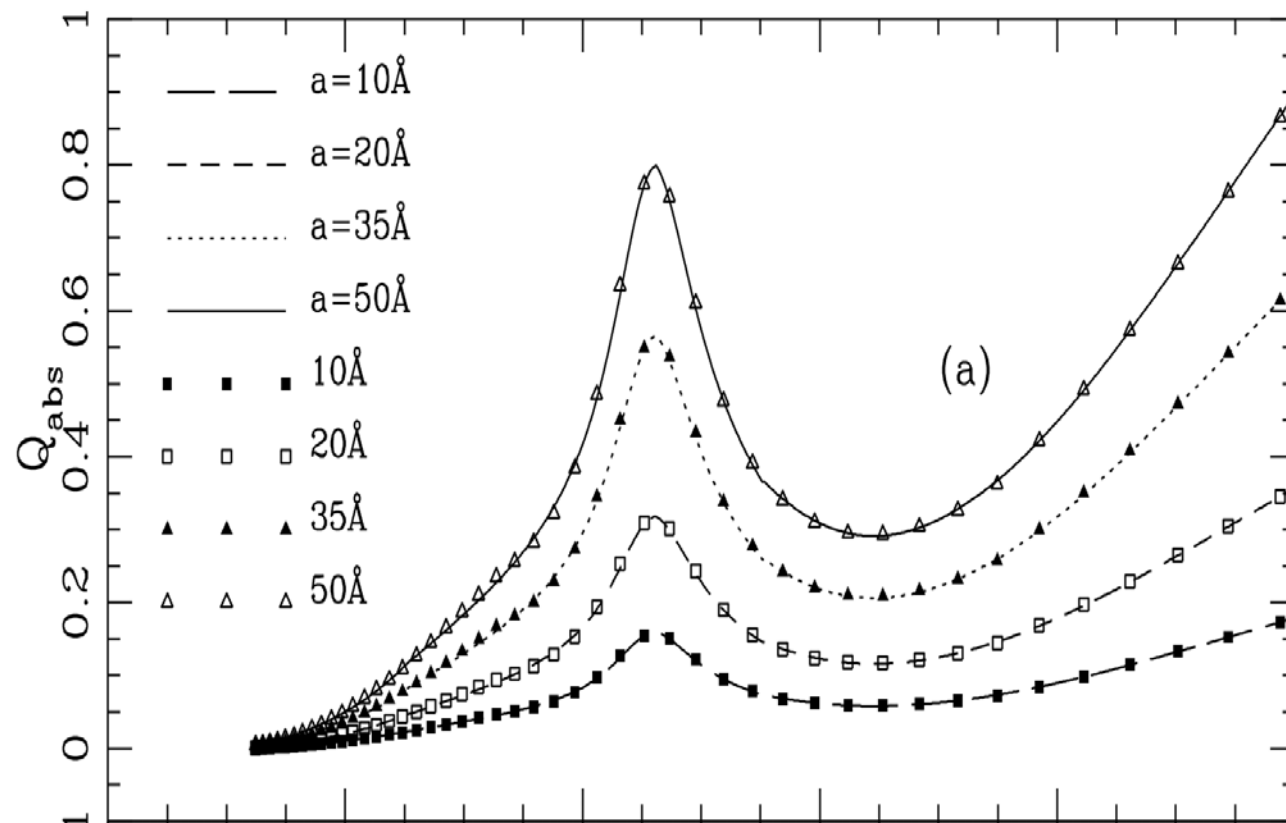
# Comparison of formulas for absorption efficiency



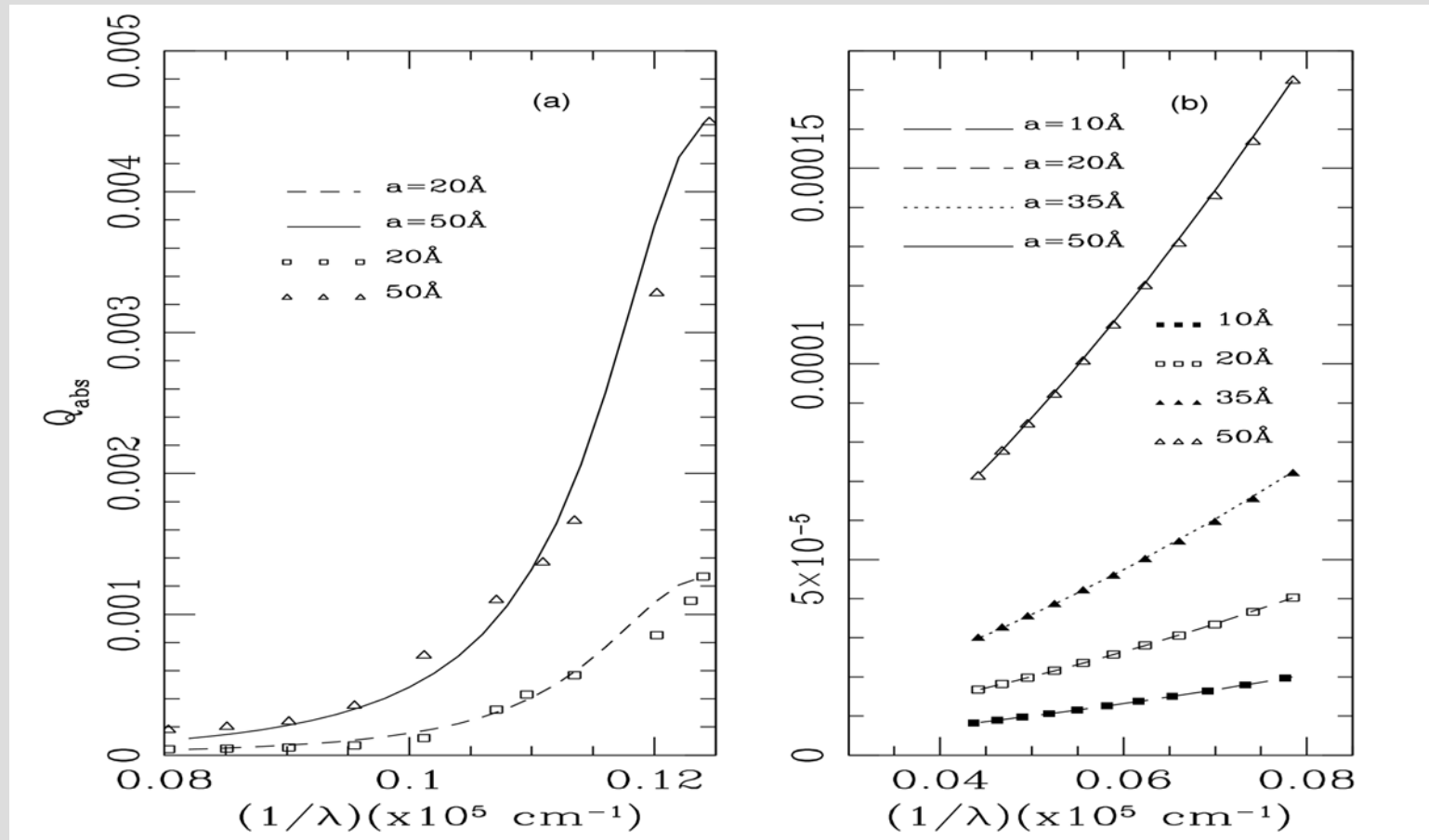
Frequency range 1000-8000 Angstrom

# Comparison of formulas for absorption efficiency

Frequency range 1000-8000 Angstrom



# Comparison of formulas for absorption efficiency



Frequency range 8000-12,500 A and 12,500-22,500A

# Absorption efficiencies of ionic PAHs

1. In the FUV and UV regions, the absorption efficiencies of ionic and neutral PAHs are identical.
2. They, however, differ in visible and infrared regions.
3. The agreement with Draine's tables is as good as in the case of neutral PAHs.

# Scattering efficiencies of PAHs

As the effective size of PAHs is small in comparison to the wavelength of radiation, the formulas for the scattering efficiency, obtained here are generally of the form

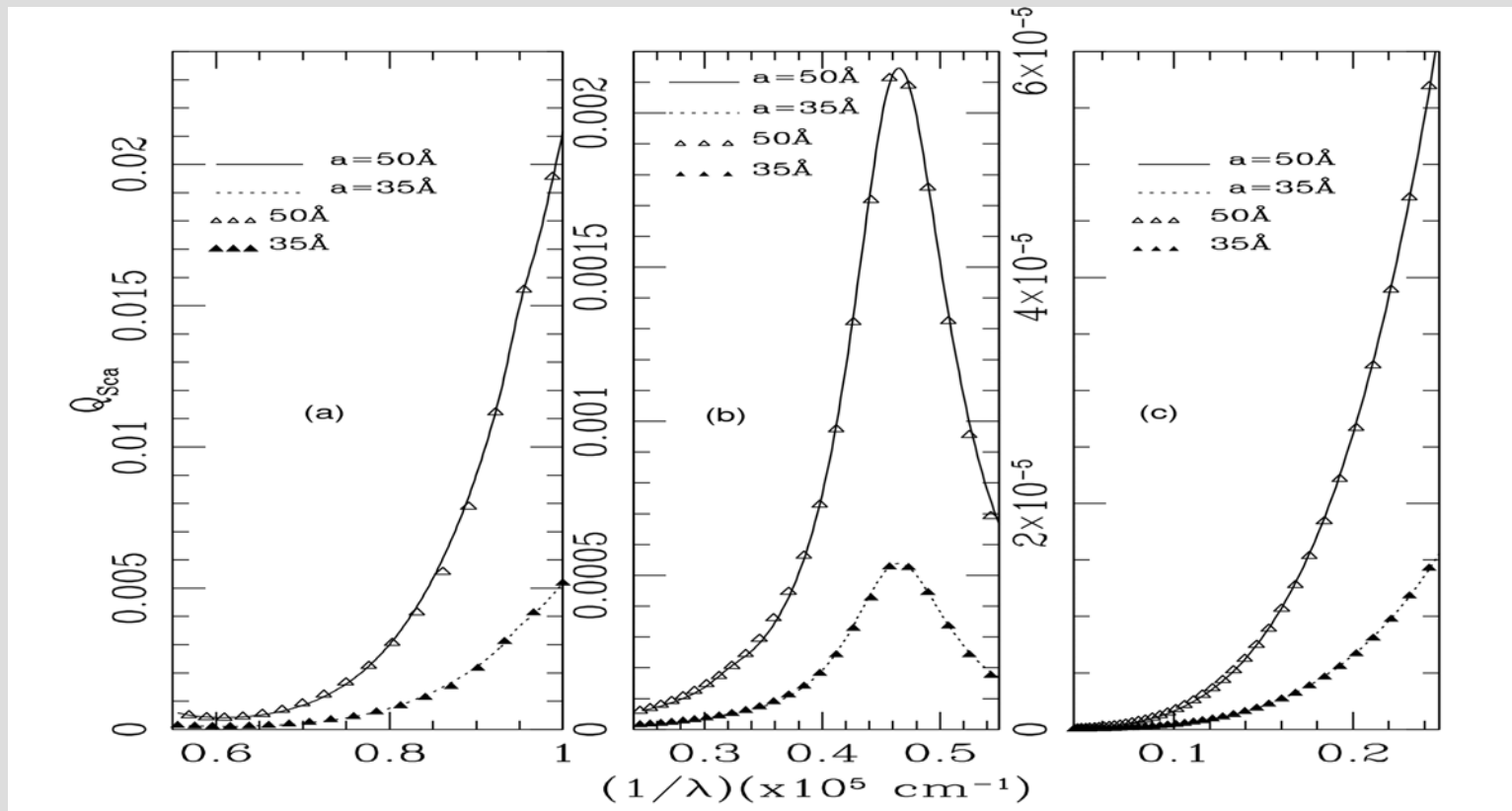
$$Q_s \sim x^4 (D + Ex^2 + Fx^2 + \dots)$$

which is in agreement with the general expression for scattering efficiency, as a power series in size parameter of Mie solution. As an example, our finding is

$$S_{sca} = 1.66x^4$$

in the range  $4000 \leq \lambda \leq 22,500 \text{ \AA}$

# Comparison of formulas for scattering efficiency



Frequency 1000-1800 A, 1800-4000 A, 4000-22,500 A

# Extinction spectral features of PAHs

Having obtained the formulas for PAHs extinction , as an example of the plausibility of use of these formula we generate extinction spectrum in UV and FUV region and compare it with the extinction spectra generated by equal volumes of other two carbonaceous components viz., graphite (perpendicular) and graphite (parallel). In this wavelength region

$$Q_{ext}^P = x \phi(\nu)$$

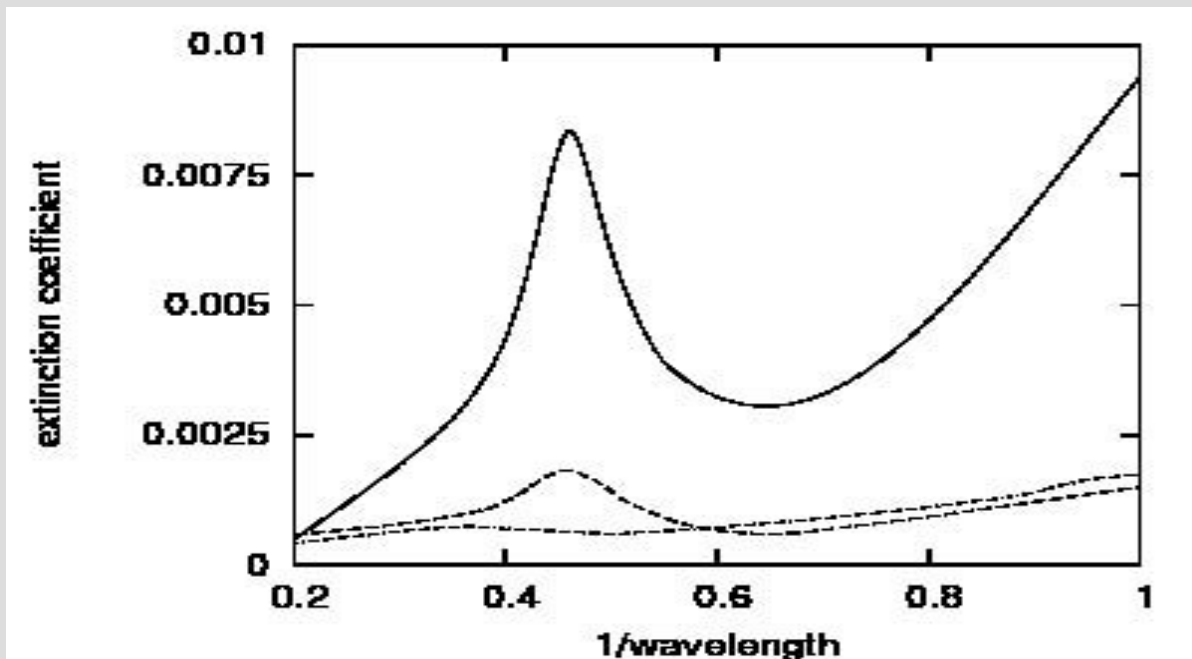
Corresponding expression for extinction spectrum is given by the simple form

$$K_{ext}^P(\nu) \propto N_P \int_{a_0}^{a_m} Q_{ext}^P a^2 f(a) da = N_P \phi(\nu) \int_{a_0}^{a_m} a^3 f(a) da = V_P \phi(\nu),$$

In other wavelength regions, however, the extinction spectra would be dependent on size distributional details in a more involved way rather than being simply proportional to volume.

# Extinction spectral features of PAHs

Comparison of extinction spectra for PAHs is with the extinction spectra generated by equal volumes of other two carbonaceous components viz., graphite (perpendicular) and graphite (parallel) for a population specified by  $N_p$ ,  $f(a)$  and  $V_p$



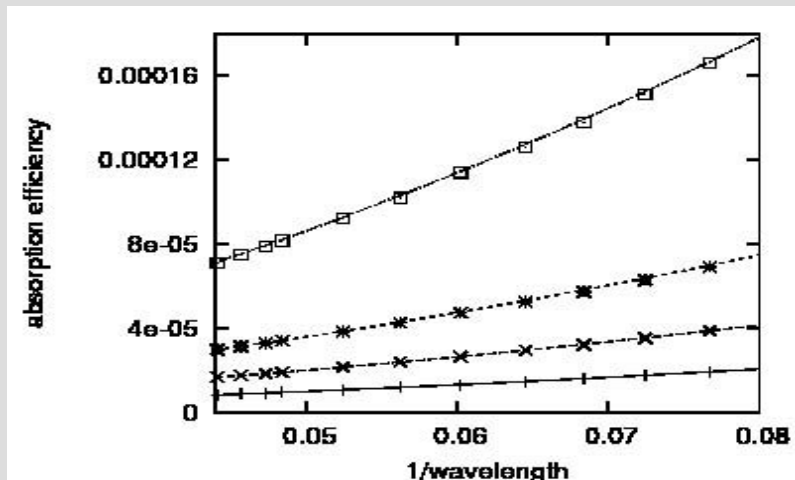
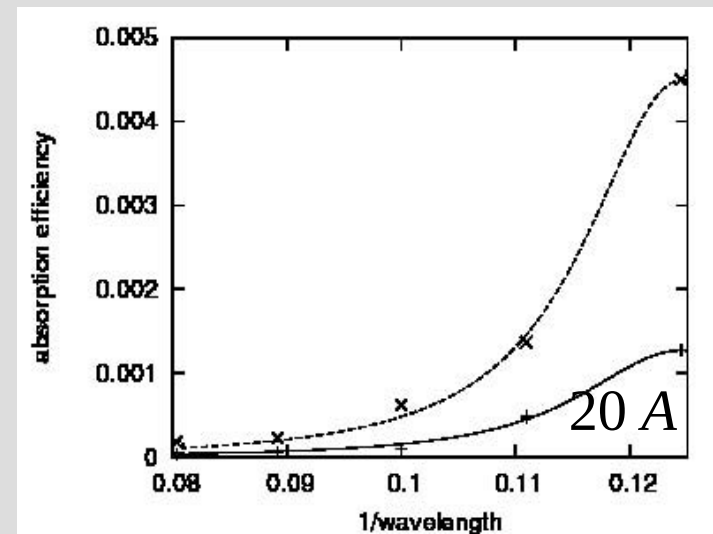
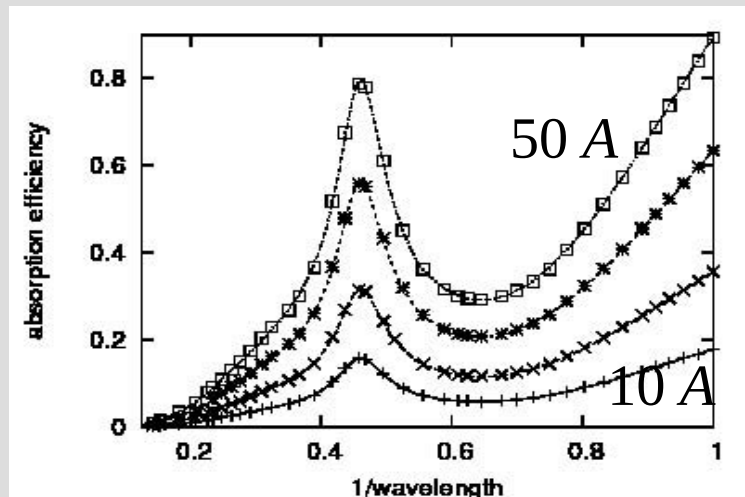
1. solid (PAHs)
2. dash- perp
3. dot- parallel

# Summary and conclusions

1. We have analyzed the extinction spectra of PAHs and obtained formulas for scattering and absorption efficiencies in terms of the size of the PAH and wavelength of the radiation.
2. This work, together with our earlier work, completes our search for a platform for interstellar dust extinction spectra analysis which employ MRN type dust models.
3. Our formulas appear to be quite accurate yet considerably simpler than expressions constructed by Li and Draine (2001)
4. It will be our future endeavor to use this framework for the analysis of extinction data corresponding to MW, LMC, SMC.
5. Exploring possibility of distorting spheres to spheroid such that extinction remains same but required ,polarization is produced?

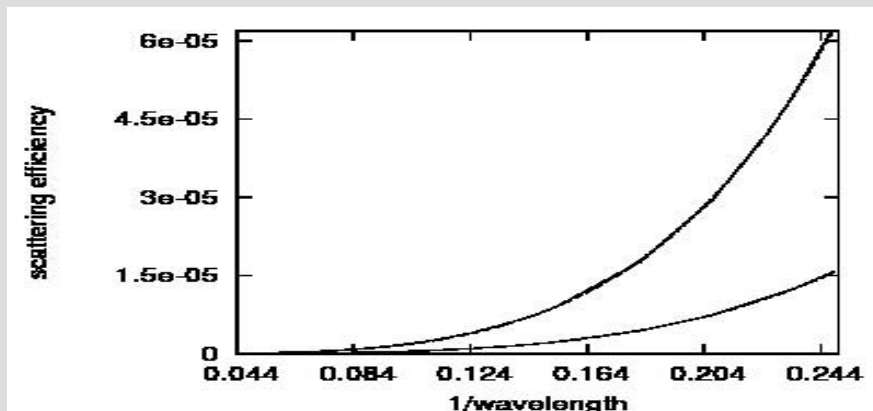
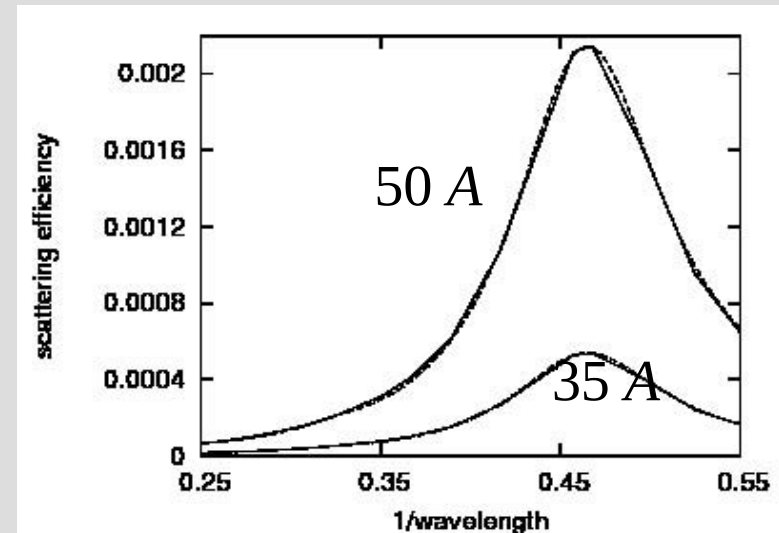
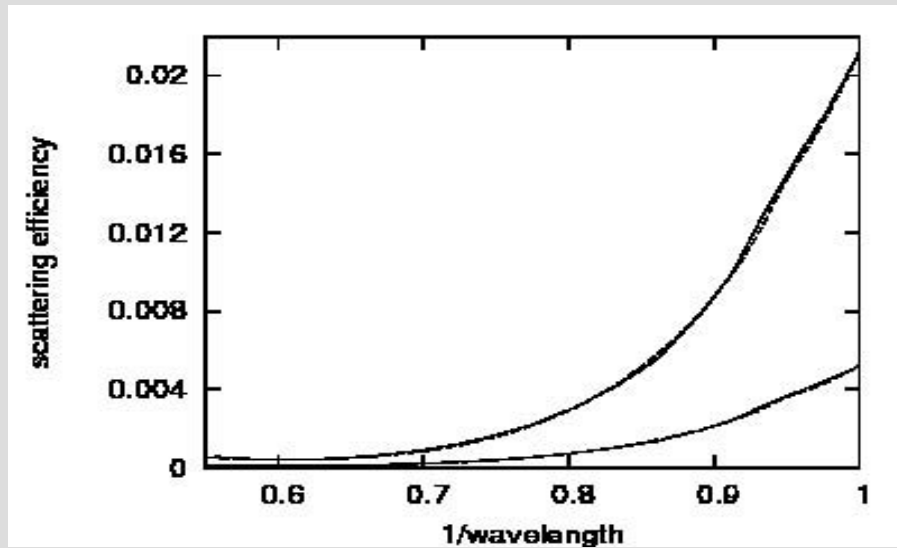
**THANK YOU**

# Comparison of formulas for absorption efficiency



1. 1000-1800 A
2. 8000-12,500 A
3. 12,000 -22,500 A

# Comparison of formulas for scattering efficiency



1. 1000-1800 Å
2. 1000-4000 Å
3. 4000-22,500 Å