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OPTICAL PROPERTIES OF IRREGULAR INTERSTELLAR GRAINS

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ABSTRACT

In order to study the interaction of light with interstellar grains, we represent an irregular particle by a network of interacting dipoles whose polarizability is determined in a first approach by the Clausius-Mossotti relationship. Typically, 10000 dipoles are considered. In the case of spherical particles, the results from Mie theory are fully recovered. The main interest of this method is to study with a good accuracy the implications of surface roughness and/or inhomogeneities on optical properties in the infrared spectral range, particularly of the silicate emission features.

INTRODUCTION

Small dust particles are known to play an important role in the interstellar extinction process, but the nature of the grains and the mechanism of interaction with light are still a matter of debate. If various models of interstellar grains have been published for the last two decades (see the reviews of Mathis, 1986 and Tielens and Allamandola, 1987) none of them is able to explain the totality of the spectral features observed in the interstellar medium from the far ultraviolet to the far infrared (Mathis et al, 1977 ; Greenberg and Chlewicki, 1983 ; Greenberg and d'Hendecourt, 1985).

So a careful study of the interaction between dust and light must be conducted. When the size of the dust particle is lower than

the wavelength of the incident light, which is the case for interstellar dust particle in the infrared spectral range, approximations are used, such as the Rayleigh theory (see for example, Bohren and Huffman, 1983) to obtain extinction, absorption and scattering cross sections as well as the scattering diagram. However this approximation cannot always be used (see for example Perrin and Lamy, 1981 ; Draine and Lee, 1984) since there exists a condition on the imaginary part of the refractive index in addition to the well-known condition that the particle is small w.r.t. the wavelength. In order to study the interaction of infrared light with interstellar dust, in a general way, we first show that the classical electrodynamic equations permit to represent a dust particle by a network of interacting dipoles as first proposed by Purcell and Pennypacker (1973). We then compare the values of the extinction cross section obtained by this method and the Mie theory (Mie, 1908) for a small, homogeneous spherical dust particle of silicate in the mid-infrared spectral range [5 - 15 μm]. Finally we use this method to study the variations to extinction introduced by fluffy particles of the same mass as the spherical one.

THE ELECTROMAGNETIC FIELD SCATTERED BY INTERACTIVE DIPOLES

We consider a dust particle with no free charge, no currents and no magnetic susceptibility and which may be composed of a inhomogeneous material of complex index of refraction $n(\vec{r})$. The electromagnetic field \vec{E} (with harmonic time dependence) interacting with the particle is solution of equations from classical electromagnetic theory :

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) - k^2 \vec{E} = k^2 [n^2(\vec{r}) - 1] \vec{E}$$

where $k = 2\pi/\lambda$ and λ is the wavelength of the incident light.

Let us represent the dust particle by a discrete collection of dipoles ; then

$$n^2(\vec{r}) = 1 + 4\pi \sum \alpha_i \delta(\vec{r} - \vec{r}_i)$$

where α_i and \vec{r}_i are respectively the polarizability and the position vector of the i^{th} dipole (in the case of an anisotropic material, the method remains valid but $n(\vec{r})$ must simply be represented by a

tensor). The scattered field is the sum of the field created by each individual dipole whose electric dipole moment \vec{d}_i is induced by the incident light and of the fields radiated by all other dipoles. When the dipoles are located at the nodes of a cubic "lattice", this method generalizes that of Purcell and Pennypacker (1973). To obtain the value of the scattered field at a point \vec{r} far away from the particle (w.r.t. the wavelength), we first calculate the dipole moment \vec{d}_i at each site :

$$\vec{d}_i = \alpha_i \vec{E}(\vec{r}_i)$$

Then the total scattered field in the direction of observation defined by the unit vector \vec{u} is found to be

$$\vec{E}_s(\vec{r}) \simeq k^2 \frac{e^{ikr}}{r} \sum \exp(-ik \vec{r}_i \cdot \vec{u}) (\mathbf{1} - \vec{u} \otimes \vec{u}) \vec{d}_i$$

The dipole moments \vec{d}_i may be obtained by solving a set of $6N$ (N = number of sites) linear equations (Shapiro, 1975).

Even with supercomputers, there is a limit to the number of dipoles which may be handled (inversion of a $6N \times 6N$ matrix). Iterative methods should be considered, as first proposed by Purcell and Pennypacker (1973) ; however as their convergence process is not always satisfied, we prefer to use the Born expansion series whose physical interpretation theoretically insures the convergence (Chiappetta, 1980 ; Chiappetta et al., 1987).

The extinction cross-section is given by the optical theorem (e.g., Born and Wolf, 1964) while the absorption cross-section follows from the formulation given for instance by Jackson (1962).

COMPARAISON WITH MIE THEORY

Using the Mie theory, we calculate the extinction cross-section of a sphere of silicate of radius $0.05 \mu\text{m}$ (Fig.1a) whose complex index of refraction in the spectral range $5\text{-}15 \mu\text{m}$ is given by Draine (1985). We now consider a cubic lattice inscribed in the same sphere such that there are 25 nodes or dipoles on a diameter. Therefore, each dipole represents a local volume whose size is $0.002 \mu\text{m}$. From

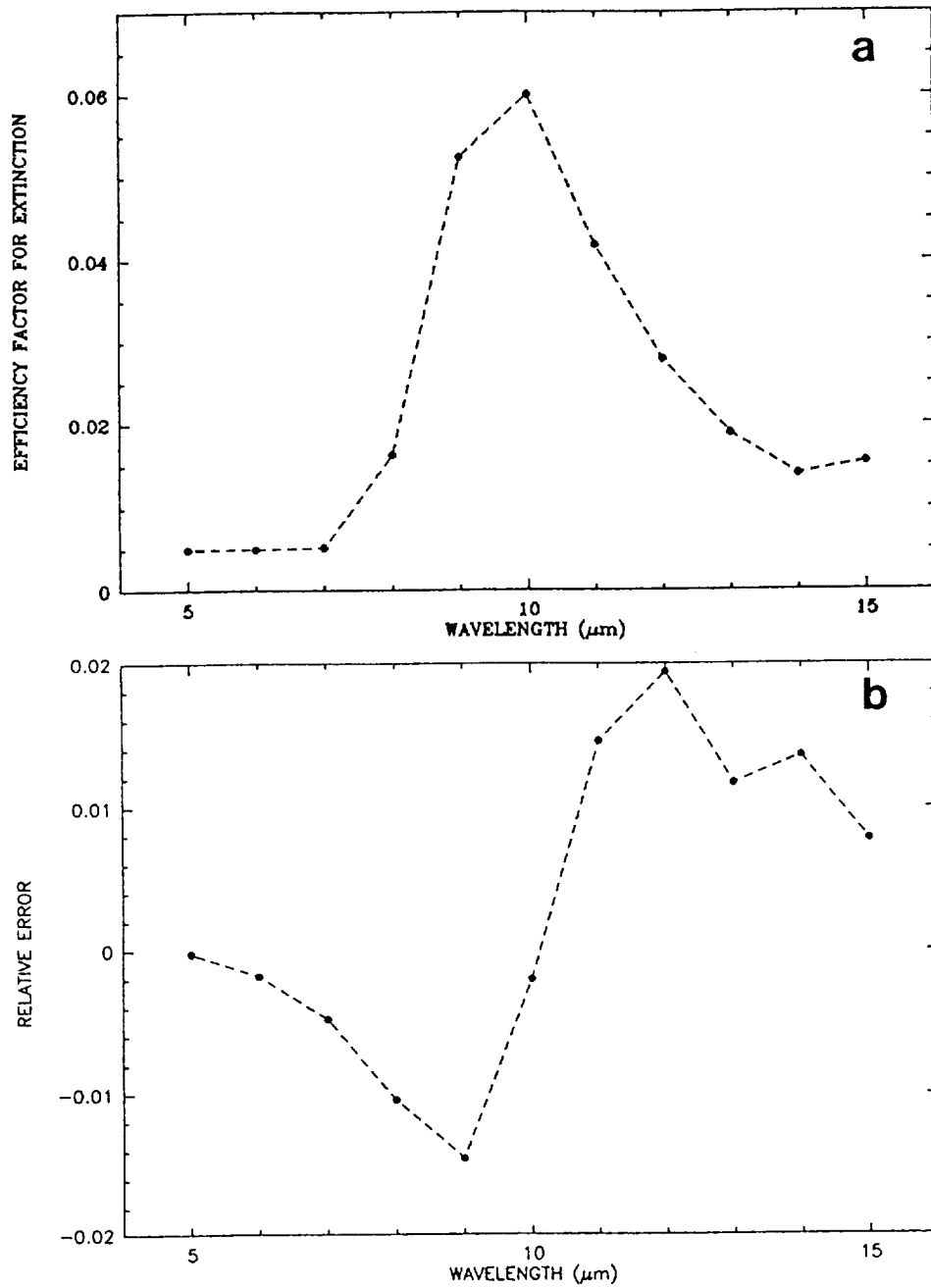


Fig. 1 : a) The efficiency factor for extinction obtained for a sphere using the Mie theory
 b) Relative error between the dipole model and the Mie result for the same sphere

the point of view of the classical electrodynamic theory (i.e., from the macroscopic point of view), this local volume is the point source of the scattered field. In the present state of physico-chemical studies, at least 1000 atoms seem to be required to obtain bulk properties (e.g., Buffat and Borel, 1976). So only dust elements whose radii are $> 0.001 \mu\text{m}$ can be studied as bulk, solid particles. Smaller particles must be considered as clusters of atoms or molecules and their optical properties cannot be described by a complex index of refraction (i.e. a macroscopic parameter).

In the present case, our sphere is homogeneous (for comparison with the Mie theory) the polarizability is the same for each dipole ; in a first stage, we define it from the Clausius-Mossotti relationship. Fig.1b gives the difference between the Mie and the present calculations of the extinction cross-section using the interactive dipoles model with the third order Born expansion series.

The maximum deviation resulting from this low order approximation is less than 2 % and illustrates well the validity of the proposed model.

IRREGULAR AND FLUFFY PARTICLES

We now consider an irregular, "fluffy" particle which contains the same number of dipoles as the spherical particle described in the previous section (i.e., same mass) located on a similar network (same spacing). Several sites are left vacant to create voids in the particle, the available dipoles being distributed on the external surface to make it irregular. Cross-sections of the two particles are given in Fig.2 to illustrate this process. The resulting roughness has a maximum amplitude equals to one third of the radius of the original spherical particle. We now compare in Fig.3 the efficiency factors for extinction of the two particles in the spectral range 5-15 μm . As it seems that the intrinsic error resulting from the dipole model at a given wavelength only depends on the total number of dipoles used in the calculation, the differences between the two particles are free of this type of error and therefore reflect the true effect of irregularity and fluffiness : a systematic decrease, by a factor of at least 10 % which depends upon the wavelength (henceforth, a color effect) ; in particular, the silicate "bump" is attenuated.

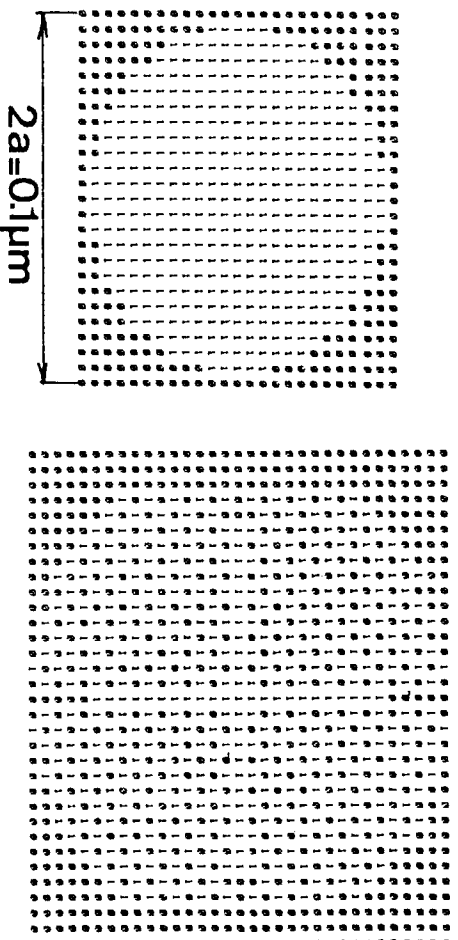


Fig. 2 : Geometrical sections of the two particles studied here : the sphere (left) and the irregular, fluffy particle (right)

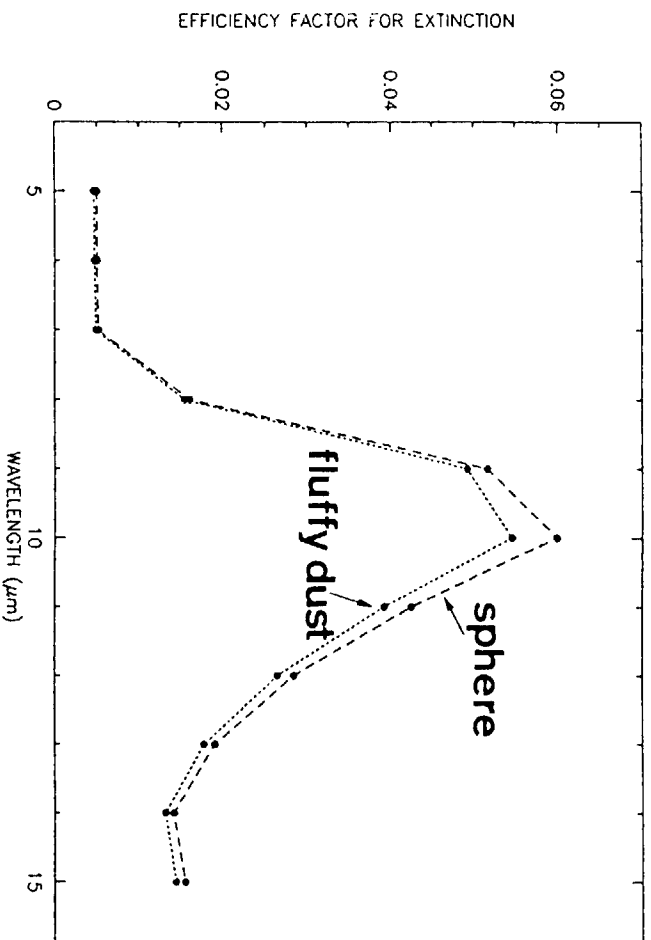


Fig. 3 : The efficiency factors for extinction for the spherical and irregular dipole models

CONCLUSION

The dipole method, originally proposed by Purcell and Pennypacker (1973) but modified by introducing the Born expansion series is shown to give very satisfactory results and therefore looks very promising for solving the problem of light interaction with irregular, fluffy particles. It is also well suited to vectorial calculation on supercomputers. Although the example discussed above corresponds to a very small size parameter ($2\pi a/\lambda \simeq 0.03$), a clear effect is noted between the sphere and the fluffy particle of the same mass which further depends upon wavelength. The method is still in its infancy and needs further improvement such as the replacement of the Clausius-Mossotti equation by a more exact expression of the polarizability. But it is extremely general as it can handle inhomogeneous particles.

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