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Monte Carlo Modelling of the Radiation Transport in Polydispersion Media

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An efficient Monte Carlo numerical method is presented for solving problems of radiative transfer in dust containing media. This method can be applied to a wide variety of astrophysical objects, as for example dust clouds, protostellar clouds, circumstellar envelopes and reflection nebulae. The computational procedure is based on the use of Mie's formulae for scattering by a single spherical particle; the interaction of photons of polarized light with dust particle is described by means of Stokes' vector. A high level of generality and the speed of the presented method is reached by the use of some improvements in the common Monte Carlo scheme.

В работе представляется мощный вычислительный метод Монте Карло для решения проблем переноса излучения в средах содержающих пыл. Этот метод приложителен к обширному классу астрофизических объектов, как например пылевым облакам, протозвездным облакам, околозвездным оболочкам и отражательным туманностям. Вычислительный процесс основан на использовании теории Ми для рассеяния отдельными шарами; взаимодейетвие фотона поляризованного света с пылевой частицей выражеатся с помощью вектор-параметров Стокса. Высокий уровень общности и скорости представляемого метода достижен некоторыми улучшениями в общепринятой схеме Монте Карло.

V práci je předložena numerická metoda Monte Carlo na řešení problémů přenosu záření v prostředích obsahujících prach. Tato metoda může být aplikována na širokou řadu astrofyzikálních objektů, jako např. prachová oblaka, protohvězdná oblaka, cirkumstelární obálky a reflexní mlhoviny. Výpočetní postup je založen na užití Mieho teorie pro rozptyl na jednotlivé sférické částici; interakce fotonů polarizovaného světla s částicemi je popsána pomocí Stokesových vektor-parametrů. Vysoká úroveň obecnosti a rychlost metody je dosažena užitím několika zdokonalení běžného schématu Monte Carlo procesu.

1. Introduction

The fundamental disadvantage of nearly all analytical solutions of the radiation transfer (RT) lies in the unavoidable necessity to make a variety of assumptions

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which may prove invalid in many objects of astrophysical interest, for example in the dust containing media with the multiple strongly anisotropic scattering. The number of simplifying assumptions can be reduced by applying statistical approach to the RT problem, in which the propagation of photons is simulated numerically in model objects. Aspects concerning light transfer and principles of this approach known as Monte Carlo method have been summarized in a comprehensive monograph by Marčuk et al. (1976), supplied by some computer routines. Despite that the monograph is aimed first of all at the terrestrial atmospheric optics, the computational procedures are applicable without dificulties to cosmic clouds, too.

Some of the first investigations of multiple scattering in optically thick reflection nebulae, based on the use of Monte Carlo method, were done by Vanýsek and Šolc (1973) and Roark, Roark and Collins (1974). Both these studies have shown that multiple scattering has an important role in the RT and that the results of the surface brightness and polarisation distribution of circumstellar dust clouds cannot be predicted assuming single scattering only. More recently, Witt (1977) used the Monte Carlo technique to determine the basic physical and optical properties of reflection nebulae. However, in his study no polarisation is taken into account what may lead to incorrect results in case of highly polarizing particles.

The problem of Monte Carlo modelling of the propagation of polarized light in the optically thick astrophysical media without symmetry both of the geometrical shape and particles density distribution, containing anisotropically scattering particles of various kinds (so-called polydisperse medium), is the aim of the present study.

2. Scattering by a Single Particle

While in the atmospheric optics the actual chemical composition and shape and size of the scattering particles (dropplets) may be measured well, those of the interstellar dust grains are essentially not known. The only way to proceed in solving the RT problem is to rely on crude theoretical considerations, i.e. to assume

1) a simple geometrical form of particles (for the sake of exact solution of scattering and absorption), and
2) the existence of certain materials in interstellar solid state particles, probably silicates and/or graphite, and
3) the theoretical distribution function of sorts and sizes of dust grains.

The role of chemical composition is included in the scattering theory by means of the refractive index; but knowledge of abundance of probable materials, if necessary, does not proceed any further than to the ad hoc constructed mixture of two or three sorts of grains. Because Monte Carlo modelling does not depend on the form of the scattering, furtheron I shall consider only one sort of material. It must be emphasized that the scattering matrix (determining all scattering properties, see below) of a mixture can be obtained as the sum of scattering matrices of the constituent materials weighed by their (normalized to 1) abundance.

As the size distribution regards, the function $n(a)$ proposed by Wickramasinghe and Nandy (1971) for the spherical grains is widely adopted in the form

$$n(a)\,\mathrm{d}a = Aa^{\alpha}\exp\left(-\frac{\alpha}{\gamma}\left(\frac{a}{\bar{a}}\right)^{\gamma}\right)\mathrm{d}a\,, \tag{1}$$

where A is a constant, a is the grain radius, $\bar{a}$ is the most frequent grain radius and α and γ are parameters characterizing the size distribution. The mixture of one sort of particles with not identical radii, called the polydisperse medium, has a scattering matrix obtained similarly by integrating the matrices belonging to various radii, weighted by $n(a)\,\mathrm{d}a$. Since the course of size distribution is not essential for the study of Monte Carlo method, only one size of spherical grains is adopted, determined by the radius a and the complex refractive index m (the monodisperse medium).

Much has been written about the theoretical and experimental investigations of scattering properties of isolated particles as well as of disperse media, as is shown for example in the basic monograph by Hulst (1957). However, when trying to study the real radiation transport, we are in need of a general theory, dealing with polarized light and particles of arbitrary size and shape. Currently only the exact analytical Mie's theory of scattering by spheres is in common use, because it is not so sophisticated as other more complex theories, and because it fairly agrees with laboratory measurements for not very oblate or prolate particles of nonregular shape, as demonstrated by Zerull, Giesse and Weiss (1977).

In order to incoroporate the Monte Carlo idea, the scattering process can be regarded as the dispersion of the photon stream to all the directions after colliding with a target particle. The "deflection" angle $\vartheta \in \langle 0^0, 180^0\rangle$ of an individual "scattered" photon is called the scattering angle. Let us denote $\boldsymbol{p}_0$ and $\boldsymbol{p}$ the unit vectors in the direction of impinging and scattered photon respectivelly, then $\boldsymbol{p}_0 \,.\, \boldsymbol{p} = \cos\vartheta$. The half-plane containing both $\boldsymbol{p}_0$ and $\boldsymbol{p}$, limited by the straight line going through the particle and parallel with $\boldsymbol{p}_0$, is called the scattering half-plane. The spatial orientation of the scattering half-plane determines the value of the tilt angle $\varphi \in \langle 0°, 360°)$ between it and a chosen reference half-plane with the same boundary line.

The intensity $I(\boldsymbol{p})$ may be defined, for instance, as the number N of photons with the direction vectors within a small solid angle $\Delta\omega$ (around the axis $\boldsymbol{p}$) and crossing perpendicularly a small area ΔS, divided by $\Delta\omega, \Delta S$

$$I(\boldsymbol{p}) = \frac{N}{\Delta\omega \,.\, \Delta S}\,. \tag{2}$$

Introducing the cross-sections C_{ext}, C_{scatt}, C_{abs} for the extinction, scattering and absorption respectivelly, for which the identity $C_{\mathrm{ext}} = C_{\mathrm{scatt}} + C_{\mathrm{abs}}$ holds, the conservation of the scattered energy may be given in the form

$$I_0(\boldsymbol{p}_0)\, C_{\mathrm{scatt}} = \int_K F(\boldsymbol{p}_0, \boldsymbol{p})\,\mathrm{d}S\,, \tag{3}$$

where $I_0(\mathbf{p}_0)$ and $F(\mathbf{p}_0, \mathbf{p})$ are the intensities before and after the scattering and $\mathrm{d}S$ is an elementary area on the sphere K with unit radius around the particle. The dimensionless function

$$\Phi(\mathbf{p}_0, \mathbf{p}) = \frac{F(\mathbf{p}_0, \mathbf{p})}{I_0(\mathbf{p}_0)\, C_{\mathrm{scatt}}}, \tag{4}$$

satisfying the obvious condition

$$\int_{4\pi} \Phi(\mathbf{p}_0, \mathbf{p})\, \mathrm{d}\omega = 1 \tag{5}$$

will be furtheron called the phase function and its diagram in spherical coordinates the indicatrix of scattering. The shape of the indicatrix is partially characterized by the assymetry factor g defined by

$$g = \int_{4\pi} \Phi(\mathbf{p}_0, \mathbf{p}) \cos \vartheta\, \mathrm{d}\omega, \tag{6}$$

allowing to distinguish the forward scattering ($g > 0$) and the backscattering ($g < 0$).

In case of spherical particle the symmetry relation reduces the $\Phi(\mathbf{p}_0, \mathbf{p})$ to the form $\Phi(\vartheta)$ with axially symmetrical indicatrix. This allows to introduce the function f

$$f(\vartheta) = \int_0^{2\pi} \Phi(\vartheta) \sin \vartheta\, \mathrm{d}\varphi = 2\pi\Phi(\vartheta) \sin \vartheta, \tag{7}$$

for which

$$\int_0^{\pi} f(\vartheta)\, \mathrm{d}\vartheta = 1, \tag{8}$$

so that

$$g = \int_0^{\pi} f(\vartheta) \cos \vartheta\, \mathrm{d}\vartheta. \tag{9}$$

The Mie's functions $i_1(\vartheta)$, $i_2(\vartheta)$ are proportional to the intensities of light polarized with the oscillation plane perpendicular and parallel to the scattering half-plane respectivelly and relate to the phase function as follows:

$$\Phi(\vartheta) = \frac{i_1(\vartheta) + i_2(\vartheta)}{2} \Big/ (k^2 C_{\mathrm{scatt}}), \tag{10}$$

where $k = 2\pi/\lambda$ is the wavenumber, λ the wavelength both of the impinging and scattered photon.

The present adaptation of Mie's formulae to the computer evaluation follows that by Deirmendjian (1969). The dependence on ϑ in the symbols i_1, i_2, σ_1, σ_2, σ,

$S_1, S_2, \pi_n, \tau_n, f_1, f_2, f$ is omitted. The Mie's functions i_1, i_2 depend only on the dimensionless parameters

$$x = ka\,, \quad y = mx \tag{11}$$

and are given by

$$i_1 = S_1^* S_1 \quad i_2 = S_2^* S_2\,, \tag{12}$$

where the asterisk denotes a complex conjugation. The complex phase functions S, expressed in the goniometrical form, are

$$S_1 = \sqrt{(i_1)}\exp(\mathrm{i}\sigma_1) \quad S_2 = \sqrt{(i_2)}\exp(\mathrm{i}\sigma_2)\,, \tag{13}$$

so that we define $\sigma = \sigma_1 - \sigma_2$ (i is the imaginary unit).

The expansion of the functions S by series in π_n, τ_n may be written in the form

$$S_1 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}(a_n\pi_n + b_n\tau_n) \tag{14}$$

$$S_2 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}(b_n\pi_n + a_n\tau_n)$$

where the real functions π, τ of the argument ϑ must fulfil the recurrence relations

$$\pi_n = \cos\vartheta\,\frac{2n-1}{n-1}\,\pi_{n-1} - \frac{n}{n-1}\,\pi_{n-2} \tag{15}$$

$$\tau_n = \cos\vartheta(\pi_n - \pi_{n-2}) - (2n-1)\sin 2\vartheta\,.\,\pi_{n-1} + \tau_{n-2}$$

with the initial values

$$\pi_0 = 0\,, \quad \pi_1 = 1\,, \quad \tau_0 = 0\,, \quad \tau_1 = \cos\vartheta\,.$$

Complex Mie's coefficients a_n, b_n are given by

$$a_n = \frac{\bar{a}\ \mathrm{Re}\ w_n(x) - \mathrm{Re}\ w_{n-1}(x)}{\bar{a}_n w_n(x) - w_{n-1}(x)}$$

$$b_n = \frac{\bar{b}_n\ \mathrm{Re}\ w_n(x) - \mathrm{Re}\ w_{n-1}(x)}{\bar{b}_n\ w_n(x) - w_{n-1}(x)}\,, \tag{16}$$

where

$$\bar{a}_n = A_n(y)/m + n/x\,,$$

$$\bar{b}_n = A_n(y)/m + n/x\,.$$

The complex functions $A_n(y)$, $w_n(x)$ are computed according to the recurrence formulae

$$A_n(y) = (n/y - A_{n-1}(y))^{-1} - n/y \tag{17}$$

with the initial value

$$A_0(y) = \cos y/\sin y\,,$$

and

$$w_n(x) = \frac{2n-1}{x}\, w_{n-1}(x) - w_{n-2}(x) \tag{18}$$

with the initial values

$$w_0(x) = \sin x + \mathrm{i}\cos x\,, \quad w_{-1}(x) = \cos x - \mathrm{i}\sin x\,.$$

Thus, the scattering matrix M expressed by i_1, i_2, σ functions (the i-normalized form M_i) is

$$\begin{pmatrix} .5(i_1 + i_2) & .5(i_2 - i_1) & 0 & 0 \\ .5(i_2 - i_1) & .5(i_1 + i_2) & 0 & 0 \\ 0 & 0 & \sqrt{(i_1 i_2)}\cos\sigma & -\sqrt{(i_1 i_2)}\sin\sigma \\ 0 & 0 & \sqrt{(i_1 i_2)}\sin\sigma & \sqrt{(i_1 i_2)}\cos\sigma \end{pmatrix} \tag{19}$$

and the efficiency factors Q, defined by means of the efficient cross-sections C as

$$Q = C/(\pi a^2) \tag{20}$$

for extinction, scattering, absorption and radiation pressure respectivelly, are

$$\begin{aligned} Q_{\mathrm{ext}} &= 2x^{-2}\sum_{n=1}^{\infty}(2n+1)\,\mathrm{Re}(a_n + b_n) \\ Q_{\mathrm{scatt}} &= 2x^{-2}\sum_{n=1}^{\infty}(2n+1)\,(a_n^* a_n + b_n^* b_n) \\ Q_{\mathrm{abs}} &= Q_{\mathrm{ext}} - Q_{\mathrm{scatt}} \\ Q_{\mathrm{pres}} &= Q_{\mathrm{ext}} - g\,.\,Q_{\mathrm{scatt}} \\ g\,.\,Q_{\mathrm{scatt}} &= 4x^{-2}\sum_{n=1}^{\infty}\left\{\frac{n(n+2)}{n+1}(\mathrm{Re}\,a_n\,\mathrm{Re}\,a_{n+1} + \mathrm{Im}\,a_n\,\mathrm{Im}\,a_{n+1} + \right. \\ &\left. + \mathrm{Re}\,b_n\,\mathrm{Re}\,b_{n+1} + \mathrm{Im}\,b_n\,\mathrm{Im}\,b_{n+1}) + \frac{2n+1}{n(n+1)}(\mathrm{Re}\,a_n\,\mathrm{Re}\,b_n + \mathrm{Im}\,a_n\,\mathrm{Im}\,b_n)\right\} \end{aligned} \tag{21}$$

$$albedo = Q_{\mathrm{scatt}}/Q_{\mathrm{ext}}\,.$$

The eq. (10), (21) may be combined to yield

$$\Phi(\vartheta) = \frac{1}{4\pi}(S_1^* S_1 + S_2^* S_2) / \sum_{n=1}^{\infty} (2n + 1)(a_n^* a_n + b_n^* b_n) . \tag{22}$$

By analogy f-normalized form of scattering matrix M_f may be written, using

$$f_j(\vartheta) = i_j(\vartheta) \sin \vartheta / (x^2 Q_{\text{scatt}}) , \tag{23}$$

where $j = 1, 2$, and

$$f = .5(f_1 + f_2) . \tag{24}$$

3. Basic Equations

According to the generally used Monte Carlo scheme, the transfer of radiation is taken as the "history" of many individual quanta, not identical with photons, but behaving in the same manner, travelling through the scattering medium until they leave it. The quantities characterizing the physical stage of the quantum are:

i) the Stokes vector-parameters I, Q, U, V (defined elsewhere, e.g. in Hulst (1957));

ii) the co-moving reference orthonormal right-handed basis $\boldsymbol{r}\,\boldsymbol{l}\,\boldsymbol{p}$, with respect to which I, Q, U, V are expressed; $\boldsymbol{p}$ represents the direction of the quantum;

iii) the coordinates x, y, z in the model of the scattering medium, e.g. the circumstellar cloud;

iv) the number N of scattering events since the emission of the quantum.

Thus, the history of each quantum emitted by the radiation source consists of a sequence of scattering-absorption events and the free motions between them. Both these events have a random nature, and specifying their probability density functions is the aim of the following paragraphs.

Every probability density function $p(A)$ of an one-dimensional random quantity $A \in \langle a, b \rangle$ must satisfy the condition

$$\int_a^b p(A)\, \mathrm{d}A = 1 . \tag{25}$$

The Monte Carlo modelling of a sequence of numbers $A_1, A_2, \ldots A_n$ with a given probability density $p(A)$ is based on the solution of equation

$$R_i = \int_a^{A_i} p(A)\, \mathrm{d}A , \tag{26}$$

where $R_i \in \langle 0, 1 \rangle$ is a number taken from the set of equally probable random numbers, supplied by a special routine. I have used the congruential algorithm of generating numbers R_i that is included in the Science Subroutine Package for IBM 360.

a) Modelling of the Free Path

In a partially absorbing medium with the absorption coefficient $\varkappa$, the length l of free path has the Poisson's distribution

$$p(l) = \varkappa(l) \exp\left(- \int_0^l \varkappa(l) \, \mathrm{d}l \right), \tag{27}$$

where l is used also as the coordinate, so that $\varkappa(l)$ is the value of absorption coefficient at the end of free path.

i) If $\varkappa = const.$, then (27) put in (26) gives

$$\ln(1 - R) = -\varkappa l ,$$

where $1 - R$ has the same probability distribution as R and therefore

$$l = -\frac{1}{\varkappa} \ln R . \tag{28}$$

$1/\varkappa$ is the mean value of the Poisson's distribution and has the meaning of the mean free path.

ii) If $\varkappa < \varkappa_{\max}$ is slowly varying, the algorithm by Coleman (1968) can be applied. Two sequences of random numbers are computed:

$$R_1, R_2, \ldots, R_n$$

defined above, and

$$Z_1, Z_2, \ldots, Z_n$$

with the probability density

$$\varkappa_{\max} \exp(-\varkappa_{\max} \cdot Z) ,$$

until the unequality in condition

$$R_n \leqq \varkappa(l_n)/\varkappa_{\max} \tag{29}$$

is reached, where $l_n = \sum_{k=1}^{n} Z_k$ is the computed value of the free path. With respect to the frequency, with which the validity of the condition (29) sets in, this algorithm reveals advantageous for $\varkappa/\varkappa_{\max} \gtrsim 0.1$ only.

iii) In case of strongly varying $\varkappa$ the cloud can be divided into a set of elementary

cartesian cells, fully described by subscripts ix, iy, iz in the reference frame of the cloud, and the corresponding values of $\varkappa(ix, iy, iz)$. Furthermore, the subscripts with respect to the starting point of the free path are needed. The free path breaks up into small segments Δl_i of varying length, to which correspond the optical equivalents $\Delta\tau_i = \varkappa(ix, iy, iz)\,\Delta l_i$. The eq. (26) can be written in the form

$$R = \Delta\tau_1 \exp(-\Delta\tau_1) + \Delta\tau_2 \exp(-\Delta\tau_1 - \Delta\tau_2) + \ldots = \sum_{n=1}^{\infty} A_n , \tag{30}$$

where for the term A_n the recurrence formula

$$A_n = A_{n-1} \frac{\Delta\tau_n}{\Delta\tau_{n-1}} \exp(-\Delta\tau_n) \tag{31}$$

is valid. Computing the actual length l, the terms in (30) must be added until the value R is reached, and then l is the sum of the corresponding number of segments Δl.

iv) In the disc-like circumstellar clouds, the absorption coefficient may depend strongly on the coordinate z perpendicular to the symmetry plane of the disc, while in this plane it varies only slowly. Let ∇_z and ∇_r denote the corresponding gradients of absorption coefficient, then $|\nabla_z| \gg |\nabla_r|$, $\nabla_z < 0$ and usually $\nabla_r < 0$. At a short distance ξ from the point P_0 (with $\varkappa_0$), $\varkappa$ is given by

$$\varkappa = \varkappa_0 + \nabla_r \xi \sqrt{(p_x^2 + p_y^2)} + \nabla_z \xi p_z = \varkappa_0 + \nabla \cdot \xi , \tag{32}$$

where $\boldsymbol{p} = (p_x, p_y, p_z)$. The eq. (32) together with (26) leads to

$$R = \int_0^l (\varkappa + \nabla \cdot \xi) \exp(-(\varkappa + .5\nabla\xi)\,\xi)\, \mathrm{d}\xi , \tag{33}$$

in which the integrand can be expanded and integrated term by term as follows:

$$R = \int_0^l (\varkappa + \nabla\xi) \sum_{k=0}^{\infty} \frac{1}{k!} (\varkappa + 5\nabla\xi)^k\, \xi^k (-1)^k \,\mathrm{d}\xi = \tag{34}$$

$$= \sum_{k=0}^{\infty} \sum_{j=0}^{k} \frac{(-1)^k}{j!(k-j)!} \varkappa^{k-j} \left(\frac{\nabla}{2}\right)^j l^{k+j+1} \left(\frac{\varkappa}{k+j+1} + \frac{\nabla \cdot l}{k+j+2}\right).$$

The first five terms have the following coefficients:

$$\begin{aligned} &1: \ \varkappa \\ &2: \ \tfrac{1}{2}(\nabla - \varkappa^2) \\ &3: \ \tfrac{1}{6}(\varkappa^3 - 3\nabla\varkappa) \\ &4: \ \tfrac{1}{24}(6\nabla\varkappa^2 - 3\nabla^2 - \varkappa^4) \\ &5: \ \tfrac{11}{120}(\varkappa^5 - 10\nabla\varkappa^3 + 15\nabla^2\varkappa) . \end{aligned} \tag{35}$$

Since the series (34) converges on an arbitrary finite interval $(0, M)$, $M < \infty$, its expression can be converted to

$$l = \alpha_1 R + \alpha_2 R^2 + \alpha_3 R^3 + \alpha_4 R^4 + \ldots \tag{36}$$

with coefficients

$$\begin{aligned}
\alpha_1 &= \frac{1}{\varkappa} \\
\alpha_2 &= \frac{1}{\varkappa^3}(-V + \varkappa^2) \\
\alpha_3 &= \frac{1}{6\varkappa^5}(-\varkappa^4 + 3V\varkappa^2 + 33\varkappa^2 - 6V\varkappa + 3V^2) \\
\alpha_4 &= \frac{1}{24\varkappa^7}(6\varkappa^6 - 11V\varkappa^4 + 18V^2\varkappa^2 - 15V^3)
\end{aligned} \tag{37}$$

The computational procedure must take also into account the higher terms in (36), since the α_1 represents only the mean free path.

b) Modelling of the New Direction of the Quantum after Scattering

In order to achieve the actual picture of scattering, one must consider the probability density function of the directions after scattering as proportional to the scattering indicatrix. The shape of the indicatrix $I(\vartheta, \varphi)$ depends, however, on the degree of polarisation of the incident beam, too. This beam can be regarded as a composition of the two following fractions: the fully linearly polarized fraction with intensity I_p, and the unpolarized fraction (including circularly polarized component) with intensity I_n; i.e.

$$\begin{aligned}
I_p &= \sqrt{(Q^2 + U^2)} \\
I_n &= I - \sqrt{(Q^2 + U^2)}\,.
\end{aligned} \tag{38}$$

In the direction given by angles ϑ, φ the intensity $I(\vartheta, \varphi)$ can be expressed as follows:

$$I(\vartheta, \varphi) = I_n \,.\, \tfrac{1}{2}(i_1 + i_2) + I_p(i_1 \sin^2 \varphi + i_2 \cos^2 \varphi)\,, \tag{39}$$

if the scattering particles are characterized by the Mie's theory.

In order to obtain probability density function which depends only on ϑ, the eq. (39) should be integrated over $\varphi \in \langle 0°, 360° \rangle$, normalized and cast into (26), which then has the following form

$$R = \tfrac{1}{2} \int_0^{\vartheta} (f_1 + f_2) \sin \vartheta \, \mathrm{d}\vartheta\,. \tag{40}$$

From (40), the random value of ϑ can be calculated by interpolating in the tables of this integral as function of the upper boundary.

Let us return to (39) and normalize it to obtain the probability density function $p(\vartheta, \varphi)$

$$p(\vartheta, \varphi) = \frac{\Phi_1 + \Phi_2}{2.\,albedo} - \frac{\Phi_1 - \Phi_2}{2.\,albedo}\, p \cos 2\varphi\,, \tag{41}$$

where p is the degree of polarisation of the incident beam. Eq. (41) and (26) give

$$4\pi R = 2\varphi - p\,.\,\frac{\Phi_1 - \Phi_2}{\Phi_1 + \Phi_2}\,.\,\sin 2\varphi\,, \tag{42}$$

from where φ can be calculated. This equation has a similar form as Kepler's equation and also the methods of solution are the same. If the incident beam is only slightly polarized, the second term on the right-hand side vanishes and (42) transforms in the simple

$$\varphi = 2\pi R\,, \tag{43}$$

the equation widely used in common Monte Carlo schemes to calculate the tilt angle φ.

The differences between (42) and (43) are shown in Table I. The values φ computed according to (43) are in the first column, the values computed according to (42) are in the remaining columns, using the same R in the whole line. The capital A denotes the value of the term $p\,.\,[(\Phi_1 - \Phi_2)/(\Phi_1 + \Phi_2)]$.

Table 1.

φ \ A	−0.05	−0.1	−0.5	−0.7	−0.8	−0.9
0	0	0	0	0	0	0
15	16	16	22	25	26	28
30	31	32	42	47	50	52
45	46	48	59	65	68	71
60	61	62	72	77	80	82
75	76	76	82	85	86	88
90	90	90	90	90	90	90

4. The Computational Procedure

Two groups of parameters are required to specify the case of a model cloud: a) parameters describing the geometry of the nebula, including the shape, the nature of the radiation source and the orientation of the whole object with respect to the

distant observer, and the space distribution of dust particles of various types within the nebula; b) parameters describing the behaviour of a dust particle in case of collision with the quantum. We have thus a very wide range of input parameters on which we need not lay any further simplifying restrictions. However, in some models it may be convenient to make the best use of the symmetry, which allows us to avoid the time consuming computations.

The versatility of the Monte Carlo scheme lies in the possibility of building-up the computer routine as a sequence of procedures, each one with its own functions. The main cycle consists of the four labelled procedures:

EMISSION:

The initial quantum space coordinates in the nebula with a pointlike source are the same for all quanta, namely $x = y = z = 0$, but in principle any other choice is possible. The emitting radiation is assumed to be unpolarized, so that the initial Stokes vector is $I = 1$, $Q = U = V = 0$. The initial reper $\boldsymbol{rlp}$ is determined. The number of quanta emitted is checked, and if the demanded number is reached, the control transfers to the procedure **LAYOUT**, otherwise the **FREE PATH** continues.

FREE PATH:

Using one of the ways listed in the part 3a (Modelling of the free path) the length of the free path is computed and the coordinates of its end are determined and checked. If the endpoint is not inside the nebula, the computation turns back to the last preceeding endpoint, where the "splitting" and the "forced last scattering" occur. The trajectory of the quantum ramifies to several fixed directions, wherefrom we wont to observe the nebula. The last scattering is therefore not random, but determined by these directions. The control transfers to the **RECORD** of Stokes parameters of emerging quantum. This procedure specifies also the output points on the surface, or on the projection of the nebula along the corresponding direction. The next step leads to **EMISSION**. The quantum remaining in the cloud continues on the **SCATTERING**.

SCATTERING:

Using the eq. (40), the scattering angle ϑ is computed and by use of (43) or (42) the tilt angle φ is determined. As the Stokes parameters before scattering must be expressed with respect to the reper, having $\boldsymbol{l}$ in the half-plane of scattering, the rotation around old $\boldsymbol{p}$ by φ is needed. Thus, if we look in the direction of the quantum motion and rotate counterclockwise the pair $\boldsymbol{r}$, $\boldsymbol{l}$ (so that φ is the angle between the old and the new vector $\boldsymbol{r}$), the new reper $\boldsymbol{rlp}$ in form of the 3×3 matrix $\begin{pmatrix} \boldsymbol{r} \\ \boldsymbol{p} \\ \boldsymbol{l} \end{pmatrix}$ is obtained by

matrix multiplication by

$$\begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{44}$$

and the new set I, Q, U, V is obtained by multiplication by

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\varphi & -\sin 2\varphi & 0 \\ 0 & \sin 2\varphi & \cos 2\varphi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{45}$$

In the course of scattering, the reper rotates around $\boldsymbol{r}$ by ϑ; the corresponding matrix multiplication must be applied using

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\vartheta & -\sin\vartheta \\ 0 & \sin\vartheta & \cos\vartheta \end{pmatrix} \tag{46}$$

Only now the Stokes parameters may be transformed by scattering matrix (19). In order to unify the scattering and absorption events, we normalize the resulting I, Q, U, V set, so that for intensity I_0 and I before and after the scattering, the relation

$$I = I_0 \,.\, albedo \tag{47}$$

must hold. Hence, the intensity is decreased as if a part the energy quantum were lost by absorption.

The control is then given to **FREE PATH.**

LAYOUT:

For each demanded fixed direction and for each surface element of the nebula, the Stokes parameters of the emerging quanta have been added and stored. The intensity, the degree of linear polarisation p_l and circular polarisation p_c can be evaluated as follows:

$$p_l = \sqrt{(Q^2 + U^2)}/I \tag{48}$$

$$p_c = V/I$$

$$\chi = (180°/\pi)\,\mathrm{arctg}\,U/Q \quad \text{for} \quad Q \neq 0$$

and

$$\chi = 45° \,.\, \mathrm{sign}\,U \quad \text{for} \quad Q = 0\,,$$

where χ is measured clockwise from $\boldsymbol{r}$, if looking in the propagation direction.

5. Discussion

The accuracy and speed of the Monte Carlo calculation depends on the geometry of the nebula and on the number N of quanta used, but the accuracy increases only as $\sqrt{N}$. In the most symmetrical case – sphere with central source, however, the number of quanta needed varies about 1000.

The choice of the actual indicatrix for the density probability function for evaluation of the new $\boldsymbol{p}$ is essential, since it minimizes the dispersion of the method, as will be shown below. If considering a particle with $g \to 1$, the indicatrix $F_g(\boldsymbol{p}_0, \boldsymbol{p})$ becomes

$$\lim_{g \to 1} F_g(\boldsymbol{p}_0, \boldsymbol{p}) = \delta(\boldsymbol{p}_0 - \boldsymbol{p}), \tag{49}$$

as the particle throws all the scattered light forward. If another probability density $p(\boldsymbol{p}_0, \boldsymbol{p})$ is applied to determine the new $\boldsymbol{p}$, then the eq. (47) must be replaced by

$$I = I_0 \,.\, albedo \,.\, \frac{F_g(\boldsymbol{p}_0, \boldsymbol{p})}{p(\boldsymbol{p}_0, \boldsymbol{p})}, \tag{50}$$

to achieve the actual energy distribution after scattering. Hence, in the limit $g \to 1$, the right-hand side converts to $\delta(\boldsymbol{p}_0 - \boldsymbol{p})$ and $I = 0$ for $\boldsymbol{p} \neq \boldsymbol{p}_0$, while for $\boldsymbol{p} = \boldsymbol{p}_0$ it remains undetermined. There are many other aspects that may be discussed only in connection with the real model of scattering nebula.

6. Conclusion

A practical method for computing the radiation transfer has been described, including the multiple and anisotropic scattering. Results of model calculation and a discussion of the importance of various model parameters will be presented in future papers.

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