FLUORESCENT SCATTERING IN PLANETARY ATMOSPHERES
I. BASIC THEORETICAL CONSIDERATIONS*

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ABSTRACT

Resonance scattering, fluorescence, and pure absorption are considered as mechanisms governing the daytime ultraviolet spectrum of a planet observed from above. It is assumed throughout that continuous absorption prevents any sunlight from being reflected by the ground (or cloud surface) and that the scattered continuum is weak compared with scattering in spectral lines. These considerations are appropriate to the ultraviolet, when ozone (or some other substance) is strongly absorbing in the high atmosphere. Such a spectrum is qualitatively different from a reflected Fraunhofer spectrum; this scattered light constitutes a daytime airglow of emission lines. To aid interpretation of such spectra, in terms of atomic and molecular relative abundances, several alternative models of line formation are investigated.

I. INTRODUCTION: LINE FORMATION IN PLANETARY ATMOSPHERES

Interpretation of the absorption spectrum of a planetary atmosphere in terms of chemical abundances is fairly straightforward when the solar continuum is diffusely reflected by a surface and when the planetary absorption lines are not saturated. But when there is a large amount of atmospheric scattering in the continuum, in addition to line absorption, the interpretation takes on an entirely different character. Van de Hulst (1952) first discussed this problem and indicated its solution for a semi-infinite atmosphere, suggesting that it might apply to the formation of CO_2 bands on Venus.

Subsequently, Chamberlain and Kuiper (1956) showed that these bands vary in equivalent width with the phase angle of the planet in rough agreement with radiative-transfer theory for a thick, scattering atmosphere. This phase variation is in the opposite sense to that expected if the absorption bands are formed by a simple traversal of light through a thin atmosphere with a reflection by a well-defined cloud layer. In the multiple scattering theory, the absorption in a weak line varies as the square root of the absorption coefficient rather than linearly. Therefore, it also appeared to be significant that the scattering theory gave a consistent interpretation of the rotational-line absorption in terms of the kinetic temperature. Although that CO_2 temperature determination has generally been adopted in theoretical discussions of Venus' atmosphere, some authors have at the same time adopted a CO_2 abundance "above the cloud layer" (Herzberg 1952) that is based on the model of simple reflection of sunlight. Unfortunately, if the multiple-scattering model is the more correct one, as present evidence would lead us to believe, our knowledge of the CO_2 abundance becomes far less definite (Chamberlain 1961a).

Another class of problems concerns an atmosphere that scatters radiation back into space at discrete line frequencies but does not reflect continuous radiation, the "surface" being effectively black. This is the group of problems we intend to investigate in detail. As with absorption-line spectra, it is not always possible to relate intensities uniquely to absolute abundances above a well-determined height, although it may be possible to derive at least the ratio of abundances for the constituent scattering in spectral lines and the substance producing continuous absorption at the same altitude.

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Among the first problems in interpreting a given set of spectra will be to ascertain whether the atmosphere is optically thick or thin in the observed emissions and whether continuous absorption is relatively important or negligible. By calculating relative intensities of lines in a band and of bands in a system and the intensity variations across the planetary disk for different models, we hope to provide a basis for such interpretations. We might emphasize here that it will be necessary to measure the intensity variations of emission lines and bands across the disk of a planet, in order to interpret the results with some confidence. Hence one would desire high angular resolution, probably necessitating measurements from space probes in the neighborhood of the planet. An alternative program would measure the intensities integrated over the disk from an orbiting earth satellite at different planetary phases. While this technique of integrated intensity is the one so far used on the absorption-line spectrum of Venus, it is not so amenable to interpretation as would be observations confined to small angles of incidence and reflection.

Throughout we shall use the terms *optically thick* and *optically thin atmospheres* as pertaining to the centers of the most strongly absorbing lines in the band system or multiplet, unless it is specifically stated that we refer to weaker lines or the wings of lines. Also, in all the problems considered, we suppose that incident radiation in the continuum is absorbed either at the same altitude or below the level at which line scattering occurs. Physically, this corresponds to absorption by O_3 or O_2, for example, in the terrestrial middle and high atmosphere. The theory would then apply to lines and bands resonantly scattered in the high atmosphere. We shall consider ordinary (Rayleigh) scattering to be negligible and suppose that atomic and molecular transitions provide the only means of radiation scattering, which will always be treated as isotropic and coherent.

The following definitions will be used throughout: I_ν is the specific intensity, and $\mathfrak{F} = \int I_\nu d\nu$ represents an integrated intensity over an entire line (or molecular band, when so stated).

The albedo for single scattering is ϖ. If there is no continuous absorption in the scattering region, ϖ is constant over an entire molecular band and depends only on the fractional number of re-emissions occurring in that band. Hence we have, for example, for a transition $v' \rightarrow v''$,

$$\varpi_{v''} = \frac{A_{v''}}{\sum_{v''=0}^{\infty} A_{v''}}, \tag{1}$$

where $A_{v''}$ is the transition probability for a particular band. (As emissions arising from different upper levels, v', will be independent of one another, we shall generally suppress v' in the subscript notation. A specific v', as well as v'', is always tacitly implied, however.)

Strictly, this albedo depends on the rotational lines as well. In a system with P and R branches, an upper level J' is populated by absorptions from initial (lower) levels $J = J' + 1$ and $J = J' - 1$. It emits with transitions to the final (lower) levels $J'' = J' + 1$ and $J'' = J' - 1$. If the incident flux is constant across the entire band, a good approximation for single scattering is to neglect changes in the rotational quantum number. Then absorption from level J is assumed to populate only $J' = J$ and to re-emit only to $J'' = J' = J$. One would then treat each branch of the band separately in this fashion, adopting the absorption coefficients appropriate to that branch. With multiple scatterings in optically thick atmospheres, this neglect of the coupling between levels will introduce some errors in a theory using pure coherent scattering (e.g., see Chamberlain 1961, pp. 442 and 444). The inclusion of coupling in the theory is treated by Sobouti in Paper II.

If there is continuous absorption given by coefficient σ per unit volume and discrete-

line absorption with a volume coefficient κ_ν, the albedo varies across the line profile and is

$$\varpi_{v'', \nu} = \frac{\kappa_\nu}{\kappa_\nu + \sigma} \varpi_{v''} = \frac{\kappa_\nu}{\kappa_\nu + \sigma} \frac{A_{v''}}{\sum_{v''=0}^{\infty} A_{v''}} . \tag{2}$$

If there is no continuous absorption, the *fluorescent emissions* (i.e., ones arising from downward transitions *not* ending on the ground vibrational level) will always have emergent intensities proportional to the emitting path length, $1/\mu$, and will have relative intensities proportional to their individual albedos. Thus the fraction of fluorescent re-emission appearing in a given transition is

$$\frac{\varpi_{v''}}{1 - \varpi_0} = \frac{A_{v''}}{\sum_{v''=1}^{\infty} A_{v''}} . \tag{3}$$

The variation of fluorescent emissions across the planetary disk and their relative intensities with respect to one another will both serve as sensitive tests for the presence of continuous absorption in or above the line-scattering region.

Optical depth,

$$t_\nu(z) = \int_z^\infty [\kappa_\nu(z') + \sigma(z')]\, dz',$$

is always referred to the vertical direction, is measured from the top of the atmosphere, and applies, of course, to the frequencies at which absorption occurs. It varies across the line profile and depends on the particular molecular line absorbed $(v', J' \leftarrow v, J)$.

We use τ_ν for the total optical thickness of the atmosphere. The ground albedo (at $t_\nu = \tau_\nu$) is zero throughout. The polar angle θ is measured from the upward normal, and throughout we write $\mu = \cos\theta$. These conventions are illustrated in Figure 1. Figure 2 illustrates the fluorescent scattering mechanism in a band system.

The incident solar flux per unit frequency interval, at the frequency of the $v' \rightarrow v''$ transition, is $\pi F_{v''}$. In this paper we assume that only $v'' = 0$ is significantly populated, so that only πF_0 will induce atmospheric fluorescence.

II. SCATTERING BY AN ATMOSPHERE OF SMALL OPTICAL THICKNESS

This section summarizes the theory for atmospheres in which τ_0, the total optical thickness at the center of a line, is small for all lines. For practical purposes this means $\tau_0 \leq 1$. With the solar flux πF_0 incident from direction μ_i, the monochromatic solution for the diffusely reflected intensity at the top of the atmosphere in the direction μ, arising from a downward transition to the ground level $(v'' = 0)$, is (R.T.,[1] p. 209)

$$I_{0,\nu}(0, +\mu) = \frac{F_0}{4\mu} S(\tau_\nu), \tag{4}$$

where the scattering function, which depends on $\varpi_{0,\nu}$, μ, and μ_i, as well as on τ_ν, is

$$S(\tau_\nu) = \frac{\varpi_{0,\nu}\mu\mu_i}{(\mu + \mu_i)} [X(\mu)X(\mu_i) - Y(\mu)Y(\mu_i)] . \tag{5}$$

[1] The basic theory for this paper is contained in Chandrasekhar's (1950) treatise, which will always be called simply "R.T."

The X- and Y-functions, tabulated by Chandrasekhar, Elbert, and Franklin (1952), are also functions of $\varpi_{0,\nu}$ and τ_ν, as well as μ or μ_i.

The total reflected intensity for a transition ending on $v'' = 0$, then, is

$$\Im_0^{(\text{ref})}(+\mu) = \frac{F_0}{4\mu} \int S(\tau_\nu)\, d\nu .$$ (6)

For a Doppler-broadened line without continuous absorption one has

$$\tau_\nu = \tau_c \exp(-x^2); \qquad x = \frac{c(\nu - \nu_c)}{U\nu_c}; \qquad U = \left(\frac{2kT}{M}\right)^{1/2} .$$ (7)

Here U is the most probable velocity for temperature T and particle mass M and x is the deviation from the center of the profile, ν_c, in units of the Doppler width $U\nu_c/c$.

Changing the variable ν to x, equation (6) becomes

$$\Im_0^{(\text{ref})}(+\mu) = \frac{F_0 U\nu_c}{4\mu c} \int_{-\infty}^{\infty} S(\tau_\nu)\, dx .$$ (8)

a) Constant Albedo across a Line: No Continuous Absorption

For the albedo given by equation (1) and constant over the line profile, a general analytic solution for equation (8) has been obtained by Brandt and Chamberlain (1958)
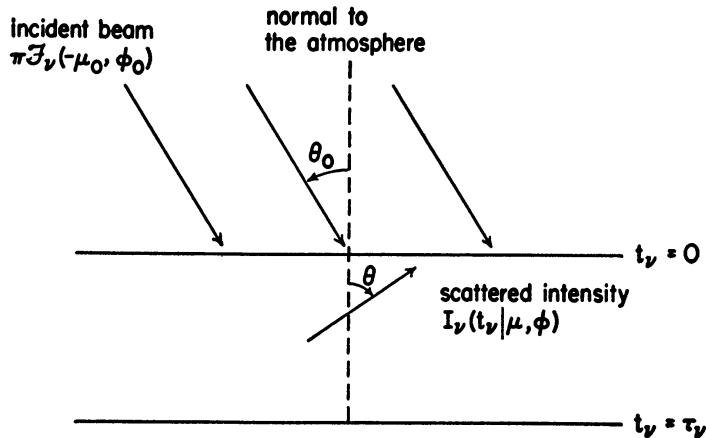

FIG. 1.—A scattering atmosphere illuminated by a parallel beam of light of flux $\pi\, F_0(-\mu_i,\ \phi_i)$, where $\mu = \cos\theta$.
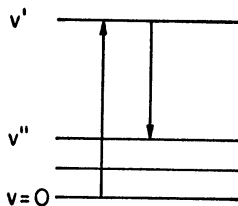

FIG. 2.—Illustration of the fluorescent mechanism treated in the text. A molecule is initially in the ground electronic state and ground vibrational level; it is given an unprimed quantum number. After absorption of a quantum, it is in level v'. After fluorescent emission, it is again in the ground state, but in vibrational level $v'' > v$.

by expanding $S(\tau_\nu)$ in a Taylor's series in τ_ν about an arbitrary point a and integrating over the profile. Letting primes denote derivatives with respect to τ_ν, we have

$$\Im_0^{(\mathrm{ref})}(+\mu) = \frac{F_0 U \nu_c}{4\mu c}\left[\pi^{1/2}\tau_c S'(a) + \frac{\tau_c^2(\pi/2)^{1/2} - 2a\,\tau_c\pi^{1/2}}{2}S''(a)\right.$$
$$\left. + \frac{\tau_c^3(\pi/3)^{1/2} - 3a\,\tau_c^2(\pi/2)^{1/2} + 3a^2\tau_c\pi^{1/2}}{6}S'''(a) + \cdots\right]. \tag{9}$$

In this fashion one may express the solution for the integrated intensity in terms of X- and Y-functions and their derivatives. In practice, derivatives higher than the first are cumbersome to work with. But, for small optical thicknesses, we may neglect $S'''(a)$ and higher-order terms. Then, adopting $a = \tau_c/2\sqrt{2}$, we write equation (9) (Brandt and Chamberlain 1958) as

$$\Im_0^{(\mathrm{ref})}(+\mu) = \frac{F_0 U \nu_c}{4\mu c}\pi^{1/2}\tau_c S'\left(\frac{\tau_c}{2\sqrt{2}}\right), \tag{10}$$

where $S'(\tau)$, in terms of the X- and Y-functions ($R.\,T.$, p. 209), is

$$S'(\tau_\nu) = \varpi_0 Y(\mu) Y(\mu_i). \tag{11}$$

Another approximate solution of equation (8), which defines an effective optical thickness for the entire line, is (Hunten 1954; Brandt and Chamberlain 1958)

$$\Im_0^{(\mathrm{ref})} = (+\mu) = \frac{F_0 U \nu_c}{4\mu c}(2\pi)^{1/2}S(\tau_c/\sqrt{2}). \tag{12}$$

This equation gives the integrated intensity in terms of the expression for the monochromatic intensity as computed for an effective optical thickness, $\tau_{\mathrm{eff}} = \tau_c/\sqrt{2}$ and a line width of $(\Delta\nu)_{\mathrm{eff}} = (2\pi)^{1/2} U\tau_c/c$.

Equations (10) and (11) or (12) and (5) form two approximate solutions (both neglecting the third and higher derivatives in Taylor's expansion) for the total reflected intensity of a Doppler-broadened resonance line with albedo $\varpi_0 = \mathrm{const.}$ and an optical thickness in the line center of τ_c. In the limit of $\tau_c \approx 0$, we find that either solution (10) or (11) varies as τ_c and the solutions represent mere single scattering. For larger values of τ_c, the linearity disappears, and relative line intensities in a band will be distorted from the usual temperature distribution. To obtain an entire band intensity, it is necessary to add the emergent intensities for the individual lines, which will depend on the rotational distribution of populations.

To obtain the emergent intensities in the fluorescent bands, $v' \to v'' \geq 1$, we note that, with no continuous absorption, the total flux emerging from the atmosphere must be equivalent to that entering it. (Continuous absorption represents, for our purposes, resonant and fluorescent photons lost to the radiation field.)

Since these bands (again with no continuous absorption) have intensities proportional to $1/\mu$ and are emitted equally at the top and bottom of the atmosphere, the sum of the fluorescent intensities is

$$2 \times 2\pi \sum_{v''=1}^{\infty}\int_0^1 \Im_{v''}^{(\mathrm{ref})}(+\mu)\mu d\mu \equiv 4\pi\sum_{v''=1}^{\infty}\Im_{v''}^{(\mathrm{ref})}(+1)$$
$$= \frac{U\nu_c\mu_i\pi F_0}{c}\int_{-\infty}^{\infty}\left[1 - \exp\left(-\frac{\tau_0}{\mu_i}e^{-x^2}\right)\right]dx \tag{13}$$
$$- 2\pi\int_0^1 \Im_0^{(\mathrm{ref})}(+\mu)\mu d\mu - 2\pi\int_0^1 \Im_0^{(\mathrm{trans})}(-\mu)\mu d\mu.$$

The first term on the right is the fraction of the incident flux (on unit area of the atmosphere) that is scattered by either resonant or fluorescent transitions in the atmosphere. The second term is the diffusely reflected *resonance* radiation. The last term represents the diffusely transmitted *resonance* flux, which is computed in a manner analogous to that diffusely reflected. The individual fluorescent bands ($v' \rightarrow v'' \geq 1$) have intensities proportional to $\varpi_{v''}/(1 - \varpi_0)$, given by equation (3).

When the monochromatic approximation (12) is adequate for the resonance transition, equation (13) for the fluorescent emissions also reduces to the analogous monochromatic expression (see Brandt 1959):

$$\mathfrak{S}_{v''}^{\mathfrak{X}(\mathrm{ref})}(+\mu)$$

$$= \frac{(2\pi)^{1/2} U \nu_c F_0 \varpi_{v''} \mu_i}{4 c (1 - \varpi_0) \mu} \{1 - \tfrac{1}{2}\varpi_0 [\alpha^{(0)} + \beta^{(0)}]\} [X(\mu_i) - Y(\mu_i)]_{\tau_\nu = \tau_c/\sqrt{2}}, \tag{14}$$

where $\alpha^{(0)}$ and $\beta^{(0)}$ are the moments of order zero of $X(\mu)$ and $Y(\mu)$, respectively (*R.T.*, p. 274), and must also be evaluated for $\tau_\nu = \tau_c/\sqrt{2}$ and an albedo ϖ_0. When $\varpi_0 \rightarrow 1$, the first bracket approaches $1 - \varpi_0$ and cancels that factor in the denominator. At the same time, $\varpi_{v''} \rightarrow 0$, and the fluorescent emission vanishes.

b) Variable Albedo across a Line: Continuous Absorption

i) *Resonant transition.*—The general solution (9) and the approximations (10) and (12) still hold in this case, provided that the calculation of $S(\tau_\nu)$ and its derivatives allows for the dependence of $\varpi_{0,\nu}$ on τ_ν. For a continuous-absorption coefficient, σ, that is constant across the line and a Doppler profile for the line-absorption coefficient, $\kappa_\nu = \kappa_c \exp(-x^2)$, the total optical thickness of the atmospheres becomes

$$\tau_\nu = \int_0^\infty (\sigma + \kappa_c e^{-x^2}) \, dz = \tau_\sigma + \tau_c e^{-x^2}, \tag{15}$$

where τ_σ and τ_c are the optical thicknesses in the continuum and in the center of the line, respectively.

The albedo of equation (2) in the presence of continuous absorption becomes

$$\varpi_{0,\nu} = \frac{\kappa_c \exp(-x^2)}{\kappa_c \exp(-x^2) + \sigma} \varpi_0 = \frac{\varpi_0}{1 + r \exp(x^2)} = \frac{\varpi_0}{1 + r \tau_c/(\tau_\nu - \tau_\sigma)}, \tag{16}$$

where $r = \sigma/\kappa_c = \tau_\sigma/\tau_c$.

In calculating the scattering function and its derivatives, these new values of optical thickness and albedo must be used. The new optical thickness, however, is introduced only in the argument of the scattering function, S, and its derivatives. The coefficients of these functions in the Taylor expansion involve only the variable part of the optical thickness, $\tau_c \exp(-x^2)$. But, since the Taylor series is developed with respect to this variable about some point a, the total optical thickness employed in the scattering function is $\tau_\sigma + a$. In view of these considerations, equation (9) becomes

$$\mathfrak{S}_0^{\mathfrak{X}(\mathrm{ref})}(+\mu) = \frac{F_0 U \nu_c}{4 \mu c} \left[\pi^{1/2} \tau_c S'(\tau_\sigma + a) \right.$$
$$\left. + \frac{\tau_c^2 (\pi/2)^{1/2} - 2 a \tau_c \pi^{1/2}}{2} S''(\tau_\sigma + a) + \cdots \right]. \tag{17}$$

In differentiating the scattering function, allowance must be made for the variations in albedo. For example, in the above general equation and in the approximate expression (10) for the total intensity, $S'(\tau)$ will no longer be given by equation (11). The new

corresponding expression is to be obtained by inserting the variable albedo, equation (16), in the scattering function of equation (5) and then differentiating with respect to τ_ν. This procedure gives

$$S'(\tau_\nu) = \varpi_{0,\,\nu} Y(\mu) Y(\mu_i) + \frac{\partial \varpi_{0,\,\nu}}{\partial \tau_\nu} [X(\mu) X(\mu_i) - Y(\mu) Y(\mu_i)]$$

$$+ \frac{\partial \varpi_{0,\,\nu}}{\partial \tau_\nu} \frac{\partial}{\partial \varpi_{0,\,\nu}} [X(\mu) X(\mu_i) - Y(\mu) Y(\mu_i)] .$$

(18)

The approximate solution (12), however, retains the same simple form, the only change being that it should now be evaluated for the optical thickness, $\tau_{\text{eff}} = \tau_\sigma + \tau_c/\sqrt{2}$, and the corresponding albedo, $\varpi_{0,\,\text{eff}} = \varpi_0/(1 + 2^{1/2} r)$:

$$\Im_0^{(\text{ref})}(+\mu) = \frac{F_0 U_{\nu c}}{4\mu c} (2\pi)^{1/2} S\left(\tau_\sigma + \frac{\tau_c}{2}\right)\Bigg|_{\varpi_0/(1+2^{1/2} r)} .$$

(19)

To illustrate the effect of continuous absorption, in Figure 3 we have plotted the ratio of the intensity of equation (19) to the intensity without continuous absorption, equation
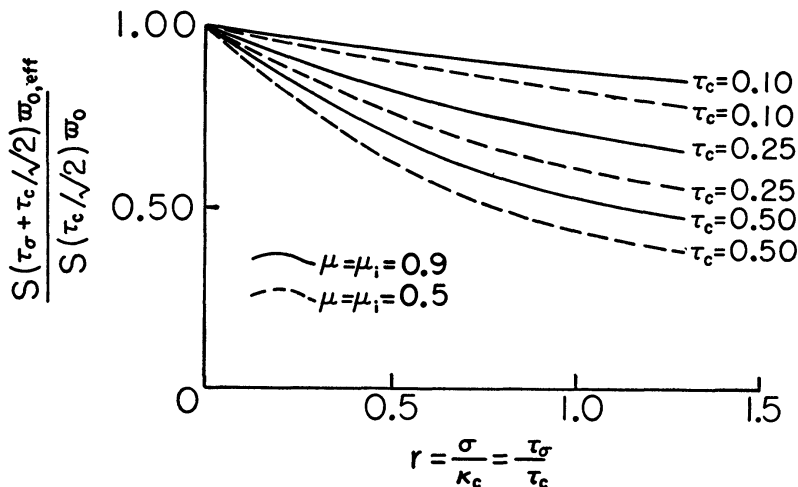

Fig 3 —The ratio of the integrated intensity for continuous absorption to that without continuous absorption The albedo in the latter case is $\varpi_0 = 1$. Solid curves are for $\mu = \mu_i = 0\,5$; $\tau = 0.10$, 0 25, 0.50 Broken curves are for $\mu = \mu_i = 0\,9$; $\tau_c = 0\,10$, 0 25, 0 50

(12), versus $r = \sigma/\kappa_c$. As the continuous absorption increases (i.e., r increases), the reflected intensity decreases, in agreement with one's intuitive expectation. This decrease is more rapid for larger values of τ_c and smaller values of μ and μ_i.

ii) *Fluorescent transitions.*—We assume that each fluorescent band has a continuous-absorption coefficient per unit volume of $\sigma_{v''}$, which gives rise to an optical thickness in the continuum at the position of the v'' band of

$$\tau(v'') = \int_0^\infty \sigma_{v''}(z')\, d z' .$$

We recall that the total optical thickness at the resonant band is

$$\tau_\nu = \int_0^\infty [\kappa_\nu(z') + \sigma(z')]\, d z' ,$$

where we shall continue to write simply σ for $\sigma_{v''=0}$. Since we assume that the atmosphere is isothermal and has the same relative chemical abundances at all scattering heights (in practice, the principal scattering will occur over a range of about one scale height), we have

$$\frac{\tau(v'')}{\tau_\nu(0)} = \frac{\sigma_{v''}}{\kappa_\nu + \sigma}. \tag{20}$$

This ratio is independent of the altitude.

The radiative-transfer equation for the resonant band is (R.T., p. 22)

$$\mu \frac{dI_{0,\,\nu}(t_\nu, \mu)}{dt_\nu} = I_{0,\,\nu}(t_\nu, \mu) - \frac{\kappa_\nu}{\kappa_\nu + \sigma} \frac{\varpi_0}{2} \int_{-1}^{1} I_{0,\,\nu}(t_\nu, \mu')\, d\mu' \tag{21}$$

$$- \frac{\kappa_\nu}{\kappa_\nu + \sigma} \frac{\varpi_0}{4} F_0 e^{-t_\nu/\mu_i},$$

where t_ν refers to optical thickness in the resonant line, $v'' = 0$. The first term on the right-hand side is the absorption rate, and the other two terms constitute the re-emission rate—the source function. A similar equation can be stated for the fluorescent intensities:

$$\mu \frac{dI_{v'',\,\nu}(t_\nu, \mu)}{dt_\nu} = \frac{\sigma_{v''}}{\kappa_\nu + \sigma} I_{v'',\,\nu}(t_\nu, \mu) - \frac{\kappa_\nu}{\kappa_\nu + \sigma} \frac{\varpi_{v''}}{2} \int_{-1}^{1} I_{0,\,\nu}(t_\nu, \mu')\, d\mu' \tag{22}$$

$$- \frac{\kappa_\nu}{\kappa_\nu + \sigma} \frac{\varpi_{v''}}{2} F_0 e^{-t_\nu/\mu_i}.$$

The source function in this equation is the same as in equation (21) except for the replacement of ϖ_0 by $\varpi_{v''}$; it depends on t_ν but not on μ. Eliminating the source function between equations (21) and (22), we find, for any depth t_ν,

$$\frac{\kappa_\nu + \sigma}{\sigma_{v''}} \mu_{v''} \frac{dI_{v'',\,\nu}(t_\nu, \mu_{v''})}{dt_\nu} - I_{v'',\,\nu}(t_\nu, \mu_{v''})$$

$$= \frac{\varpi_{v''}}{\varpi_0} \frac{\kappa_\nu + \sigma}{\sigma_{v''}} \left[\mu_0 \frac{dI_{0,\,\nu}(t_\nu, \mu_0)}{dt_\nu} - I_{0,\,\nu}(t_\nu, \mu_0) \right]. \tag{23}$$

We have written subscripts on μ to emphasize that the equation is valid for any direction, $\mu_{v''}$, of $I_{v'',\,\nu}$ and any direction, μ_0, of $I_{0,\,\nu}$. The last equation yields a solution for $I_{v'',\,\nu}(t_\nu, \mu)$ of the form

$$I_{v'',\,\nu}(t_\nu, \mu_{v''}) = \frac{\varpi_{v''}}{\varpi_0} \frac{\kappa_\nu + \sigma}{\sigma_{v''}} I_{0,\,\nu}(t_\nu, \mu_0), \tag{24}$$

for $\mu_0 = (\kappa_\nu + \sigma)\mu_{v''}/\sigma_{v''}$. This solution may be verified by substituting equation (24) on the left side of equation (23).

We may now express the the reflected fluorescent intensities in terms of X- and Y-functions by means of equations (24), (4), and (5). Replacing μ_v'' with simply μ, we have

$$I_{v'',\,\nu}(0, +\mu)$$

$$= \frac{F_0}{4} \frac{\varpi_{v''} \kappa_\nu \mu_i}{(\kappa_\nu + \sigma)\mu + \sigma_{v''}\mu_i} \left[X\left(\frac{\kappa_\nu + \sigma}{\sigma_{v''}} \mu\right) X(\mu_i) - Y\left(\frac{\kappa_\nu + \sigma}{\sigma_{v''}}\mu\right) Y(\mu_i) \right]_{\varpi_0,\,\nu}. \tag{25}$$

The X- and Y-functions appearing in this equation (and which are evaluated for thickness τ_ν) will often have arguments greater than unity. If so, we define them to

satisfy the same equations as the X- and Y-functions with arguments less than unity and later show that this generalization does indeed render meaningful results. The X- and Y-functions with arguments greater than unity are expressible in terms of those with arguments less than unity. Let us define[2]

$$\xi^{\pm}(\mu) = \frac{\varpi\mu}{2} \int_0^1 \frac{X(\mu')\,d\mu'}{\mu \pm \mu'}, \qquad \mu \geq 0, \quad (26)$$

$$\zeta^{\pm}(\mu) = \frac{\varpi\mu}{2} \int_0^1 \frac{Y(\mu')\,d\mu'}{\mu \pm \mu'}, \qquad \mu \geq 0. \quad (27)$$

Substituting these expressions in the defining equations for the X- and Y-functions ($R.T.$, p. 181; they are also quoted as eqs. [35] and [36] of Paper II) gives

and
$$X(\mu) = 1 + X(\mu)\,\xi^{+}(\mu) - Y(\mu)\,\zeta^{+}(\mu), \qquad \mu \geq 0,$$
$$Y(\mu) = e^{-\tau/\mu} + Y(\mu)\,\xi^{-}(\mu) - X(\mu)\,\zeta^{-}(\mu). \qquad \mu \geq 0. \quad (28)$$

For $0 \leq \mu \leq 1$, these equations constitute two integral equations; but for $\mu > 1$ they are two ordinary, linear equations of the first order, which give X- and Y-functions in terms of $\xi^{\pm}$ and $\zeta^{\pm}$.

A numerical evaluation of ξ- and ζ-functions is needed to get the fluorescent intensities. In one special case, however, one can find these intensities in terms of known functions. From equations (28), we have

$$X(\infty) = Y(\infty) = \left\{ 1 - \frac{\varpi_{0,\nu}}{2}[\alpha^{(0)} - \beta^{(0)}] \right\}^{-1}, \quad (29)$$

where $\alpha^{(0)}$ and $\beta^{(0)}$ are the zeroth moments of the X- and Y-functions, respectively. Thus, letting $\sigma_{v''} \to 0$, equation (25) becomes

$$I_{v'',\nu}(0,+\mu) = \frac{F_0\varpi_{v''}\varpi_{0,\nu}\mu_i}{4\mu\varpi_0}[X(\infty)X(\mu_i) - Y(\infty)Y(\mu_i)]_{\varpi_{0,\nu}}$$
$$= \frac{F_0\varpi_{v''}\varpi_{0,\nu}\mu_i}{4\mu\varpi_0}\left\{ \frac{X(\mu_i) - Y(\mu_i)}{1 - \frac{1}{2}\omega_{0,\nu}[\alpha^{(0)} - \beta^{(0)}]} \right\}_{\varpi_{0,\nu}}, \quad (30)$$

where we have used equation (2) with $v'' = 0$, in writing the line-profile portion of the albedo. This is the monochromatic solution for the special case of no continuous absorption at the frequencies of the fluorescent emissions, although not necessarily at the resonant frequency. If the optical thickness τ_ν in the resonance transition is sufficiently small that the approximate solution (19) holds, the integrated fluorescent intensities can then be obtained from equation (30) by adopting the effective thickness and albedo $\tau_{\text{eff}} = \tau_\nu + \tau_c/\sqrt{2}$ and $\varpi_{0,\text{eff}} = \varpi_0/(1 + 2^{1/2}r)$ and the effective line width $\Delta\nu_{\text{eff}} = (2\pi)^{1/2}U\nu_c/c$, as was done for the resonant band, equation (19). We then have an integrated reflected intensity for a line in the v'' band of

$$\Im_{v''}^{(\text{ref})}(+\mu) = \frac{(2\pi)^{1/2}U\nu_cF_0\varpi_{v''}\varpi_{0,\text{eff}}\mu_i}{4c\varpi_0\mu}\left\{ \frac{X(\mu_i) - Y(\mu_i)}{1 - \frac{1}{2}\varpi_{0,\text{eff}}[\alpha^{(0)} - \beta^{(0)}]} \right\}_{\tau_{\text{eff}},\,\varpi_{0,\text{eff}}}, \quad (31)$$

valid for no continuous absorption except at the resonant frequency.

From equation (27) of $R.T.$ (p. 187), the denominator of equation (31) may be written

$$\frac{1}{1 - \frac{1}{2}\varpi_{0,\text{eff}}[\alpha^{(0)} - \beta^{(0)}]} = \frac{1 - \frac{1}{2}\varpi_{0,\text{eff}}[\alpha^{(0)} + \beta^{(0)}]}{1 - \varpi_{0,\text{eff}}}. \quad (32)$$

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[2] The ξ- and ζ-functions are discussed also in the appendix to Paper II.

When this expression is inserted in equation (31) and when the continuous absorption in the resonant band approaches zero (i.e., when $\tau_{\text{eff}} \to \tau_c/\sqrt{2}$ and $\varpi_{0,\,\text{eff}} \to \varpi_0$), the integrated intensity of equation (31), as one would expect, reduces to that in equation (14). This emergence of solution (14) as a special case of the more general one of equation (31) (which itself is derived as a special case of eq. [25]) supports the validity of our generalization of the X- and Y-functions to arguments greater than unity.

III. SCATTERING BY AN ATMOSPHERE OF LARGE OPTICAL THICKNESS

When the optical thickness at the line center becomes very large ($\tau_0 \gg 1$), the problem acquires a rather different character. Again we shall consider separately the cases of the albedo being constant (ϖ_0) and variable ($\varpi_{0,\,\nu}$), since most appropriate approximations are rather different in the two situations.

a) Constant Albedo across a Line: No Continuous Absorption

If there is no continuous absorption in the line-scattering portion of the atmosphere, all the incident radiation in and near the line center will be diffusely reflected—either in the resonant line or in one of the fluorescent transitions. For the central portion of the lines, the monochromatic solution is thus given in terms of Chandrasekhar's H-functions.

For the entire line profile, an approximate solution of the integrated line intensity, $\mathfrak{F}$, may be found by estimating in what portion of the line the atmosphere remains optically thick ($\tau_\nu > 1$, say) and then neglecting the optically thin wings ($\tau_\nu < 1$). If $t_c \gg 1$, little error is introduced by this approximation of the reflected profile as being rectangular.

The monochromatic intensity is still given by equations (4) and (5), except that, as $\tau_\nu \to \infty$, $X \to H$ (Chandrasekhar's H-functions) and $Y \to 0$. The integrated resonant intensity is thus

$$\mathfrak{F}_0^{(\text{ref})}(+\mu) = \frac{\Delta\nu F_0 \varpi_0 \mu_i}{4(\mu + \mu_i)} H(\mu) H(\mu_i), \tag{33}$$

where $\Delta\nu$ is the effective width of the line, defined as the interval between the two frequencies where $\tau_\nu = 1$. It should be emphasized that when τ_c is extremely large, $\Delta\nu$ may extend between the far wings. It is then necessary to compute the line-absorption coefficient with allowance for the wings produced by natural damping (or, in the case of moderately high pressures, collisional damping). Harris (1948) has published convenient tables for this purpose. The H-functions are tabulated by Chandrasekhar ($R.T.$, p. 125), by Harris (1957), and by Stibbs and Weir (1959).

The fluorescent-band intensities are obtained by substituting equation (33) in equation (13) for $\tau_c \gg 1$ and $\mathfrak{F}_0^{(\text{trans})}(-\mu) = 0$ and then integrating over a range of $\Delta\nu$. Using a form of the integral equation for $H(\mu)$ ($R.T.$, p. 107) and equation (3), we obtain, for the fluorescent intensities,

$$\mathfrak{F}_{\nu''}^{(\text{ref})}(+\mu) = \frac{F_0 \Delta\nu \varpi_{\nu''} \mu_i}{4\mu(1-\varpi_0)^{1/2}} H(\mu_i). \tag{34}$$

As usual, the H-function in this equation is to be evaluated for an albedo ϖ_0.

b) Variable Albedo across a Line: Continuous Absorption

In the following we suggest an approximate solution for the integrated intensity of the reflected resonant and fluorescent transitions.

i) *Resonant transition.*—In semi-infinite atmospheres with variable albedo $\varpi_{0,\,\nu}$ given by equation (16), the scattering function of equation (5) reduces to

$$S(\mu,\,\mu_i) = \frac{\varpi_0}{1 + r \exp(x^2)} \cdot \frac{\mu\mu_i}{(\mu+\mu_i)} |H(\mu) H(\mu_i)|_{\varpi_{0,\,\nu}}. \tag{35}$$

Substituting this in the expression for the integrated intensity of equation (8) gives

$$\Im_0^{(\mathrm{ref})}(+\mu) = \frac{F_0 U \nu_c \varpi_0 \mu_i}{4\,c\,(\mu+\mu_i)} \int_{-\infty}^{\infty} \frac{|\,H(\mu)\,H(\mu_i)\,|_{\varpi_0,\,\nu}}{1+r\,\exp\,(x^2)}\,dx\,. \tag{36}$$

Extending the integration limits to infinity, as indicated, requires that continuous absorption be dominant enough to cut off the emission profile in the Doppler wings. Otherwise it is more appropriate to stop the integration rather arbitrarily at the frequency corresponding to $\tau_\nu = 1$, i.e., at the transition from an optically thick to an optically thin atmosphere; that was the procedure used for equation (33). The use of equation (36) is therefore justified only when $\tau_\sigma + \tau_c \gg 1$ and $\tau_\sigma > 1$, and even then the denominator must be modified if the damping wings contribute. For the intermediate situation of $0 < \tau_\sigma < 1$, the integration is carried to a total optical thickness of

$$\tau_\sigma + \tau_c \exp\,(-x_{\mathrm{max}}^2) \approx 1 \quad \text{or} \quad x_{\mathrm{max}} = \left(\ln\frac{\tau_c}{1-\tau_\sigma}\right)^{1/2}. \tag{37}$$
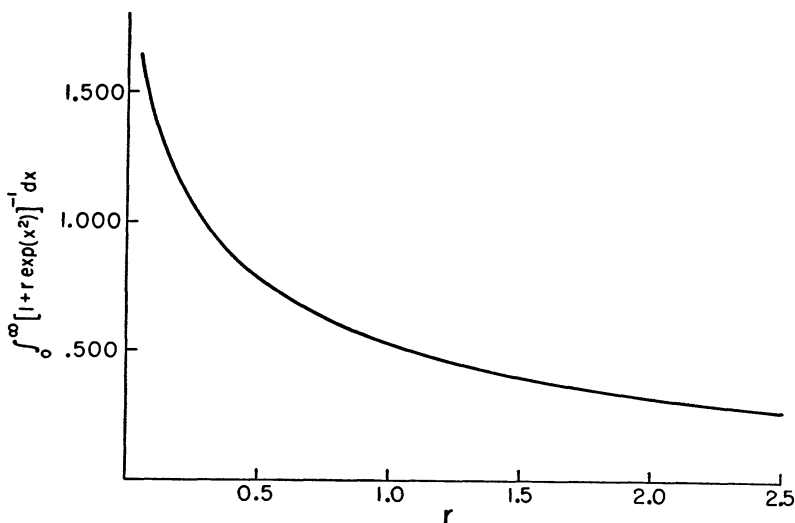

FIG. 4.—The integral $\int_0^\infty (1+r\exp x^2)^{-1}\,dx$ of equation (38)

In equation (36) the H-functions are frequency-dependent through $\varpi_0,\,\nu$, but they vary only gradually with albedo. (For example, as the albedo varies from zero to 0.95 $H[1]$ varies from 1 to 2.) Thus as an approximation we may consider the H-functions as constant and write equation (36) as

$$\Im_0^{(\mathrm{ref})}(+\mu) = \frac{F_0 U \nu_c \varpi_0 \mu_i}{2\,c\,(\mu+\mu_i)}\,|\,H(\mu)\,H(\mu_i)\,|_{\varpi_0,\,\mathrm{av}} \int_0^\infty \frac{dx}{1+r\,\exp\,(x^2)}\,. \tag{38}$$

The integral in this equation must be evaluated numerically. In Figure 4 we have plotted the integral as a function of r. Here the H-functions are to be evaluated for a suitably averaged albedo. For this average we suggest

$$\varpi_{0,\,\mathrm{av}} = \frac{\varpi_0}{1+r\,\exp\,(\chi^2)}\,, \tag{39}$$

where χ is given by

$$2\int_0^\chi \frac{dx}{1+r\,\exp\,(x^2)} = \int_0^\infty \frac{dx}{1+r\,\exp\,(x^2)}\,. \tag{40}$$

That is, χ is the frequency which halves the integral in equation (38). In Figure 5 we have plotted $\varpi_{0,\,av}$ as a function of r.

ii) *Fluorescent transitions.*—Monochromatic intensities may be obtained from equation (25) by passing to the limit of large optical thicknesses,

$$I_{v'',\,\nu}(0,\,+\mu) = \frac{F_0}{4} \frac{\varpi_{v''}\kappa_{\nu}\mu_i}{(\kappa_{\nu}+\sigma)\mu+\sigma_{v''}\mu_i}\left| H\left(\frac{\kappa_{\nu}+\sigma}{\sigma_{v''}}\mu\right)H(\mu_i)\right|_{\varpi_{0,\,\nu}}, \quad (41)$$

where again the H-function may have arguments greater than unity. It is defined by the limit of equation (28) as the optical thickness grows large:

$$H(\mu) = 1 + H(\mu)\eta^{+}(\mu) \quad (42)$$

or

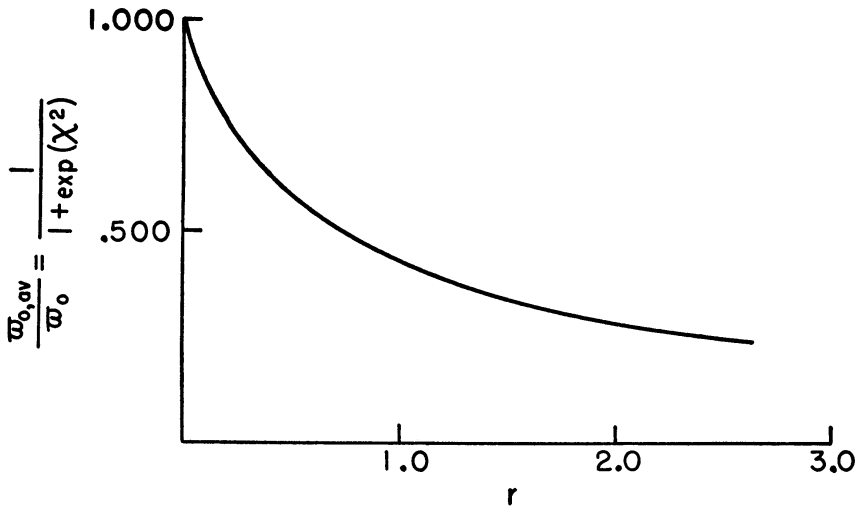$$H(\mu) = \frac{1}{1+\eta^{+}(\mu)}, \quad \mu \geq 0. \quad (43)$$

FIG. 5.—The average albedo of equation (39) where $\chi(r)$ is given by equation (40) and Fig 4

The function η introduced here is the analogue of the ξ- and ζ-functions,

$$\eta^{\pm}(\mu) = \frac{\varpi\mu}{2}\int_0^1 \frac{H(\mu')}{\mu \pm \mu'}\,d\mu' \quad \mu \geq 0. \quad (44)$$

Equation (41) may now be written as

$$I_{v'',\,\nu}(0,\,+\mu) = \frac{F_0\varpi_{v''}\varpi_{0,\,\nu}\mu_i H(\mu_i)}{4\varpi_0[\mu+\sigma_{v''}\mu_i/(\kappa_{\nu}+\sigma)]\{1-\eta^{+}[(\kappa_{\nu}+\sigma)\mu/\sigma_{v''}]\}}\bigg|_{\varpi_{0,\,\nu}}. \quad (45)$$

The factor $H(\mu_i)/(1-\eta^{+})$ is a slowly varying function of albedo and therefore ν. Thus, using the same procedure as for the resonant line, we find the approximate expression for the integrated fluorescent intensities:

$$\mathfrak{F}_{v''}^{(\mathrm{ref})}(+\mu)$$

$$= \frac{F_0 U\nu_c\varpi_{v''}\mu_i H(\mu_i)}{2c\{1-\eta^{+}[(\kappa_{\nu}+\sigma)\mu_i/\sigma_{v''}]\}}\bigg|_{\varpi_{0,\,av}}\int_0^{\infty}\frac{\varpi_{0,\,\nu}\,dx}{\varpi_0[\mu+\sigma_{v''}\mu_i/(\kappa_{\nu}+\sigma)]}, \quad (46)$$

where the average albedo $\varpi_{0,\,av}$ is defined by equation (39) and is plotted in Figure 5. The integral in equation (46) is to be evaluated numerically. The restrictions on the problem for the integration limit to be infinite, as indicated, are summarized below equation (36).

If the continuous absorption in the fluorescent bands, $\sigma_{v''}$, tends to zero, equation (46) reduces to

$$\Im_{v''}^{(ref)}(+\mu) = \frac{F_0 U \nu_c \varpi_{v''} \mu_i \, | H(\mu_i) | \, \varpi_{0,\,av}}{2\,c\mu(1-\varpi_{0,\,av})^{1/2}} \int_0^\infty \frac{dx}{1+r\exp(x^2)} . \tag{47}$$

In deriving this equation we have used the relation (see *R.T.*, p. 106)

$$1 - \eta^\pm(\infty) = 1 - \frac{\varpi_{0,\,av}}{2} \int_0^1 H(\mu')\,d\mu' = (1-\varpi_{0,\,av})^{1/2} . \tag{48}$$

Equation (47) gives the integrated reflected intensity of a line in the v'' fluorescent transition, when there is continuous absorption only at the resonant frequency. It is the fluorescent analogue of equation (38), and it is the extension to optically thick atmosphere of equation (31). The integral in equation (47) is plotted in Figure 4.

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