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Interstellar dust extinction problem: benchmark of (semi)analytic approaches and regularization method

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Abstract. Interstellar extinction curves have a typical so-called bump at a constant wavelength of about 220 nm. This indicates that cosmic dust particles distributed in space must be quite small in comparison with the wavelengths of visible radiation. The well-known Mie theory, or its approximations, are usually employed to simulate an interaction of electromagnetic radiation with such particles. However, the conventional Mie theory is applicable only for spherical and homogeneous particles, and, as known, the spherical geometry is very rare in space. Utilization of any approximation in solving the inverse problem for interstellar extinction may therefore lead to questionable results. To evaluate possible differences between retrieved size distributions, we performed a benchmark of three various techniques. The first one is based on the anomalous diffraction approximation and offers a semi-analytical solution. The profile of an extinction curve is scalable: a simple parametrization uses the modified gamma function as a substitute for the real distribution. The second approach extends the first one, but the distribution function is not expressed in an analytical form. The final profile of size distribution is computed using Mellin's transform of kernel of the integral equation. The third solution follows the modified Tikhonov's regularization and can be applied to both spherical and non-spherical particles. There is no requirement placed on a distribution function. It is shown that direct consequences of the above discussed approximations are: i) underestimation of the amount of large particles, ii) a reduced value of the modal radius of the retrieved size distribution, and iii) quite narrow distrubution functions.

Key words: interstellar dust – extinction – inverse problems

1. Introduction

The starlight penetrating through the cosmic space is influenced by interstellar extinction. Presence of dust grains in the universe is one of the crucial factors which affects the form of extinction curves. A theoretical analysis of the interstellar extinction is a powerful tool for obtaining information on the nature of the material and the size distribution of particles in the Universe. Various dust populations obviously differ in chemical composition and physical properties of the particles. In the interstellar medium iron-rich phases will be susceptible to oxidation and carbonization and will therefore be partially or totally chemically metamorphosed, whereas sulphide and oxygen rich phases are likely to be more robust (Jones, 1988). Heterogeneousness of physical and chemical properties of cosmic dust particles results in a complex spectral behaviour of extinction curves. Recent information on chemical processes acting during particle generation enables us to start a simulation of interstellar extinction.

It is assumed that a great part of dust is produced in circumstellar shells of luminous carbon stars (Gail and Sedlmayr, 1987). Past years have shown that interstellar particles are probably small enough when compared a typical size of the interplanetary particles in the Solar System. For instance, the circumstellar extinction in the envelope of AB Aur suggests the presence of small silicate grains ($a \approx 0.02\mu m$) (Catala, 1983). Usually a dust population is characterized by its own environment-specific size distribution function. One of the well-known model accommodated in the dust community is the so-called MRN (Mathis et al., 1977). This MRN model uses two separate mixtures of silicates and graphitic grains with the size distribution

$$f(a) = K\ a^{-n} \quad , \tag{1}$$

where a is the particle radius and K is a proportionality factor. It seems that $n \approx 3.5$ is a more generic value, which can reproduce various galactic extinction curves (Mezger et al., 1982). Nevertheless, the model is expected to be valid in a limited range of particle radii (Maccioni and Perinotto, 1994). Apart from Eq. (1) the regular solution of the inverse problem for extinction data often results in mono- or bi-modal functions (Zubko et al., 1998). Zubko et al. (1996) also indicating that silicate grains of the spherical shape may have a distinct peak in their size distribution centered around 0.2 μm. However, it must be stressed that similar results were reached by Kim and Martin (1995) when assuming non-spherical cosmic dust grains.

It is important to analyse a behaviour of extinction curve in the UV band, where the main mode of the extinction is positioned ($\lambda \approx 0.2\ \mu m$ - Blanco et al., 1996). The attenuation of the radiation can be caused by grains in an interstellar cloud obscuring a far field star. In these cases, the extinction curves show a bump whose strength and width are largely variable from star to star (Fitzpatrick and Massa, 1986), but with a peak wavelength very stable at about 217.5 nm (Cardelli et al., 1989), regardless of the direction of observation - which means that it is a certain more general characteristic of interstellar dust. In the spectral region from IR to UV, the extinction efficiency of such dust grains usually grows up. The extinction is later on reduced, after reaching the modal wavelength (Désert et al., 1990). However, the dust size distribution is not an unique factor responsible for a particular course of the extinction curve. The spectral behaviour of an extinction curve can also be interpreted by means of structural inhomogeneity of dust particles. The agreement between the wavelength dependence of interstellar extinction and the wavelength dependence of absorption in amorphous carbon implies that carbon layers must be on the surface of very small particles - most likely those particles that produce a 220 nm feature (Duley, 1987). Hecht (1981) concluded that also graphite particles have small coatings. Probable occurence of graphite in cosmic dust grains was confirmed by Perrin and Sivan (1989).

The presence of very small grains ($\approx 0.01 - 0.1 \mu m$) in cosmic space is evident because of linear increase of the attenuation coefficient in the UV spectral region. However, the submicron fraction of the dust population isn't negligible because it enables to explain the spectral behaviour of the extinction curve in visible. Except for the particles' shape (Draine, 1988), the extinction curve is really considerably influenced by optical properties of dust grains. Swamy (1970) pointed out that grains have no simple chemistry. They should have a mixed structure, as the primitive graphite dust model is not sufficient to simulate the extinction curve as a whole. In particular, it was shown by some authors that the computed extinction curve was inconsistent with the measured data in shortwave spectrum (Stecher and Donn, 1965; Swamy and O'dell, 1967). For instance, the iron sulphide pyrrhotite, $Fe_{1-x}S$, a common material in interplanetary grains, could also be an important component of interstellar grains (Jones, 1988).

2. Retrieval of dust size distribution using extinction data: theory

The dry dust particles of the interstellar origin are almost exclusively irregular. It is well known that the main processes of the formation of grains in cosmic space do not favour formation of perfectly spherical (or spheroidal) homogeneous dust particles. Particle characteristics, such as physical, optical, chemical properties, internal distribution of the inhomogeneities, and, especially, morphology, are important parameters for determining the wave front of radiation scattered by the particle (extinction is observed when the light is scattered at the scattering angle - forward transmitted radiation). As well-known dust non-sphericity eliminates the interference structure and ripple typical for monodisperse scattering patterns. Such matter may result in disappearance of a subsidiary mode, which is usually the case with Mie particles. Borghese et al. (1979) calculated the efficiency factors for extinction Q_{ext} for some model particles (e.g. cavity spheres) and found out that particle non-sphericity reduces values of Q_{ext} for particles' size which is less than the incident wavelength.

At present, several methods are known to solve the problem of light scattering and absorption by irregular particles. Mishchenko and Travis (1998) have developed a fortran implementation of the T-matrix method for randomly oriented, rotationally symmetric scatterers. There is a list of various computational methods - DDA (Discrete Dipole Approximation), FDTD (Finite Difference Time Domain), and EBCM (Extended Boundary Condition Method), which can be applied to calculate the light scattering by arbitrarily shaped particles (Wriedt and Comberg, 1998). Although the scattering properties of the individual non-spherical particles vary significantly with the particle orientation, the polydisperse ensembles of small spheroids exhibit essentially the same scattering behaviour as their equivalent-volume spheres (Krotkov et al., 1999). Nevertheless, the original Maxwell equations must be explicitly solved when computing light scattering by objects the size of which is comparable to wavelength λ of incident radiation (not less than 0.03 λ). As for chemical composition, we assume in our simulations that small-scale inhomogeneities are evenly distributed over the particle volume. In such a case it is possible to define an effective refractive index $\overline{m}$ of the particle, for which the numerical calculations can be performed with sufficient accuracy (Kolokolova, 2001).

2.1. Anomalous diffraction theory: simplest size distribution models

The theory of anomalous diffraction was worked out by van de Hulst (1957) and is applicable to spherical homogeneous particles. Spherical particles are mainly assumed for making the theoretical modelling possible. The homogeneity approximation needs some more comments. We suppose that those of structural inhomogeneities are much smaller than sizes of interstellar grains. It is then reasonable to invoke the small-scale asymptotic approximation. When suffciently small-scaled structures are evenly distributed, the inhomogeneous material still causes simple effects of a phase retardation and attenuation of an electromagnetic wave. It is, therefore, possible to find an "effective" refractive index to represent such materials. Despite of real progress in dust chemistry modelling, one must take into account any evolutionary changes in the dust properties. A more plausible dust model should take into account a detailed physical and chemical behaviours of grains during their passage through various environments: diffuse and/or molecular clouds, star-forming regions and so on. Although the iron-rich silicates or magnesium-rich silicates are representative for pure interstellar dust, their optical properties can considerably be modified in dense interstellar clouds. Under such conditions, the original particles are coated by dirty ice (Sorrell, 1995). A real part of the complex refractive index of these particles will be reduced. The cosmic dust particles are usually assumed to be dielectric objects and this assumption can significantly affect the retrieval of the particle characteristics such as the size distribution. In the visible, both the silicates and dirty ices are mostly non-absorbing media. The most useful result obtained in the theory of anomalous diffraction is the expression for the extinction efficiency factor for such spheres, namely,

$$Q_{sca}(\rho) = \frac{2\overline{m}(\lambda) - 1}{\overline{m}(\lambda)} \left[2 - \frac{4}{\rho} sin\rho + \frac{4}{\rho^2}(1 - cos\rho) \right] \quad , \tag{2}$$

where $\rho = 4\pi(\overline{m} - 1)a/\lambda$, see e.g. van de Hulst (1957). Formula (2) is predominately suitable for optically soft particles. However it gives a good results also for $m \to 2$. The dust extinction τ is a simple function of the toward-the-star dust size distribution function $f(a)$,

$$\tau(\lambda) = \pi \int_0^\infty Q_{ext}(a, \lambda, m)\ a^2\ f(a)\ da \quad , \tag{3}$$

where $Q_{ext}(a, \lambda, m)$ refers (as stated above) to the efficiency factor for extinction, λ is the incident wavelength, a the particle effective radius and m the mean particle refractive index. Weingartner and Draine (2001) have constructed the size distribution for carbonaceous and silicate grain populations in different regions of the Milky Way, and have found a mode of the particle size distribution in the submicron range. The results demonstrate that such a distribution cannot be simulated by the MRN model. Any model size distribution should be at least monomodal. We have therefore systematically performed computations on size distributions constructed as a linear combination of several simple modified gamma functions

$$f(a) = a \sum_{n=1}^{N} k_n \exp\{-b_n a\} \quad . \tag{4}$$

The series (4) satisfies the usual condition $f(0) = f(\infty) = 0$ and, simultaneously enables us to fit a large scale of real distributions (in dependence on N). Employing the above given formula for the most elementary case (N=1) the extinction acquires the form

$$\tau(\lambda) = 4\pi \frac{\overline{m} - 1}{\overline{m}} \frac{k_1}{b} \frac{15h^4 + 10h^2 + 3}{(h^2 + 1)^3} \quad , \tag{5}$$

where $b \equiv b_1$, $h = \lambda b/[4\pi(\overline{m} - 1)]$ and the modal radius of the dust distribution accommodates the form $a_m = b^{-1}$. The approximate modal radius of the toward-the-star dust size distribution can be found by minimizing the differences between measured and theoretical extinction curves (Eq. 5). The parameter b for the above mentioned modified gamma function corresponds to minimum of the functional

$$\delta(b) = \frac{\sum_{i=1}^{M} \left[\tau^m(\lambda_i) - \tau_a^r(\lambda_i, b)\right]^2}{M} \quad , \tag{6}$$

where $\tau^m(\lambda_i)$ and $\tau^r(\lambda_i, b)$ are the measured and recalculated dust extinctions, respectively. Although the modal radius is relatively well-catched, the theoretical extinction curve usually isn't able to follow the real data. On the other hand, the more convenient size distribution model, the more complex analytical representation of the the extinction. For example, one can find an analytical expression for τ in the case of $f(a) = k_1 a^2 e^{-ba}$ as follows

$$\tau(\lambda) \sim \frac{8\pi k_1}{b^5} \left\{ 6 + h^2 + h^6 \frac{15 - 10h^2 - h^4}{(h^2+1)^4} \right\} \quad . \tag{7}$$

2.2. Anomalous diffraction theory: solution for size distribution

Many of the inverse problems in astrophysics of dust particles can be formulated in terms of a Fredholm integral equation of the first kind (Eq. 3). The extraction of information on the particle size distribution from multispectral extinction measurements is, in general, an ill-posed problem, which is notoriously difficult to solve. Such problems fail to fulfill at least existence of a solution, uniqueness of the solution, and continuity of the solution on the data function. Several methods were developed to solve such inverse tasks, although no general rules can be formulated. The singular-function theory or eigenfunction theory (Box et al., 1992; Box and Box, 1985) are well-applicable. But one must be aware that the extinction is usually measured in a restricted spectral region $\lambda \in \langle \lambda_1, \lambda_2 \rangle$. An inversion of the measured data will therefore produce a distribution function $f(a)$ restricted in particle size: $a_1 \rightarrow a_2$. Eq. (3) represents a mapping in a Hilbert space from $L^2[\lambda_1, \lambda_2]$ to $L^2[a_1, a_2]$ constructed over the set of quadratically integrable and continuous functions $f(a)$. Accepting that the measured extinction data cover the visible spectrum range, the size distribution can be successfully retrieved in the submicron range.

The fast calculation of the efficiency factor $Q_{ext}(a, \lambda, m)$ is based on rigorous Mie's theory (Bohren and Hufmann, 1983, McCartney, 1977), where kernel of the integral equation (3) can be transformed into a product-type kernel when the anomalous diffraction approximation is accommodated. Then the efficiency factor for the extinction depends on the ratio a/λ (Schmeidler, 1955). For such kernels, the Mellin transform is employed to significantly simplify the solution of the integral equation (Shifrin, 1971). It is important to obtain the data concerning $\tau(\lambda)$ in the domain of its maximum to improve the stability of the obtained solution. Shiffrin and Perel'man (1964) have shown that the procedure can be applicable in the case if: i) the relative error of the measured data is about 1-5%, ii) the particle polydispersive system has not too narrow a distribution with the evident mode, iii) the measured extinction data cover the region containing a mode of $\tau(\lambda)$.

In the case of the product-type kernel, Eq. (3) can be transformed as follows

$$\tau(s) = 2\pi \int_0^\infty Q_{ext}(as)\; a^2\; f(a)\; da \quad , \tag{8}$$

where $s = 2\pi(\overline{m} - 1)/\lambda$, and

$$Q_{ext}(y) = 1 - \frac{sin(2y)}{y} + \frac{1 - cos(2y)}{2y^2} \quad . \tag{9}$$

Finally, including the Mellin transform based on two-dimensional Laplace's transformations, the solution of the integral equation (3) takes a form

$$af(a) = \frac{1}{\pi^2} \int_0^\infty p(2as)\; q(s) ds \quad , \tag{10}$$

where

$$p(z) = \frac{1 - cos(z)}{z} - sin(z) \tag{11}$$

and

$$q(s) = s\,[\tau(s) - \tau(\infty)] \quad . \tag{12}$$

Using the asymptotic formulae for extinction

$$\tau(s) \approx Bs^2 \quad , \quad s \in \langle 0, s_1) \tag{13a}$$

$$\tau(s) \approx C_0 + \frac{C_2}{s^2} \quad , \quad s \in (s_M, \infty) \tag{13b}$$

integral (10) can be split into three individual integrals, i.e. $I_0(0, s_1)$, $I_1(s_1, s_2)$ and $I_3(s_N, \infty)$, where the interval $s_1 - s_M$ is covered by measured extinction data. It is possible to express a sum of integrals $I_0(0, s_1)$ and $I_3(s_N, \infty)$ in an analytical form which enables us to formulate Eq. (10) as follows

$$af(a) = \frac{B}{\pi^2} \left\{ \frac{s_1^2}{6a} + \frac{1}{a^2} \left(\frac{1}{2a^2} - s_1^2 \right) \sin(2as_1) + \frac{s_1}{a} \left(\frac{s_1^2}{2} - \frac{1}{a^2} \right) \cos(2as_1) \right\} +$$

$$+ \frac{C_0}{\pi^2} \left\{ \frac{1}{2a^2} \sin(2as_M) - \frac{s_M}{2a} \cos(2as_M) - \frac{s_M}{2a} \right\} + \frac{C_2}{2as_M\pi^2} \left[1 - \cos(2as_M) \right] +$$

$$+ \frac{1}{\pi^2} \int_{s_1}^{s_M} p(2as)\; q(s)\; ds \quad . \tag{14}$$

We calculated the last term in equation (14) numerically using Lagrange's polynomials to fit the measured extinction data at discrete wavelengths with a continuous smooth function. The results of theoretical calculations show that the greater particle modal radius the greater wavelength belonging to the mode position of the function $\tau(\lambda)$. It is not too difficult, nor time-consuming, to solve an integral equation of the 1-st kind using the above given technique. Nevertheless, with Mellin's transform it is not guaranteed that the solution will be positive, i.e. will have a physical meaning.

2.3. Regularization technique for non-spherical randomly oriented particles

The major complexity to the solution brings the asphericity of the particles. A substantial fraction of dust in space is composed of solid materials, thus implying non-spherical particle shapes, and it must be expected that these particles will have a size distribution, a shape distribution, and an orientation distribution as well. Grain morphology may be described by characteristic diameters (e.g. aerodynamic, mobility and volume equivalent diameters). The non-sphericity of dust particles raises the question of applicability of the conventional Mie theory to compute their radiative properties. In fact, the light scattering by polydisperse systems of non-spherical particles need to be investigated. Averaging over the shapes provides a more realistic model of natural ensembles of scattering particles since it eliminates the interference structure and ripple typical for monodisperse scattering patterns, thus enabling us to derive meaningful conclusions about the effects of particle non-sphericity on light scattering and extinction.

The characteristics of radiation scattered by irregular particles can be calculated using the Discrete Dipole Approximation (DDA) (Draine, 1988). The principal advantage of the DDA is that it is completely flexible regarding the geometry of the target, being limited only by the need to use an interdipole separation d small compared to i) any structural lengths in the target, and ii) the wavelength λ. Numerical studies (Draine and Flatau, 1994) indicate that the second criterion is adequately satisfied if $|m|kd < 1$, where $k = 2\pi/\lambda$ is a wave number. Interstellar environment contains a mixture of particles with different sizes, shapes, orientations, and refractive indices, so the efficiency factor for extinction must be averaged over the particle ensemble. Computation of ensemble averages is, in principle, rather straightforward. In the absence of external forces such as magnetic, electrostatic, or aerodynamic forces, all orientations of a nonspherical particle are equiprobable, so then Q_{ext} for the set of randomly oriented particles of the same shape, size, and composition is a triple integral

$$Q_{ext} = \frac{1}{8\pi^2} \int_0^{2\pi} d\beta \int_{-1}^{1} d\cos\Theta \int_0^{2\pi} Q_{ext}(\beta, \Theta, \Phi)\, d\Phi \quad , \tag{15}$$

where Euler angles β, Θ, and Φ specify particle orientations with respect to the laboratory reference frame.

However, there are several disadvantages of DDA: limited numerical accuracy for certain particle sizes, especially when calculating the scattering matrix elements; slow convergence of results with an increasing number of dipoles; and a need to repeat the entire calculation for each new direction of incidence. Nevertheless it was shown by Draine and Flatau (2003) that for dielectric materials ($|m| \leq 2$), the DDSCAT code (based on DDA) permits calculations of scattering and absorption accurate to within a few percent.

Calculations based on DDA have shown that Q_{ext} for nonspherical dust grains is approximately 2 times smaller than that for equivalent spheres. Such a behaviour was found for optically hard materials (Mg-Fe silicates) as well as for optically soft dust (containing the dirty ice). This fact has important and evident consequences in solving integral Eq. 3. Namely, the change of Q_{ext} in a range of some tenth percent has a basic impact on retrieval of particle size distribution. It is a sufficient motivation to analyse how the particle shape influences processing of extinction data. To guarantee the representativeness of our numerical simulations, the computations cannot be performed for standard geometrically well defined objects - which never render the natural irregularities of interstellar particles. Anyway, no simple analytical model exists to fit the real particle morphology as any model particle is still too regular to represent a real rough grain (Chamaillard et al. 2001).

To calculate the interstellar extinction by non-spherical particles we used a true cosmic dust sample (originally retrieved during a series of flights in the Earth's stratosphere along the west coast of North America (Clanton et al., 1984). The shape of particles we finally selected to coincide well with the results of mid-infrared spectropolarimetry of the interstellar grains obtained by Hildebrand and Dragovan (1995). These authors found that the grains are oblate and the best fit for a ratio of particle axes is 2:3. The kernel of integral equation (3) for non-sherical grains is quite complex and must be calculated numerically. Fredholm integral equation can then be split into a system of linear equations

$$\tau(\lambda_i) = \mathbf{A}_{ij} f_j + \epsilon \quad , \tag{16}$$

where $\mathbf{A}$ is a matrix of type $\mathbf{A}_j(\lambda_i)$ and ϵ is an error which arises due to the difference between the measured τ and theoretical $\tau(= \sum \mathbf{A}_{ij} f_i)$. Eq. (3) for non-spherical particles was solved using an adapted Tikhonov's regularization method. This method has been proved to be useful for spherical particles and is used by many authors (Zubko, 1997, 1999; Groetsch, 1984). The only difference is a different kernel for the particles of a non-spherical shape. A method of solution follows the minimization of the functional

$$R_\alpha = \sum_{i=1}^{M} \left[\sum_{j=1}^{N} \mathbf{A}_{i,j} s_j - f_i \right]^2 + \alpha \left\{ p_0 \sum_{j=1}^{N} \Delta'_j s_j^2 + p_1 \sum_{j=1}^{N-1} \frac{(s_j - s_{j-1})^2}{\Delta_j} \right\} \quad , \tag{17}$$

where M is the total number of wavelengths at which the extinction data are measured, i.e. $\tau(\lambda_{i=1..M})$, and N is a number of nodes $a_{j=1..N}$ at which the function $s(a) = \pi a^2 f(a)$ is calculated. The components of the matrix $\mathbf{A}$ are given as follows (Kabanov et al, 1988)

$$\mathbf{A}_j(\lambda_i) = \mathbf{G}_{j-1,j}(\lambda_i) + \mathbf{G}_{j,j}(\lambda_i) + \mathbf{G}_{j+1,j}(\lambda_i), \quad j \neq 1, j \neq N \tag{18a}$$

$$\mathbf{A}_1(\lambda_i) = \mathbf{G}_{1,1}(\lambda_i) + \mathbf{G}_{2,1}(\lambda_i) \tag{18b}$$

$$\mathbf{A}_N(\lambda_i) = \mathbf{G}_{N-1,N}(\lambda_i) + \mathbf{G}_{N,N}(\lambda_i) \tag{18c}$$

and

$$\mathbf{G}_{j,k}(\lambda_i) = \int_{a_j'}^{a_j''} Q_{ext}(a, \lambda_i)\; h_{j,k}(a)\; da, \tag{19}$$

where functions

$$h_{j,k}(a) = \frac{\omega_j(a)}{(a - a_k)\; \omega_j'(a_k)} \tag{20a}$$

$$\omega_j(a) = (a - a_{j-1})(a - a_j)(a - a_{j+1}), \quad j = 1..N \tag{20b}$$

are constructed using Legendre's polynomials. The nodes a_j' and a_j'' are calculated as follows

$$a_j' = \frac{a_{j-1} + a_j}{2}, \quad a_j'' = \frac{a_j + a_{j+1}}{2} \quad , j = 1..N. \tag{21}$$

The functions used in Eq. (17) represent the differences $\Delta_j' = a_j'' - a_j'$, $\Delta_j = a_j - a_{j-1}$, $p_0 = a_{N+1} - a_0$, $p_1 = (a_{N+1} - a_0)^3$ and α is the so-called parameter of the regularization. The vector of regularized solution s_α, which minimizes the functional (17) fulfill the condition of a system of linear algebraic equations

$$(\mathbf{A}^*\mathbf{A} + \alpha\mathbf{C})s = \mathbf{A}^* f, \tag{22}$$

where $\mathbf{A}^*$ is the matrix transposed to $\mathbf{A}$ and the matrix $\mathbf{C}$ has the form $\mathbf{C} = p_0\mathbf{C}_0 + p_1\mathbf{C}_1$, where $\mathbf{C}_0 = \text{diag}\ \{\ \Delta_1', \Delta_2', ..., \Delta_N'\ \}$ is a diagonal matrix. The components of the matrix $\mathbf{C}_1 = ||c_{i,j}||$ are given as follows

$$c_{i,j} = -\Delta_i^{-1}, \ j = i - 1, \ i = 2, ..., N \tag{23a}$$

$$c_{i,j} = \Delta_i^{-1} + \Delta_{i+1}^{-1}, \ j = i, \ i = 1, ..., N \tag{23b}$$

$$c_{i,j} = -\Delta_j^{-1}, \ j = i + 1, \ i = 1, ..., N - 1 \tag{23c}$$

$$c_{i,j} = 0, \ |i - j| > 1, \ i, j = 1, ..., N. \tag{23d}$$

The parameter of regularization α is chosen in conformity with the error margin δ of the input data. The value α can be obtained simply by the numerical method solving the equation

$$||\mathbf{A}s_\alpha - f_\delta|| = \delta, \tag{24}$$

by utilizing a strict monotonous course of the functional $\rho_1(\alpha) = ||\mathbf{A}s_\alpha - f_\delta||$. As usual, each method of regularization may give the negative regions too. But, if the method of regularization is suitable for a specified ill-posed problem, the errors of inversion, including the negative regions, are actually negligible.

3. Numerical example - discussion and conclusions

A choice of the inversion technique depends on many factors. The simple parametrization method (sec. 2.1) is very efficient in analysis of statistically very large sets of experimental data, to get e.g. the database of effective modal radii of various dust populations. Whereas the extinction is expressed in an analytical form, it has a great advantage in theoretical astrophysical modelling. On the other hand, the modified gamma function probably only rarely fits an interstellar dust size distribution. It is more-less necessary to retrieve a size distribution using a certain inversion algorithm. When assuming a spherical shape of the dust particles one can use Mellin's transform (sec. 2.2) of the kernel of integral equation (Eq. 3). Anyway, the solution is based on an anomalous diffraction approximation (Van de Hulst, 1957), so it is applicale only to a certain type of particles. Although this approximation was originally developed for optically soft particles with $|m-1| \ll 1$, there exists an extension partially valid for optically hard dust too (McCartney, 1977), i.e. for $|m| < 2$. Unlike the parametrization described in sec. 2.1, two-dimensional Laplace's transformation (applied in sec. 2.2) doesn't guarantee that the size distribution will be positive at the whole solution interval. As for a limited spectral region (in which the extinction data are collected), there exists a strong constraint for the size interval on which the solution can be accepted. A more generic approach is referred to regularization techniques. Here the kernel of integral equation is calculated numerically – in this way we can avoid any crucial restriction charged to the solution. While Mie theory takes place for spherical particles, the specific kernel will be employed in Eq. 3 for non-spherical grains. Although the regularization techniques represent a powerful tool usable for various dust populations, it features a number of disadvantages. First of all, the solution is slower when compared with the above discussed methods. Besides, it is almost impossible to simulate any dust environments. There must be indirect indicia on particle properties, such as chemical composition or prevailing morphology. Especially, interstellar grains are usualy prolonged in one axis (particles are either oblate or prolate). The aspect ratio vary from case to case, grains are often porous with cavities accidentally distributed over the dust body. In certain situations, the dust grains may have non-random orientation because of interstellar magnetic field. The more free dust system has to be covered by our computations, the greater database of precalculated efficiency factors for extinction has to be archived. To have the solution schema operable, we focused to most dominant particles in space, aspect ratio of which is about 1.4-1.5.

We developed the program Inverse v1.2 which accepts both the spherical and non-spherical particles. The kernel function for spherical particles is computed automatically. The efficiency factors for extinction for non-spherical particles are pre-calculated using DDA and later on they are read from an external data file. A case study of the extinction curve measured toward the star HD 202904 (Zubko et al., 1998) is employed to demonstrate functionality of all the above

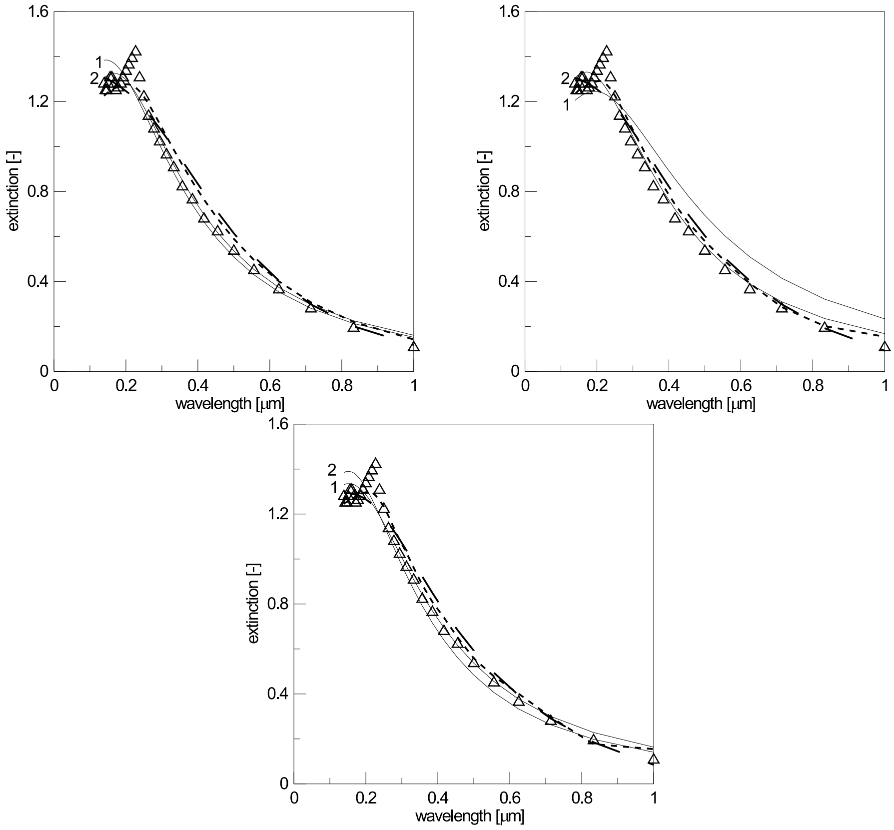

Figure 1. a,b,c) Original extinction toward the star HD 202904 (triangles, after Zubko, 1998) and recalculated extinction curves for: a) dirty ice, b) magnesium-rich silicates, c) iron-rich silicates. Solid curves: 1 (minimization based on Eq. 5), 2 (minimization based on Eq. 7). Bold dashed curves: short dashes (modified Tikhonov's regularization for spherical particles), large dashes (the curve obtained from a regularized solution for non-spherical grains; aspect ratio 1.4).

listed solutions. Both the original data (triangles) and theoretical extinction curves are drawn in Fig. 1a,b,c. The theoretical extinction curves were obtained by optimization of free parameters of the model gamma size distributions (1: Eq. 5 and 2: Eq. 7). The bold-dashed curves correspond to regularized solution $f(a)$ for both, non-spherical particles and their spherical equivalents. As the optical properties are mostly unknown, we performed the computations for three typical interstellar materials: dirty ice, magnesium-rich silicates, and iron-rich silicates.

One can see that the model gamma function for dirty ices works well when simulating the extinction curve at wavelengths in the domain beyond the max-

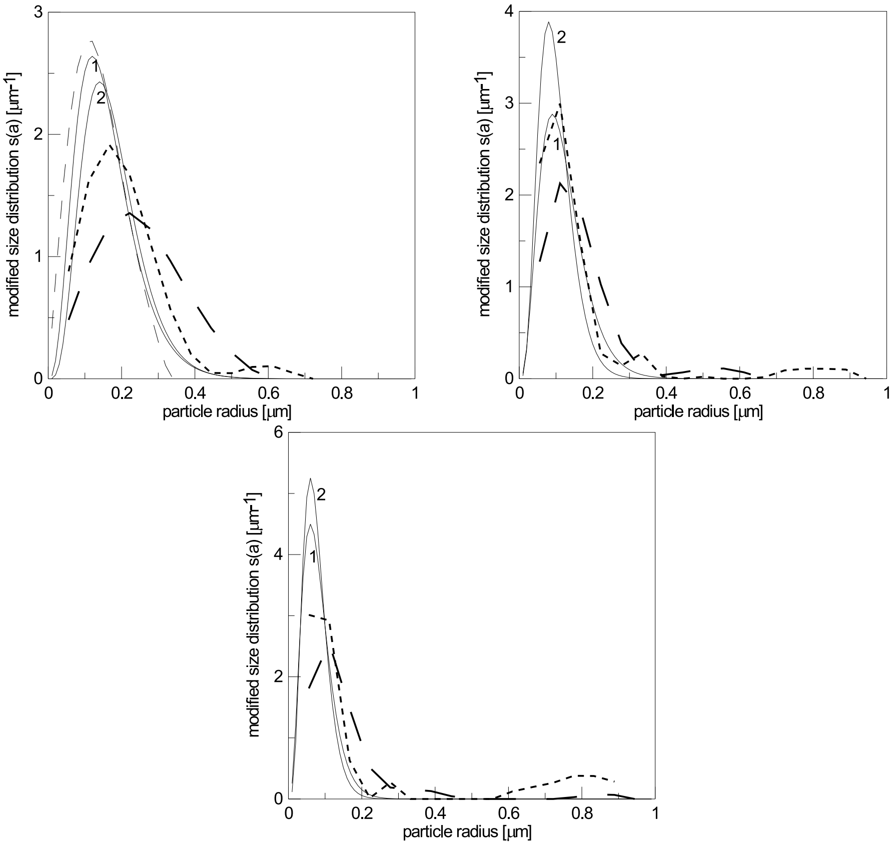

Figure 2. a,b,c) Size distribution functions retrieved from the extinction measured toward the star HD 202904 (after Zubko, 1998): a) dirty ice, b) magnesium-rich silicates, c) iron-rich silicates. Solid curves: 1 (minimization based on Eq. 5), 2 (minimization based on Eq. 7). Dashed curves: thin dashes (direct integration using Mellin transform, Eq. 14), bold short dashes (modified Tikhonov's regularization for spherical particles, Eq. 24), bold large dashes (regularized solution for non-spherical grains; aspect ratio 1.4; Eq. 24). The "Mellin's" distribution functions are not drawn in Figs 2b) and 2c) as the maximum values of s(a) were about 10-12 in these cases.

imum, but it is not optimal in the neighbourhood of the peek. In general, for all analysed materials, the model function $f(a) = k_1 a^2 e^{-ba}$ fits the measured extinction data better than the simple distribution referred to Eq. 4 for $N = 1$. Besides, there are evident differences between quality of data-fits when using the model gamma functions for various chemical compositions. While the system consisting of icy particles reproduces the extinction curve with a sufficient accuracy, this is not true for interstellar magnesium-rich silicates. On the other hand, the regularization technique gives appropriate results (comparable in accuracy) for any material.

The solution methods can be unambiguously distinguished when computing the final size distributions (Figs. 2a,b,c). As well-known the monomodal extinction curves are usually produced by polydisperse systems with not very narrow size distributions. It is quite important to get the experimental data with a sufficient spectral-density, i.e. the wavelength grid interval should not exceed 50 nm in the zone around the maximum of an extinction curve. This requirement is referred to the existence of possible subsidiary maxima which might be missed. As expected, the retrieved size distributions are mostly monomodal (Figs. 2), but the individual curves differ considerably. Although there is no fatal difference in gained modal radii of size distributions, the model gamma functions are quite narrow - it probably leads to an underestimation of the amount of large particles in space. The similar results are obtained when Mellin's transforms are employed in a solution of the integral equation. Both the above discussed approaches are based on the conventional Mie theory for homogeneous spherical particles, for which the anomalous diffraction approximation is assumed to be applicable. However, almost surely one of the pre-conditions in such modelling is violated in reality. Particles are neither spherical, nor homogeneous, nor optically soft,...

A solution of the inverse problem appears to be complex since we deny the anomalous diffraction approximation. The kernel of integral equation completely loses an analytical form, so a special retrieval algorithm is necessary. When applying the modified Tikhonov's regularization we constructed the size distributions for both, spherical and non-spherical particles. In comparison to the methods based on an anomalous diffraction approximation there are two effects associated with the new approach: the modal radius of $f(a)$ increases, and the size distribution function takes a less narrow form. As a consequence, the total amount of the most frequent particles (the radius of which is equal to a_m) is reduced. Also the subsidiary modes occur in the profile of $f(a)$. The widest distributions are typical for an ensemble of non-spherical particles. Whereas the interstellar dust have a predominately irregular shape, one can easily conclude that amount of large particles will be significantly underestimated when replacing realistically shaped grains by spherical particles of equivalent volume. On the other hand, the amount of small spherical particles is overestimated because of the above mentioned facts, but also due to the specific behaviour of the efficiency factor for extinction. Namely, the Q_{ext} for non-spherical submicrometer-sized particles is approximatelly 2-times smaller than that for spheres.

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