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MULTIPLE SCATTERING IN REFLECTION NEBULAE. I. A MONTE CARLO APPROACH

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ABSTRACT

A method is described which permits the calculation of the surface brightness distribution on a plane-parallel reflection nebula of uniform density, illuminated by a single star located in front of, behind, or arbitrarily inside the nebula. The multiple scattering problem is solved by the Monte Carlo technique in a three-dimensional simulation. The models are completely parametrized by describing particle properties by their single-scattering albedo and by an analytic phase function with one or three parameters. The computations are thus independent of wavelength or assumed size distributions of the scattering particles and are therefore particularly suited for the analysis of observations of the surface brightness of reflection nebulae in spectral regions, such as the ultraviolet, for which detailed particle models are still uncertain.

Subject headings: interstellar: matter — nebulae: general — radiative transfer

I. INTRODUCTION

One of the oldest methods for investigating the nature of interstellar grains has been the study of reflection nebulae. For a thorough review of the subject up to 1967 we refer to Vanysek (1969) and the references contained therein. Since then, much of the work has concentrated on the analysis of color differences between nebulae and illuminating stars and on nebular polarization (e.g., Greenberg and Hanner 1970; Hanner 1971; Zellner 1973). The principal weakness of these studies has been the dependence on single-scattering radiative transfer models which were applied to some of the brightest, certainly *not* optically thin reflection nebulae. The important influence of multiple scattering on nebular polarization has been evaluated by Vanysek and Solc (1973), and Roark, Roark, and Collins (1974) have shown that multiple scattering has a significant effect on nebular surface brightness gradients, because the multiplicity of scattering is increasing strongly with angular distance from the illuminating star. The last two investigations were based on the use of the Monte Carlo method for the treatment of the multiple scattering problem. This versatile technique has been applied to other cases of interstellar scattering by Mattila (1970) and Witt and Stephens (1974), and examples of the successful application of Monte Carlo models to the interpretation of observational data are contained, for example, in the studies of FitzGerald, Stephens, and Witt (1976) and Andriesse, Piersma, and Witt (1977).

The present paper, a brief description of the computational approach, is the first in a series devoted to the surface brightness of reflection nebulae in the presence of multiple scattering. We shall use the Monte Carlo technique to find solutions to the radiative transfer problem for a wide range of parameters describing the star-nebula geometry. However, we shall deviate from the practice of most previous investigators, in particular that of Roark, Roark, and Collins (1974), by using a simple parameter description of the scattering particles instead of employing grains of an assumed composition with an ad hoc size distribution. Our approach will have the advantage of avoiding the unnecessary uncertainties inherent in using scattering properties calculated by Mie's theory for homogeneous, spherical particles for properties of real grains, especially in wavelength regions where optical constants are poorly known or even unavailable. Instead, we are providing fully parametrized models for reflection nebulae, applicable to a wide range of wavelengths and/or optical depths which will allow the prediction of actual surface brightness isophotes and the quantitative evaluation of multiple scattering effects as a function of each individual model parameter. We shall begin by studying the case of a plane-parallel nebula of uniform density illuminated by a star located either in front of, behind, or arbitrarily inside the scattering medium.

II. RADIATIVE TRANSFER IN A PLANE-PARALLEL REFLECTION NEBULA

a) The Monte Carlo Principle

Following the detailed discussion by Cashwell and Everett (1959), we will describe the transfer of radiation by following the history of many individual photons until these leave the scattering medium. Quantities describing the photon trajectories such as direction of original emission, direction following scattering, and path length between scatterings may be considered as random variables, each being characterized by some probability density function $p(x)$

defined for an interval (a, b) such that

$$\int_a^b p(\xi)d\xi = 1 . \quad (1)$$

We can simulate a random event for which the variable falls with frequency $p(x)dx$ in the interval $(x, x + dx)$ by choosing a random number R from a uniform distribution $0 \leq R \leq 1$, and requiring

$$R = \int_a^x p(\xi)d\xi . \quad (2)$$

Sequences of pseudo-random numbers can easily be produced as part of the model calculations, using one of various congruential generators which are supplied as part of the operating system of large digital computers. Janson (1966) gives an extensive account of such random number generators and the method of testing them.

b) Model Parameters

Three groups of parameters are required to specify the case of a simple plane-parallel reflection nebula: (i) parameters describing the star-nebula system; (ii) parameters describing the scattering properties of the nebular grains; (iii) parameters describing the orientation of the star-nebular system with respect to a distant observer. Only the first two categories of parameters actually affect the radiative transfer, while the third set of parameters becomes important for the observed appearance of the nebula.

The star-nebula geometry is illustrated in Figure 1. For practical purposes the nebula is assumed to be finite and the cylindrical boundary is chosen for its symmetry properties. As in the study of Roark, Roark, and Collins (1974), only photons leaving the front or back surface will be considered, while photons escaping through the cylindrical wall will be disregarded. If one chooses the nebular radius r sufficiently large, this photon leakage will not noticeably affect the surface brightness in the observationally interesting portions of the nebula. The star's position on the cylinder axis at a distance z_* from the back face of the cylinder, combined with the cylinder thickness z_c, defines the relative geometry. The density of the scattering particles in the plane-parallel cylinder is assumed to be uniform and is measured by τ_0/z_c, where τ_0 is the optical thickness of the model nebula measured along the cylinder axis.

The scattering properties of the nebular particles can be parametrized in the simplest manner by specifying the albedo, a, for single scattering and the phase function $\phi(\alpha)$. A very versatile yet simple analytical form for $\phi(\alpha)$ has been suggested by Henyey and Greenstein (1941):

$$\phi(\mu, g) = [(1 - g^2)/4\pi](1 + g^2 - 2g\mu)^{-3/2} . \quad (3)$$

Here, $\mu = \cos \alpha$, where α is the scattering angle measured with respect to the original photon direction

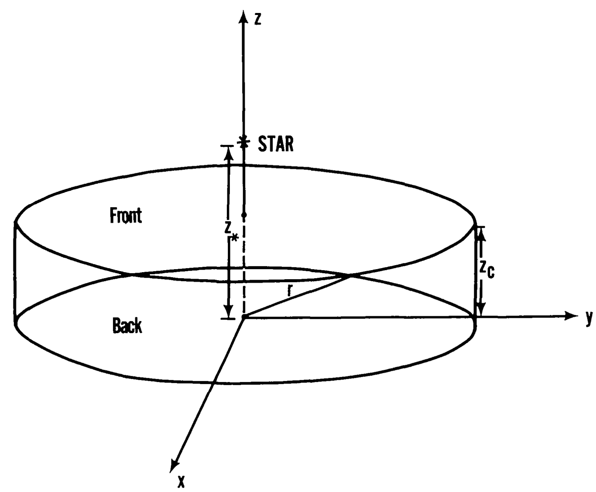

FIG. 1.—Definitions of the coordinate system and the geometric parameters describing the star-nebula system.

and g is the asymmetry factor. With g in the range $-1 < g < +1$ it is possible to characterize phase functions ranging from a completely backward-throwing to a completely forward-throwing form. However, with the one-parameter function in equation (3) it is not possible to describe simultaneous forward and backward lobes which are typical in many cases of Mie scattering as well as Rayleigh scattering. For this reason we have also studied selected cases using a three-parameter analytic phase function which was previously suggested by Irvine (1965, 1968, 1971) and was recently discussed by Kattawar (1975). This function results from the superposition of two Henyey-Greenstein phase functions,

$$\phi(\mu, g_1, g_2) = f\phi(\mu, g_1) + (1 - f)\phi(\mu, g_2) , \quad (4)$$

where $\phi(\mu, g_1)$ and $\phi(\mu, g_2)$ each are of the form given by equation (3) and f is a suitably chosen number $0 < f < 1$. The particles are assumed to be randomly oriented in the nebula so that the phase function can be assumed to be independent of the azimuthal angle of scattering.

The third set of parameters, shown in Figure 2, includes the radial coordinate of the exit position, r_f or r_b, of the photon on the front or back surface of the nebula, respectively; the azimuth angle, θ, of this exit position measured in the plane of the nebula with respect to the y-axis; the azimuth angle, Ω, of the exit direction measured at the exit position in the same sense as θ; and, finally, the polar angle, Ψ, between the photon exit direction and the nebular axis. Polar angles in the range $0° \leq \Psi < 90°$ correspond to exits from the "front" surface of the nebula, while angles $90° < \Psi \leq 180°$ correspond to exits from the "back" surface. For this work it will be assumed that the observer is located somewhere in the y-z plane.

c) Photon Source

The positions and directions of individual photons are measured by their coordinates (x, y, z) and direction

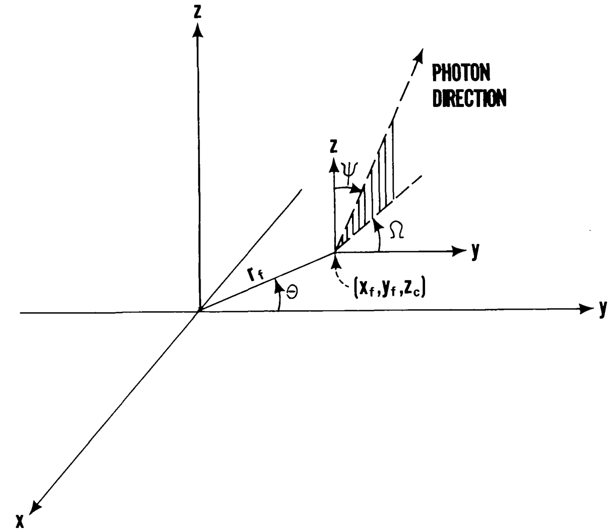

FIG. 2.—Parameters used in the classification of photons after leaving the nebula. The x-y plane is identical with the nebular front surface.

cosines (u, v, w) as defined by the coordinate system in Figure 1. The illuminating star is considered a point source located at $(0, 0, z_*)$, emitting photons isotropically.

Two cases must be distinguished. If the star is inside the nebula, or $0 < z_* < z_c$, source photons are characterized by $-1 \leq (u_0, v_0, w_0) \leq +1$ and the directions (u_0, v_0, w_0) of individual photons must be uniformly distributed on the unit sphere $u_0^2 + v_0^2 + w_0^2 = 1$. If R_i is a random number in the interval [0, 1], this is accomplished by letting

$$w_0 = 2R_i - 1\,, \tag{5}$$

and if R_{i+1} is another random number in the same interval,

$$u_0 = (1 - w_0^2)^{1/2} \cos [\pi(2R_{i+1} - 1)]\,, \tag{6}$$

$$v_0 = (1 - w_0^2)^{1/2} \sin [\pi(2R_{i+1} - 1)]\,. \tag{7}$$

The initial photon space coordinates in the nebula in this case are the same for all photons, namely $x_0 = 0$, $y_0 = 0$, $z_0 = z_*$.

A second case arises when the star is outside the nebula, or $z_* \geq z_c$. Now, we are interested only in those photons which are radiated isotropically into the solid angle subtended by the "front" surface of the nebula as seen from the star, or $-1 \leq (u_0, v_0) \leq +1$, but $-1 \leq w_0 \leq w_L$. The limiting direction cosine with respect to the z-axis is given by

$$w_L = \cos [\![\pi - \cos^{-1}\{(z_* - z_c)/[r^2 + (z_* - z_c)^2]^{-1/2}\}]\!]\,. \tag{8}$$

If R_i and R_{i+1} are some random numbers as before, we find isotropically directed photons for the solid angle under consideration from

$$w_0 = R_i[1 + w_L] - 1\,, \tag{9}$$

and by applying equations (6) and (7) for this value of w_0.

Photons emitted from a star with $z_* \geq z_c$ will in general enter the "front" surface of the nebula at different points. With the direction cosines u_0, v_0, w_0 of these photons, the entry coordinates are

$$x_0 = u_0(z_* - z_c)/\cos (\pi - \cos^{-1} w_0)\,, \tag{10}$$

$$y_0 = v_0(z_* - z_c)/\cos (\pi - \cos^{-1} w_0)\,, \tag{11}$$

$$z_0 = z_c\,. \tag{12}$$

d) First Scattering

If the optical thickness of the nebula along a given photon direction originating in the star is designated τ_1, a fraction $\exp(-\tau_1)$ of the photons emitted in this direction traverses the nebula without a single scattering. We are interested in the remaining fraction $[1 - \exp(-\tau_1)]$ of photons which are scattered at least once and shall concentrate on these, using the concept of *forced first scattering* described by Cashwell and Everett (1959).

We can find the free path length $\tau \leq \tau_1$ to the point of forced first scattering from equation (2) by letting

$$R = \frac{\int_0^\tau e^{-\xi} d\xi}{\int_0^{\tau_1} e^{-\xi} d\xi} = \frac{1 - \exp(-\tau)}{1 - \exp(-\tau_1)}\,, \tag{13}$$

which reduces to

$$\tau = \ln\{1 - R[1 - \exp(-\tau_1)]\}\,. \tag{14}$$

In this manner all photons entering the nebula will be scattered at least once. One corrects for this unnatural situation by reducing the weight, W_0, of each original photon from unity to $W_0 = 1 - \exp(-\tau_1)$. A significant enhancement of computing efficiency results from this procedure, especially in the case of small optical thickness. Analytical expressions for τ_1 in the geometry illustrated in Figure 1 for both cases $z_* \geq z_c$ and $z_* < z_c$ can be found using elementary trigonometric relationships, and these will not be reproduced here.

The physical path length l corresponding to the optical free path is given by

$$l = \tau \frac{z_c}{\tau_0}\,, \tag{15}$$

where τ_0 is as before the optical thickness of the model nebula measured along the cylinder axis. We can then find the space coordinates (x_1, y_1, z_1) of the point of first scattering from

$$x_1 = x_0 + u_0 l\,, \quad y_1 = y_0 + v_0 l\,, \quad z_1 = z_0 + w_0 l\,, \tag{16}$$

where (x_0, y_0, z_0) and (u_0, v_0, w_0) are the entry space coordinates and initial direction cosines, respectively.

e) Weight, Photon Direction, and Path Length after First Scattering

The photons interact with particles having a single-scattering albedo a. Each time there is a probability

$(1 - a)$ that the interaction is an absorption, resulting in the elimination of a photon from the radiation field. Rather than simulating actual absorption, we shall retain all photons with their accumulated history by simply reducing their weight following each interaction by multiplying the previous weight with the probability for scattering. After the first scattering we have, therefore, the reduced weight

$$W_1 = aW_0\,. \tag{17}$$

The probability distribution for the direction change following scattering is determined by the phase function. For the Henyey-Greenstein phase function (3) and a random photon, we can set

$$R = 2\pi \int_{-1}^{\mu_1} \phi(\mu, g)d\mu\,, \tag{18}$$

and we find upon integration that

$$\mu_1 = \{(1 + g^2) - [(1 - g^2)/(1 - g + 2gR)]^2\}/2g\,. \tag{19}$$

Here, $\mu_1 = \cos \alpha_1$, where α_1 is the deflection angle of the new photon path with respect to the previous direction, measured in the plane formed by the old and new photon paths. Due to the assumed azimuthal symmetry of the phase function, the azimuthal orientation of this plane is taken at random from a uniform distribution.

When the three-parameter analytic phase function (4) is used, we find

$$R = \frac{f}{2g_1}[(1 - g_1^2)(1 + g_1^2 - 2g_1\mu_1)^{-1/2} - (1 - g_1)] + \frac{(1-f)}{2g_2}[(1 - g_2^2)(1 + g_2^2 - 2g_2\mu_1)^{-1/2} - (1 - g_2)]\,. \tag{20}$$

This equation was used to supply the program with a detailed table relating values of μ_1 over the interval $[-1, +1]$ to numbers R from the interval $[0, 1]$. Subsequently, deflections μ_1 were obtained by entering this table with random numbers R, using a linear interpolation technique.

The computation of new direction cosines is discussed in full detail by Cashwell and Everett (1959) in chapter 7 of their monograph, and we shall quote their results for completeness. If u_0, v_0, w_0 are the initial direction cosines as determined in § II*c*, if α_1 is the deflection angle found above, and if ϕ_1 is the change in azimuth derived from

$$\phi_1 = \pi(2R - 1)\,, \tag{21}$$

then the new direction cosines are

$$u_1 = (\sin \alpha_1 \cos \phi_1 w_0 u_0 - \sin \alpha_1 \sin \phi_1 v_0)/(1 - w_0)^{1/2} + \cos \alpha_1 u_0\,,$$

$$v_1 = (\sin \alpha_1 \cos \phi_1 w_0 v_0 + \sin \alpha_1 \sin \phi_1 u_0)/(1 - w_0)^{1/2} + \cos \alpha_1 v_0\,,$$

$$w_1 = -\sin \alpha_1 \cos \phi_1 (1 - w_0)^{1/2} + \cos \phi_1 w_0\,. \tag{22}$$

As w_0 approaches unity, equations (22) break down and are replaced by

$$u_1 = \sin \alpha_1 \cos \phi_1\,, \quad v_1 = \sin \alpha_1 \sin \phi_1\,, \quad w_1 = \cos \alpha_1 w_0 \quad \text{for } w_0 \geq 0.99\,. \tag{23}$$

The free path length, τ_2, following first scattering is now computed according to equation (2) as

$$R = \int_0^{\tau_2} e^{-\xi} d\xi = 1 - \exp(-\tau_2)\,, \tag{24}$$

which leads to

$$\tau_2 = -\ln R\,. \tag{25}$$

f) Final Photon Classification

Following the initial scattering, the coordinates of the site of a potential second scattering can be found using equations (15) and (16). Second and higher order scatterings occur as long as the coordinates of the photon fail to satisfy at least one of the following conditions:

$$z_n > z_c\,, \quad z_n < 0\,, \quad x_n^2 + y_n^2 > r^2 \quad (n = 2, 3, 4, \ldots)\,, \tag{26}$$

which indicate that the photon is outside the nebula. If scatterings subsequent to the first take place, the photon behavior can be followed by repeating the procedures described in § II*e*.

Once a photon has left the nebula, its coordinates will satisfy one or more of the conditions of equation (26). It now needs to be classified according to its exit direction and the location of its exit point on the nebular surface. If u_n, v_n, w_n are the final direction cosines, photons with $0 \leq w_n \leq +1$ exited through the front surface of the nebula or the cylinder wall. We can eliminate those leaving through the cylinder wall by retracing the respective photon paths to a point $z_f = z_c$ for the first group and finding their corresponding coordinates x_f and y_f at the level of the front surface. If the point (x_f, y_f) lies outside the periphery of the front surface, the photon has made its exit through the cylinder wall. Similarly, photons with $0 \geq w_n \geq -1$ include those having left through the back surface as well as through the wall. Similarly, we retrace the photon paths to a point $z_b = 0$ for this group with corresponding coordinates x_b and y_b. Countable front surface photons are characterized by

$$x_f^2 + y_f^2 = r_f^2 \leq r^2\,, \tag{27}$$

and those having left through the back surface by

$$x_b^2 + y_b^2 = r_b^2 \leq r^2\,, \tag{28}$$

where r_f and r_b are the respective radial distances of the exit positions from the cylinder axis.

The angle between the photon direction and the positive z-direction is given by

$$\Psi = \cos^{-1} w_n , \qquad (29)$$

while the azimuthal angle of the photon direction is

$$\Omega = \cos^{-1}\left[\frac{v_n}{(1 - w_n^2)^{1/2}}\right], \quad u \leq 0 ,$$

or

$$\Omega = 2\pi - \cos^{-1}\left[\frac{v_n}{(1 - w_n^2)^{1/2}}\right], \quad u > 0 . \qquad (30)$$

In this form, the azimuthal angle is counted in the counterclockwise sense with respect to the z-y plane as shown in Figure 2.

A classification parameter more important than the azimuthal angle, Ω, itself is the difference between Ω and the azimuthal angle, θ, of the exit position (x_f, y_f, z_c) or $(x_b, y_b, 0)$. Due to the cylindrical symmetry, photons exiting into an element of polar angle, $d\Psi$, through an element of radial distance, dr_f, on the front surface can be considered part of the same pencil of radiation, as long as they are part of the same element of azimuth difference $d(\Omega - \theta)$. The same consideration naturally applies to the back surface. The azimuth θ of the exit position can be found by elementary means from the exit coordinates, and it should be counted in the same sense as Ω, the azimuth of the exit direction.

By grouping photons for a given polar angle interval according to radial coordinate and azimuth difference and by adding their final weights, it becomes possible to construct a map of the surface brightness distribution across the entire front and back face of the model reflection nebula.

g) Mean Numbers of Scatterings

The final weight of a photon at exit is

$$W_E = [1 - \exp(-\tau_1)]a^{n_i} \qquad (31)$$

where n_i is the number of times the particular photon has been scattered inside the nebula. The scattering multiplicity will vary from photon to photon and so will the distribution of photons over multiplicities for different parts of the nebula and different geometries. A useful measure for the importance of multiple scattering, however, can be defined by

$$m = \log\left(\frac{\sum_1^N a^{n_i}}{N}\right)\bigg/\log a , \qquad (32)$$

where N is the total number of photons leaving the nebula in a given exit bin defined by radial position, polar angle, and differential azimuthal angle. We shall refer to m as the *effective multiplicity* of scattering for a sample of N photons, each of which has been weighted according to the probability of its being lost due to absorption in the nebula. The parameter m may be used to assess the effect which changes in the albedo, optical depth, phase function, and geometry have on the importance of multiple scattering in reflection nebulae, and it can help to identify cases where single scattering approximations may be used with confidence. A detailed discussion of the variation of m with different model parameters and its relationship to the more frequently used mean number of scatterings is contained in Paper IV of this series (Witt 1977).

III. CALIBRATION OF PHOTON OUTPUT

a) Surface Brightness

The accumulated weights of photons per unit area and unit solid angle leaving different parts of the nebula surface are equivalent to a relative distribution of surface brightness and may be used to derive surface brightness gradients, as was done by Roark, Roark, and Collins (1974). Their work showed that different particle models produced rather similar relative surface brightness distributions, and it is clearly desirable to use the *calibrated* surface brightness itself as a distinguishing quantity. We accomplish this calibration by relating the nebular surface brightness per steradian to the flux from the illuminating star seen by a distant observer.

For the Monte Carlo model we define the intrinsic stellar luminosity, $\mathscr{L}$, as the number of photons emitted per steradian per model. If P is the total number of photons emitted by the star per model calculation, we have for the case $z_* \geq z_c$

$$\mathscr{L} = \frac{P[(z_* - z_c)^2 + r^2]}{\pi[\![r^2 + \{[(z_* - z_c)^2 + r^2]^{1/2} - (z_* - z_c)\}^2]\!]}, \qquad (33)$$

while the case with the star inside the nebula, $z_* < z_c$, reduces to

$$\mathscr{L} = \frac{P}{4\pi} . \qquad (34)$$

If the star is inside or behind the nebula, the observable luminosity is reduced by the nebular extinction factor $\exp(-\tau)$, where τ is the optical depth due to the nebula between star and observer.

The stellar flux received by the observer is of course distance-dependent, while the surface brightness of the nebula is not. We include this distance dependence into the ratio of these quantities by relating the intrinsic stellar luminosity, reduced for extinction, if required, to the number of nebular photons scaled as if these were emitted through an area corresponding to one steradian as seen at the position of the observer into a solid angle of one steradian. The ratio of the nebular photon luminosity thus defined to the stellar luminosity is equivalent to the quantity S/F, the ratio of nebular surface brightness per steradian to observed stellar flux as used in observational studies of reflection nebulae. While the model calculations are initially done for a standard distance, d_0, between nebula and observer, the predicted ratio S/F can be scaled to any other distance, d, through multiplication by $(d/d_0)^2$.

b) *Projected Nebular Face*

By classifying photons leaving the nebula according to their polar angle Ψ, we are able to study the effect of tilting the nebular face with respect to the plane of the sky. Since the tilt axis is the x-axis in Figure 1 according to our azimuth definition, the star's position will be projected onto the positive or negative y-axis depending on the star's location relative to the nebula.

The nebular face itself will be projected into an elliptical shape. If θ is the azimuth of the exit position as before, and Ψ is the polar angle under consideration, radial coordinates relative to the center of the nebular face are scaled by a factor

$$S = \left(\frac{\cos^2 \Psi}{\cos^2 \theta + \cos^2 \Psi \sin^2 \theta}\right)^{1/2} . \tag{35}$$

The tilt of the nebular surface also affects the calculation of the area filling a solid angle of 1 steradian for the observer. This area increases inversely proportional to $\cos \Psi$. All relations of angular scales in the sky to linear scales on the nebular face are, in addition, distance-dependent and must be changed in proportion to (d_0/d).

IV. CONCLUSION

We have described in some detail a practical method for computing the radiative transfer, including multiple scattering, for a reflection nebula which can be approximated by a plane-parallel slab of uniform density and which is illuminated by a single star. This method allows the computation of the surface brightness distribution across the face of such nebulae in units of the brightness of the illuminating star, and makes a comparison with observed surface brightness of actual reflection nebulae possible. Results of extensive model calculations and a discussion of the importance of multiple scattering effects will be presented in subsequent papers.

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