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Computation of Synthetic Spectra for a Semi-Infinite Atmosphere

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Computation of Synthetic Spectra for a Semi-Infinite Atmosphere[1]

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ABSTRACT

The computation of absorption spectra in a model planetary atmosphere is shown to be feasible using the Neumann series (successive orders of scattering) solution to the equation of radiative transfer for semi-infinite atmospheres. The method may be applied for arbitrary single scattering albedo and phase function. For orders of scattering $n \gg 1$, the terms of the Neumann series assume an asymptotic form. With the aid of this asymptotic form, simple expressions are given for the reflection function of the layer and the mean number of scatterings in the atmosphere. Computations illustrating the approach to the asymptotic form, the shape of a Lorentz-broadened absorption line, the mean number of scatterings in an atmosphere, and the equivalent width of a Lorentz line are presented graphically for both isotropic scattering and phase functions typical of clouds and hazes.

1. The problem

The traditional approach to the analysis of planetary absorption spectra in the visible and near infrared has been through use of a model atmosphere consisting of a molecular layer overlying a plane parallel cloud deck. The latter is assumed to reflect solar radiation specularly, while the absorption features are assumed to arise in the superposed molecular layer.

Chamberlain and Kuiper (1956), Chamberlain (1965) and Belton (1968) have emphasized the necessity for considering a more realistic model in which scattering particles and absorbing gas are mixed in the atmosphere. Besides being physically more satisfactory, such a model provides better agreement with the observational data in the case of Venus and Jupiter.

The difficulty with the multiple scattering model arises in the necessity for solving the equation of radiative transfer at as many distinct frequencies as is necessary for defining the shape of the absorption line or band being investigated. If we let $I_\nu(\tau_\nu,\Omega)$ be the specific intensity at frequency ν and optical depth τ_ν in direction $\Omega=(\arccos\mu,\phi)$, $\tilde{\omega}_\nu$ the single scattering albedo, $p(\Omega,\Omega')$ the phase function (scattering indicatrix), and $\Omega_0=(\arccos\mu_0,\phi_0)$ the angle of incidence of solar radiation, this equation takes the form

$$\mu\frac{dI_\nu}{d\tau_\nu}=-I_\nu(\tau_\nu,\Omega)+\frac{\tilde{\omega}_\nu}{4\pi}\times\int_{4\pi}d\Omega' I_\nu(\tau_\nu,\Omega')p(\Omega,\Omega')+\frac{\tilde{\omega}_\nu p(\Omega,\Omega_0)e^{-\tau_\nu/\mu_0}}{4\pi\mu_0}, \quad (1)$$

for a plane parallel, homogeneous atmosphere. Although methods for solving this problem are now available (for example, van de Hulst, 1963; van de Hulst and Grossman, 1968; Hansen, 1969a; Twomey *et al.*, 1966), solution at a large number of frequency points is still a difficult and time consuming problem. This difficulty could be avoided if it were possible to separate the multiple scattering problem [solution of Eq. (1) in the continuum] from the computation of absorption line shape. One method of effecting such a separation has been suggested by Irvine (1964); an alternative approach is described below, making use of the Neumann series solution to (1).

2. The Neumann series and its asymptotic form

It is well known that the solution to Eq. (1) may be expanded in successive orders of scattering [the Neumann series; see, for example, van de Hulst and Irvine (1962)]:

$$I_\nu(0,\Omega)\equiv R_\nu(\Omega,\Omega_0)=\sum_{n=1}^{\infty}\tilde{\omega}_\nu{}^n R^*(n,\Omega,\Omega_0), \quad (2)$$

where we have denoted the total reflected intensity by R_ν and the reflection function for nth order scattering by $R^*(n)$. It is important to note that the R^* are computed for the conservative case ($\tilde{\omega}_\nu=1$). In general, the R^* will be functions of the total optical thickness of the atmosphere; this dependence obviously drops out in the present model, where we confine attention to semi-infinite atmospheres.

Eq. (2) provides the desired separation between effects of multiple scattering and effects of true absorption. The equation of transfer may be solved for the conservative case to obtain the $R^*(n)$; the desired reflection function is then obtained by the simple sum-

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mation in (2). Such a summation may be rapidly performed for as many frequency points as is necessary. The difficulty with this approach lies in the slow convergence of (2) for a thick atmosphere and near conservative scattering $[(1-\tilde{\omega})\ll 1]$.

The purpose of the present paper is to point out that the following asymptotic expression holds for R^*:

$$R^*(n)\sim A(\Omega,\Omega_0)n^{-\frac{3}{2}}[1-d(\Omega,\Omega_0)/n+O(n^{-2})], \quad (3)$$

where A and d are determined by the phase function. Clearly, once the $R^*(n)$ have been computed for n sufficiently large that (3) holds, A and d may be obtained from the numerical computations, Eq. (3) substituted into (2), and the problem is solved.

A means for deriving (3) has been suggested by van de Hulst[3]. When $(1-\tilde{\omega}_\nu)\ll 1$ we may write (cf. van de Hulst, 1949; Rozenberg, 1962; Sobolev, 1968):

$$R_\nu(\Omega,\Omega_0)=\left[\sum_{n=1}^{\infty} R^*(n,\Omega,\Omega_0)\right][1-s(\Omega,\Omega_0)(1-\tilde{\omega}_\nu)^{\frac{1}{2}}], \quad (4)$$

where $s(\Omega,\Omega_0)$ is determined by the phase function. Setting

$$\sum_{n=1}^{\infty} R^*(n,\Omega,\Omega_0)=R_0(\Omega,\Omega_0), \quad (5)$$

and

$$\frac{R_\nu}{R_0}=y, \quad \frac{R^*(n)}{R_0}=y_n, \quad (6)$$

we may equate Eqs. (2) and (4) to obtain

$$y=\sum_{n=1}^{\infty} \tilde{\omega}^n y_n=1-s(1-\tilde{\omega})^{\frac{1}{2}}, \quad (7)$$

where we drop for convenience the explicit dependence upon angle and frequency. Expanding the right side of (7) and equating the coefficients of like powers of $\tilde{\omega}^n$, we obtain

$$\frac{y_n}{s}=\frac{(2n-3)!}{2^{2n-2}n!(n-2)!}, \quad n\geq 2. \quad (8)$$

Use of Stirling's formula then yields

$$\frac{y_n}{s}\sim(2n^{\frac{3}{2}}\pi^{\frac{1}{2}})^{-1}, \quad (9)$$

which is equivalent to the leading term of Eq. (3).

Two problems still remain. First, it is necessary to obtain the $R^*(n)$ for small n. The traditional approach involving repeated iteration with the Λ operator (i.e., repeated integration over both angle and optical depth) is cumbersome for a semi-infinite atmosphere. Uesugi and Irvine (1969) have been shown that the $R^*(n)$ may be obtained from the $R^*(n')$, for $n'<n$, by integrations over the angular variables only. The resulting equations are

$$(\mu+\mu_0)R^*(1,\Omega,\Omega_0)=p(\Omega,-\Omega_0), \quad (10)$$

$$(\mu+\mu_0)R^*(2,\mu,\mu_0)=\frac{\mu}{4\pi}\int_{2\pi} R^*(1,\Omega,\Omega')p(\Omega',\Omega_0)d\Omega' + \frac{\mu_0}{4\pi}\int_{2\pi} R^*(1,\Omega_0,\Omega')p(\Omega',\Omega)d\Omega', \quad (11)$$

$$(\mu+\mu_0)R^*(n,\Omega,\Omega_0)=\frac{\mu}{4\pi}\int_{2\pi} R^*(n-1,\Omega,\Omega')p(\Omega',\Omega_0)d\Omega' + \frac{\mu_0}{4\pi}\int_{2\pi} R^*(n-1,\Omega_0,\Omega')p(\Omega',\Omega)d\Omega'+\frac{\mu\mu_0}{16\pi^2} \times\sum_{n'=1}^{n-2}\int_{2\pi} R^*(n-n'-1,\Omega',\Omega_0)d\Omega' \times\int_{2\pi} R^*(n',\Omega,\Omega'')p(\Omega'',-\Omega')d\Omega'', \quad n\geq 3. \quad (12)$$

Finally, assuming that (3) holds for $n\geq n^*$, substitution of (3) into (2) still results in a summation which, for near conservative scattering, may require many thousand terms. Sufficient accuracy will ordinarily be attained (see below) by approximating this sum by an integral of the form

$$\sum_{n=n^*+1}^{\infty} \tilde{\omega}^n n^{-\frac{3}{2}}(1-d/n) \simeq \int_{n^*}^{\infty} dx x^{-\frac{3}{2}}e^{-ax} - d\int_{n^*}^{\infty} dx x^{-\frac{5}{2}}e^{-ax}, \quad (13)$$

where we have set

$$a=-\ln\tilde{\omega}. \quad (14)$$

3. Sample results

Computations have been made for both isotropic scattering and two phase functions of the form

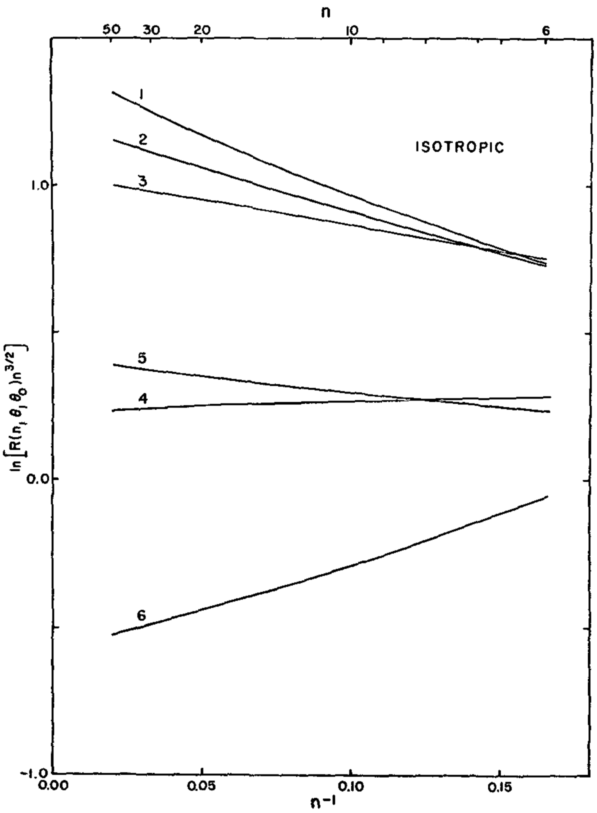
$$p(\cos\alpha)=bp_{\mathrm{HG}}(g_1;\cos\alpha)+(1-b)p_{\mathrm{HG}}(g_2;\cos\alpha), \quad (15)$$

where (Henyey and Greenstein, 1941)

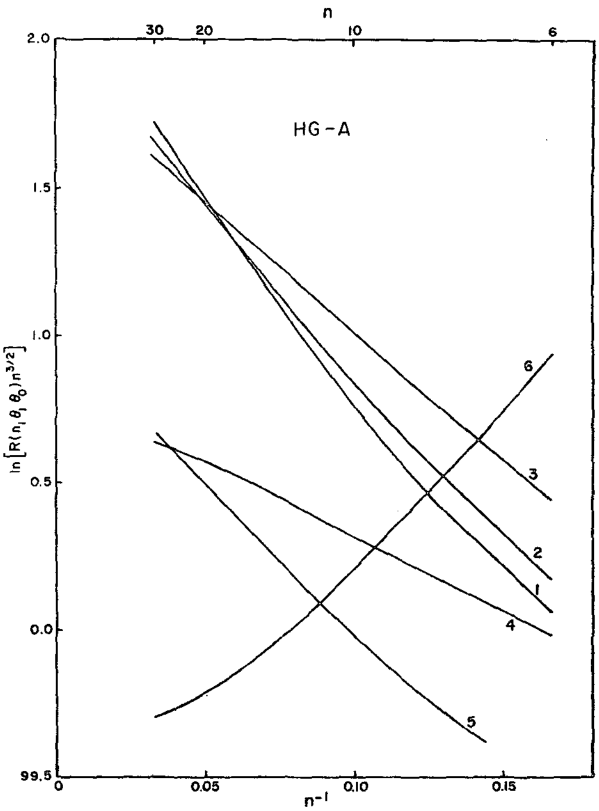
$$p_{\mathrm{HG}}(g;\cos\alpha)=\frac{1-g^2}{(1+g^2-2g\cos\alpha)^{\frac{3}{2}}}, \quad (16)$$

and $b\leq 1$ is a constant. The phase function labeled HG-A in Figs. 1–4 corresponds to the parameters $g_1=0.824$, $g_2=-0.55$ and $b=0.9724$ and is similar to the phase function of maritime haze at 0.7 μ (see Irvine, 1965 and Dermendijian, 1964). The function labeled HG-B corresponds to $g_1=0.9$, $g_2=-0.75$ and $b=0.95$ and is similar to the phase function of a cumulus cloud at 0.7 μ, although the forward peak is not quite as sharp

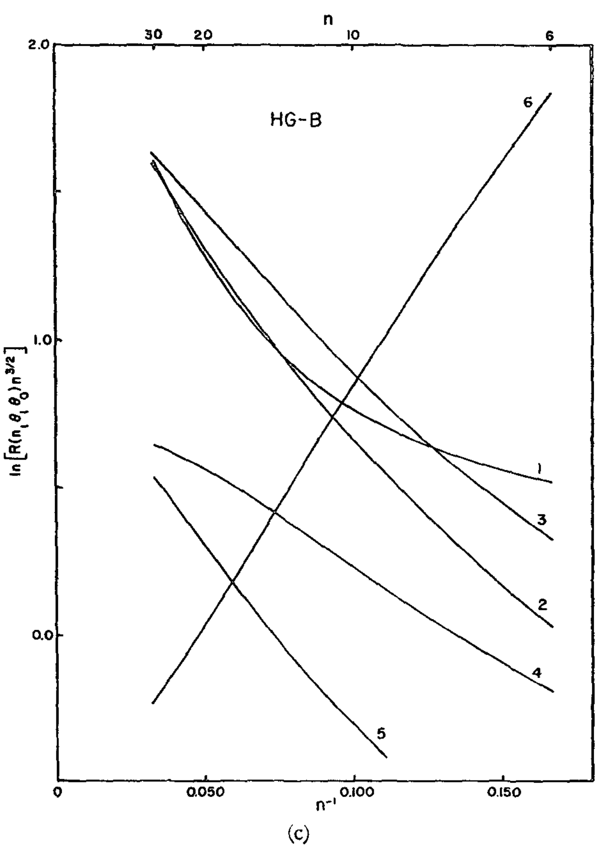
[3] Private communication.



(a)



(b)



(c)

FIG. 1. Verification of the asymptotic relation [Eq. (3)] for three choices of phase function: isotropic, a.; HG-A, b.; HG-B, c. The following pairs of angles of incidence θ and reflection θ_0 were used: 1, (0°,0°); 2, (0°,45°); 3, (45°,45°); 4, (45°,89°); 5, (0°,89°); 6, (89°,89°). See text for definitions of phase functions HG-A and HG-B.

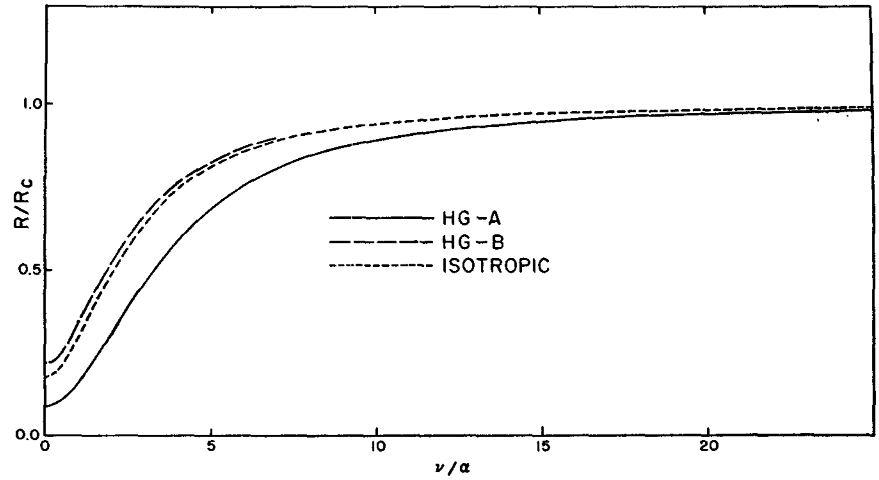


FIG. 2. Absorption profiles for a Lorentz-broadened line with $\eta = NS[\pi\alpha(\kappa_c+\sigma)]^{-1}=1$ formed in reflection from a semi-infinite atmosphere with continuum single scattering albedo $\tilde{\omega}_c=0.95$ for normal incidence and reflection. Three choices of phase function are illustrated.

as that for such a cloud. These phase functions have also been used in numerical computations by Irvine (1968a, b). The computations of $R^*(n)$ described below were made from Eqs. (10)–(12) using a Guassian-type integration formula with the interval $\theta = \arccos \mu = (0-\pi/2)$ divided into 14 points for isotropic scattering and 28 points for the phase function (15); azimuthal symmetry was assumed. From computations utilizing different numbers of integration points and by comparison with the results of Irvine (1968a), we find that our results are correct to at least 0.1% for isotropic scattering and about 1% for the anisotropic phase functions.

In Fig. 1 we plot $\ln[R^*(n)n^{\frac{3}{2}}]$ vs n^{-1}. We see from (3) that in the asymptotic regime this relation should give us a straight line. The asymptotic regime is evidently reached for isotropic scattering for $n \simeq 20$, and for slightly higher orders of scattering (depending on θ and θ_0) for the more asymmetric phase functions HG-A and HG-B.

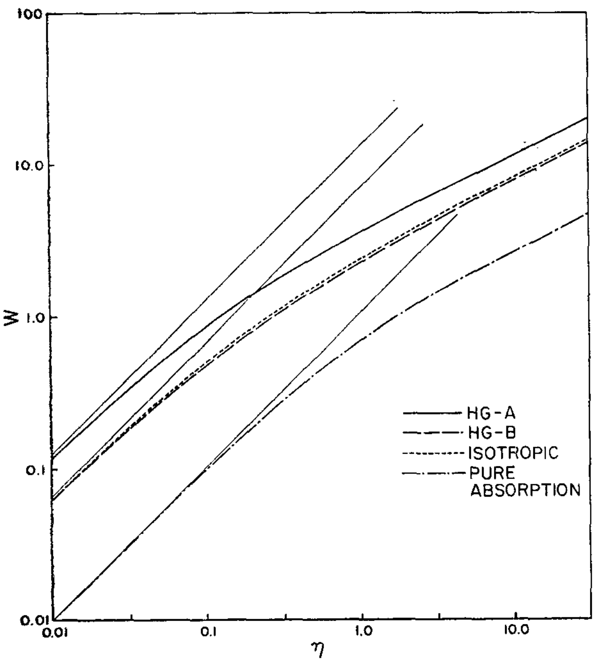


FIG. 3. Equivalent width of a Lorentz-broadened line as a function of η [see Eqs. (21) and (22)]. Tangents to the linear part of the curves of growth are shown.

To obtain the total reflected intensity at a given frequency we substitute (3) and (13) into (2) for $n > n^* \gg 1$. After an integration by parts we find that

$$R(\Omega,\Omega_0) = \sum_{n=1}^{n^*} \tilde{\omega}^n R^*(n) + 2A^* n^{*-\frac{1}{2}}[e^{-an^*} - (\pi a n^*)^{\frac{1}{2}} \mathrm{erfc}\sqrt{(an^*)}] - \tfrac{2}{3}A^* d n^{*-\frac{3}{2}}[(1-2an^*)e^{-an^*} + 2\sqrt{\pi}(an^*)^{\frac{3}{2}} \mathrm{erfc}\sqrt{(an^*)}], \quad (17)$$

where we evaluate $A^*(\Omega,\Omega_0)$ from

$$R^*(n^*,\Omega,\Omega_0) = A^*(\Omega,\Omega_0) n^{*-\frac{3}{2}} e^{-d/n^*},$$

d and a being defined by Eqs. (3) and (14), respectively, and erfc$x$ is the complementary error function. Fig. 2 shows the corresponding profile of a Lorentz-broadened line, for which R_c is the continuum intensity and

$$\tilde{\omega}_\nu = \frac{\sigma}{\sigma + \kappa(\nu) + \kappa_c}, \quad (18)$$

where κ_c is the continuum absorption coefficient and

$$\kappa(\nu) = \frac{NS\alpha}{\pi(\nu^2+\alpha^2)}. \quad (19)$$

As might be expected, the forward scattering peak in phase function HG-A makes the line both deeper and broader. Note, however, that the line profile for phase function HG-B, which is more peaked in the forward direction than HG-A but also has a more pronounced back scattering peak, closely mimics the behavior of the profile for isotropic scattering for the particular value of continuum albedo chosen. This points out the danger of using an oversimplified phase function in computations of synthetic spectra.

Curves of growth corresponding to the three phase functions considered are illustrated in Fig. 3. The equivalent width

$$W=\int_0^\infty d\nu\frac{(R_c-R_\nu)}{R_c} \tag{20}$$

is expressed as a function of η, where

$$\eta=\frac{NS}{\pi\alpha Q},\quad Q=(\kappa_c+\sigma)^{-1}, \tag{21}$$

for the multiple scattering models considered here and where

$$\eta=\left(\frac{NS}{\pi\alpha}\right)\ell \tag{22}$$

in the case of pure absorption (as for a specularly reflecting cloud layer model). In (22) ℓ is the geometric path traveled. As Belton (1968) and Hansen (1969b) have pointed out, the transition region between the linear and square root regimes is much larger in the multiple scattering case than for the case of pure absorption. We note also, as in Fig. 2, that the results for the phase function with both a pronounced forward and backward peak (HG-B) closely mimic those for isotropic scattering when the continuum albedo $\tilde{\omega}_c=0.95$.

Fig. 4 illustrates computations for the mean number of scatterings

$$\langle n\rangle=\sum_{n=1}^{\infty} n\tilde{\omega}^n R^*(n)\Big/\sum_{n=1}^{\infty}\tilde{\omega}^n R^*(n), \tag{23}$$

for the three phase functions. Although for nearly conservative scattering $\langle n\rangle$ is greater for the asymmetric than for the isotropic phase function, because of the deeper penetration into the cloud for such phase functions, this is not necessarily true for smaller values of $\tilde{\omega}_\nu$ if the cloud phase function has a large backward peak. It is interesting to note that when $\tilde{\omega}_\nu\simeq 0.95$, the mean number of scatterings for the HG-B phase function is practically equal to $\langle n\rangle$ for the isotropic phase function. This leads to the near equality of the absorption line profiles and curves of growth for these phase functions shown in Figs. 2 and 3.

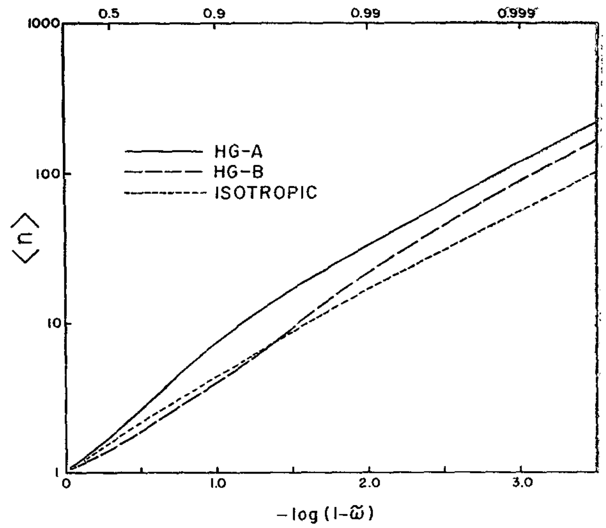


FIG. 4. Mean number of scatterings $\langle n\rangle$ undergone by radiation reflected from a semi-infinite atmosphere for normal incidence and reflection and three choices of phase function.

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