(NEW) METHODS OF RADIATIVE TRANSFER IN EXPANDING ATMOSPHERES

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ABSTRACT The principle difficulties of radiative transfer in expanding atmospheres are discussed. Standard methods of calculating the radiation field in lines (Sobolev approach, Comoving frame method, Monte Carlo simulation) are compared and the influence of line-blocking and multi-line (ML) processes on the radiation field is investigated. It turns out that ML processes can -in principle- accelerate the winds of WR stars even at large distances from the star. Finally, a newly developed operator is presented which is able to solve for all aspects of the radiation field in *one single step.*

I. INTRODUCTION

The general principle of calculating stellar atmospheres is given by the self-consistent solution of at least three different sets of equations:

i) the rate equations, from which we find - for given atmospheric model and radiation field- the occupation numbers.
ii) the equation of radiative transfer, which yields - for given atmospheric model and occupation numbers - the radiation field.
iii) the hydrodynamical equations (in case of no mass-outflow the equation of hydrostatic equilibrium), which define - for given radiation field and occupation numbers - the atmospheric model.

To obtain the correct temperature stratification, additionally the constraint of energy conservation has to be accounted for.

This paper deals (exclusively) with item ii), the solution of the equation of radiative transfer. In contrast to plane-parallel, hydrostatic atmospheres (HSA), where several standard methods are available for solving this problem (Feautrier, Rybicki, Auer-Heasley,...) the introduction of a *velocity field* in rapidly expanding spherical atmospheres leads to additional complications for which these methods become inefficient.

Firstly, the density decreases $\sim r^{-2}$ in a large part of the atmosphere (HSA: $\rho \sim \exp(-r/H)$), so that the continua forming layers may become *spatially extended* and optically thick up to several stellar radii (Pauldrach, 1987).
Much more important in this context, however, are the effects of the Doppler-shifts of frequencies induced by the velocity field, leading to an *intrinsic coupling* of *frequency* and *location* of absorption/emission processes, which follows from the well known Doppler formula

$$\nu_A = \nu_O \left(1 - \frac{\mu V(r)}{c}\right) \tag{1}$$

where ν_A is the atomic transition frequency and ν_O the observer's frame frequency.
The intrinsic profile width of b-b transitions leads then to the concept of *interaction zones of definite width*, dependent only on the velocity field and rather small compared to atmospheric dimensions. In contrast, the "interaction zone" in HSA extends throughout the total atmosphere.
Furthermore, equ.(1) implies that for given ν_O and specified ray a large number of b-b transitions with transition frequencies in the range of $\nu_O(1 \pm \mu V_\infty)$ can take place at different locations on this ray. This feature which is known as *line-overlap* leads to an intrinsic coupling of different species of ions via the equations of statistical equilibrium. In HSA, line overlap is possible only for lines where the profile-functions are overlapping in the oberver's frame itself.
Finally, the evaluation of profile-weighted and frequency integrated quantities in lines such as $\bar{J}$, $\bar{H}$ requires a frequential and spatial *micro-resolution* due to the small width of the interaction zone, which will be considered in detail below. On the other hand, in HSA the radiative transfer for both continua and lines is similar.

II. THE PROBLEM

Before discussing the difficulties of radiative transfer caused by the expansion in more detail, we want to consider briefly which quantities of the radiation field are needed to perform stellar wind calculations. In the following we will restrict ourselves to the assumption of spherical symmetry and stationary flows (i.e $\partial/\partial t \equiv 0$). The problems arising from a fully time-dependent treatment are discussed in the contribution by S.Owocki et al. to these proceedings.
In principle, two different kinds of quantities are required, at least when the outflow velocities are well below the speed of light, so that the frequency shift of continuum quantities such as opacity, emissivity and cross-sections can be neglected. (Nevertheless, attention must be paid to at ionization edges!)
The first type then consists of the frequential integral of mean intensity J_ν or flux H_ν multiplied by one of those continuous quantities to describe the radiative acceleration by the continuum ($\sim \int d\nu\, \chi_\nu^{cont} H_\nu$), the ionization rates ($R_{ik} \sim \int d\nu\, \alpha_{ik}/h\nu\, J_\nu$) and the continous part of the radiative (non-)equilibrium ($\sim \int d\nu\, \chi_\nu (S_\nu - J_\nu)$).

The second type is the more sophisticated one which describes the processes connected with b-b transitions, where the difficulty arises from the frequency and velocity-field dependent profile function Φ. It typically appears to be of the form

$$1/2 \int_{\nu_{min}}^{\nu_{max}} d\nu_O \int_{-1}^{+1} (\mu) d\mu \; \Phi(\nu_O - \nu_A \frac{\mu V(r)}{c}) \; I(\nu,\mu,r) \quad , \tag{2}$$

where the integration is performed over the total observer's frame line width (P-Cygni type) and the profile function is evaluated at the corresponding comoving frame frequency. This type of quantity yields the radiative line pressure, the scattering integral $\bar{J}$ ($\rightarrow$ rate equ.) and the cooling (heating) rates of lines in the equation of radiative (non-)equilibrium.
Finally, for a comparison to observations, the flux itself is required at $r = R_\infty$, and for separate albedo calculations (cf. the contribution by D.Husfeld) one may need the quantity $I_\nu^-(\mu)$ at the sonic point.

Summarizing, the ideal operator to solve the radiative transfer should yield, for given opacity and emissivity, the specific intensity $I(\nu,\mu,r)$ with *sufficient resolution* concerning ν,μ,r such that *all* integral and frequential quantities could be easily derived. The question now is which resolution is actually sufficient?

III. THE DIFFICULTIES

A. The Minor Problem: J_ν, H_ν

1. The Problem *Without* Lines

The pure continuum case is rather easy to handle. J_ν and H_ν can be calculated by standard methods (Feautrier, Rybicki,...), and the necessary frquency grid is found by taking into account *all* relevant ionization edges (ground state + excited levels) in the range from $\lambda_{min} \approx 70$ Å (ionization edge of SiV) up to $\lambda_{max} \approx 100{,}000$ Å required for flux conservation. In total, with ~ 30 elements, 3 main ionization stages, 5 main ionizing levels per ion and a factor of 2 more points to perform the ionization/recombination integrals, we end up with ca. 1,000 frequency points in this case.

2. The Problem *With* Lines: *Line-Blocking*

Taking into account the actual line-distribution function to treat the problem of line-blocking (photospheric + wind) correctly, the solution becomes more difficult. Line-blocking can have a large influence on the photoionization rates of trace ions such as CIII, NIII, SiIV (see the contribution by A.Pauldrach) and must be considered for the calculation of the frequential and total flux. Its main importance, however, is given by its influence on the line formation itself, as will be seen below.-

A given observer's frame frequency ν_o is influenced by lines with transition frequencies $\nu_A = \nu_o \pm \Delta\nu_{max}$, $\Delta\nu_{max} = \nu_o v_\infty/c$ or $\Delta\lambda = \pm\lambda v_\infty/c$, which for typical hot star winds is of order 1% of rest wavelength (e.g. ±15Å at 1,500 Å).

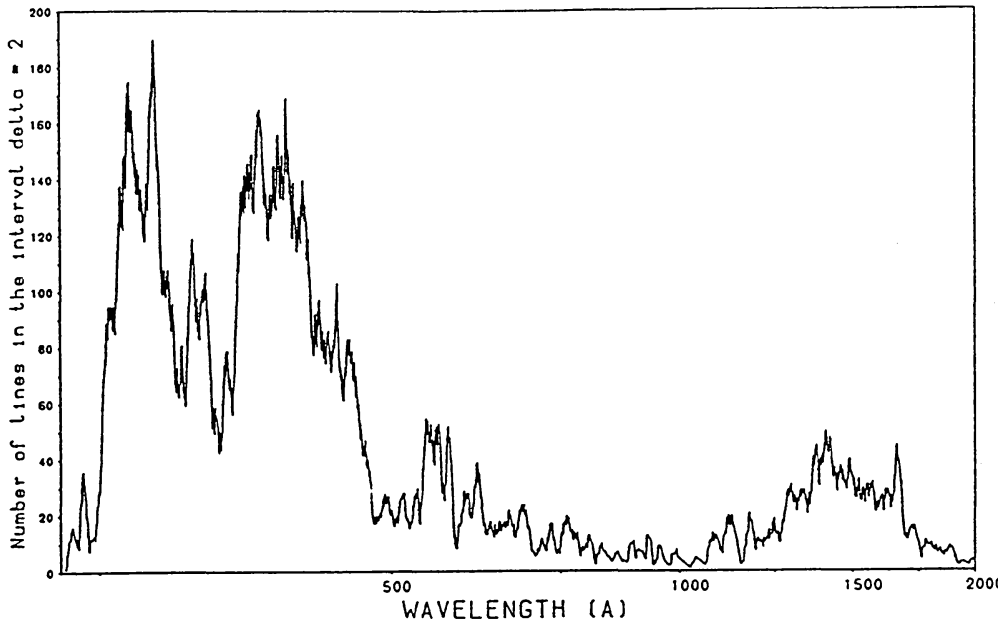

Fig.1 Line distribution function for ζ Pup and $228 \le \lambda \le 2{,}000$ Å

As an example, Fig.1 gives the actual line-distribution function for our standard model of ζ Pup (cf. the contribution by A.Pauldrach). In this figure, the number of *important* (i.e. stronger than e^--scattering) lines in the interval $\lambda_o \pm \Delta\lambda_{max}$ is plotted over wavelength (228...2,000 Å). Most stikingly, just at the ionization edges of the trace ions between 260 and 280 Å, this function shows an extreme peak with ca. 150 lines per $\Delta\lambda$-interval, which should influence the ionization crucially.

To calculate the essential frequential resolution, we estimate the minimum number of grid points per $\Delta\lambda$-interval to be of order 5. The number of these intervals themselves is given by (cf. Puls, 1987)

$$n = \log(\lambda_{max}/\lambda_{min}) \;/\; \log(1 + v_\infty/c) \;, \qquad (3)$$

so that for typical values of O/WR stars (line blocking important between $\lambda_{min} \approx 200$ Å and $\lambda_{max} \approx 2{,}000$ Å, $v_\infty \approx 2{,}000$ km/s) n amounts to 350 and the total number of frequencies to perform line-blocking calculations is given by 350 * 5 = 1750 (plus some 500 points in the range below 200 and beyond 2,000 Å).

Although this number is easily to manage with today's computers, the introduction of overlapping lines in the radiative transfer has some significant effect on the solution method. In fact, at least in the observer's frame, standard methods on a *fixed* grid are no longer applicable. As the typical width of the interaction zone (of order $v_{th} \approx 5$ km/s) is small compared to the typical velocity spacing of the radial grid points, a difference operator would simply miss the resonance zone. Instead of differential operators, *integral operators on a variable grid* must be applied in this case (see sect.5).

B. The Major Problem: $\bar{J}$, $\bar{H}$ for *All* Lines

The major problem, however, arises if we want to calculate profile weighted and frequency integrated quantities such as $\bar{J}$, $\bar{H}$ in each line at each grid point. In addition to the *spatial* microresolution (see above), in this case also a *frequential* microresolution is necessary due to the fact that the specific intensity varies rapidly on the "fast" frequency scale $\Delta\nu_{Profile} = \Delta\nu_{Dop}$, which has to be considered for the integration of terms like $I_{\nu_0} * \Phi(\nu_0 - \nu_A \mu V/c)$ (cf.eq.(2)). In this case, the required number of intervals is given by (eq.(3))

$$n = \log(\lambda_{max}/\lambda_{min}) \;/\; \log(1 + v_{Dop}/c)$$

which results with $v_{dop} \approx 5$ km/s (in absence of micro-turbulence) in NF = 140,000*5 = 700,000 frequencies, a number much too large to be even thought of.

IV. STANDARD METHODS OF CALCULATING $\bar{J}$, $\bar{H}$

In order to calculate $\bar{J}$, $\bar{H}$ on a reasonable time-scale, two different techniques are commonly applied which will be discussed in the following: the Sobolev-approximation (SA) and the comoving frame (CMF) method. Also, advantages and disadvantages of using Monte-Carlo simulations in radiative transfer will be considered. (For a detailed discussion, see Puls, 1987)

A. The Sobolev Approach

The general principle of the Sobolev approach (based on the pioneering work by Sobolev, 1958) is well known. Assuming the so-called "macro-variables" such as opacity, source-function S, velocity and its derivative to be constant in each interaction zone of a specific line (- which is justified because of its small width compared to spatial dimensions-), the profile weighted and frequency integrated specific intensity $I(\mu,r)$ can be calculated *analytically* and its angular moments $\bar{J}$, $\bar{H}$ are found by simple angular quadrature.
Hence, *no* microresolution - neither spatial nor frequential - has to be taken into acount and the required number of operations is proportional to the number of radial gridpoints times the number of lines. Depending on the specific situation, different levels of sophistication have been developed in the last years.

1. SA *Without* Continuum

This most simple approach is justified if the continuum is optically thin in the line forming (spatial+frequential) region, which is true for O/B stars beyond the sonic point and longwards from 228 Å (or 504, 911 Å , depending on ionization). In result, the desired quantities are given by

$$\begin{aligned} \bar{J}(r) &= (1 - \beta(r))\, S_L(r) + \overline{\beta_c I^{inc}(r)} \quad , \\ \bar{H}(r) &= \overline{\gamma_c I^{inc}(r)} \quad , \end{aligned} \tag{4}$$

where β is the local escape probability in SA and $\overline{\beta_c I^{inc}}$, $\overline{\gamma_c I^{inc}}$ are defined as

$$\left.\begin{matrix} \overline{\beta_c I^{inc}} \\ \overline{\gamma_c I^{inc}} \end{matrix}\right\} = \frac{1}{2} \int_{-1}^{+1} \begin{pmatrix} d\mu \\ \mu d\mu \end{pmatrix} \frac{1 - e^{-\tau_S(\mu)}}{\tau_S(\mu)} I^{inc}(\mu) \quad , \tag{5}$$

with τ_S the optical depth in SA and $I^{inc}(\mu)$ the specific intensitiy at the beginning of the considered interaction zone. This last quantity — the actual crux of the problem - is approximated by nearly all authors in the so-called *single-(line)*-scattering (SL) approach, neglecting the contribution of all lines prior to (and beyond of) the specified interaction zone. This approximation then yields

$$I^{inc}(\mu) = \begin{cases} I^{core}(\nu_{CMF}, \mu) & \text{for } 1 \le \mu \le \mu_* \\ 0 & \text{else} \end{cases} \tag{6}$$

and has to be compared to the so-called *multi-line* (ML) approach (Rybicki and Hummer, 1978; Olson, 1982; Puls, 1987) which takes into account the actual intensity at the beginning of the interaction zone (calculated in SA), processed by overlapping lines.

Fig.2 compares the total line acceleration obtained by different approaches for the case of ζ Pup. It is normalized to the value given by the SL approach defined in (6). The term "single-(line)-scattering is somewhat misleading, as the actual approximation *is not* the event of a *single* scattering in the wind, but the assumption that *all lines* are irradiated by the *full* photospheric intensity. The *real* single scattering force where the photon is actually scattered only once is given by the dashed-dotted curve. It has the same value as the SL force in the photosphere, but is much smaller in the outer layers due to the apparent line-blocking in zones below. The force arising by detailled ML calculations is shown by the bold curve. In the photospere, it is smaller than the SL value due to the diffuse radiation field scattered back from above, whereas in the outer wind it is much larger than the *real* single-scattering force due to the multiple momentum transfer — but still smaller than the approximate SL value. Hence, we find in this case —

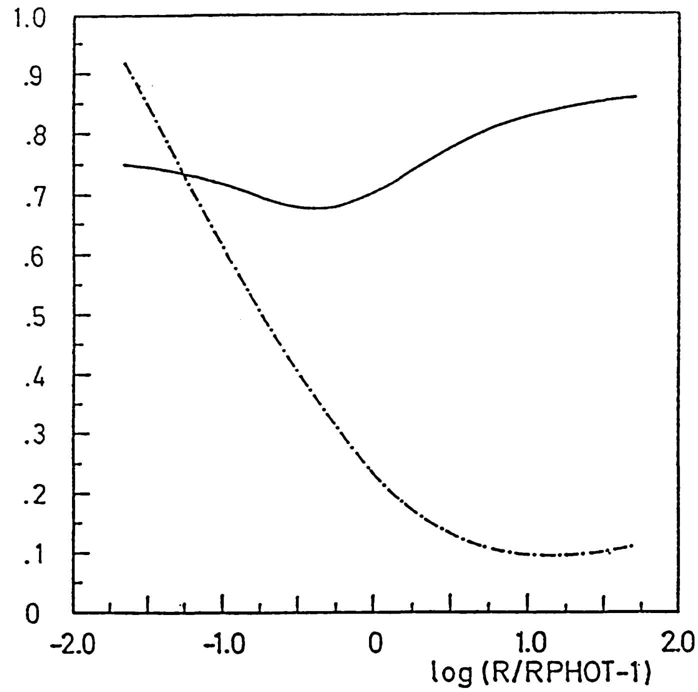

Fig.2 Ratio of line accelerations: *real* single scattering/g_{Rad}(SL) (-.-.) and multi-line scattering/g_{Rad}(SL) (——)

despite of the increase of the line force by ML scattering processes — a smaller line acceleration than the approximate value used e.g. by Pauldrach (1987) in all parts of the wind.—
This behaviour, however typical for O/B stars, is not necessarily true under all circumstances and is essentially connected with the question: what is the *maximum value of the line force* can be theoretically achieved . In this context, the reader may note that the so-called *single-scattering limit* $\dot{M} v_\infty/Lc$ (≡ 1 means that the total momentum of the stellar radiation field is transferred *once* to the stellar wind) which is of order 0.1...0.5 for O/B stars can reach values of 3...50 for WR-stars (high $\dot{M}$ + high v_∞). Although it is (in principle) possible to obtain the large mass loss rates by either claiming that these objects are situated close to the Eddington limit (in contrast to today's evolutionary calculations) or by including the rather large continuum force in the lower atmosphere (but far beyond the sonic point), the acceleration of this $\dot{M}$ to observed v_∞'s is not feasible in the usual SL approach. In the following, we will discuss under which circumstances the radiation force obtained by multi-line momentum transfer can exceed the SL value. Comparing the resulting line forces, we find

$$g_{Rad}^{SL} \sim \sum_{\substack{\text{all}\\ \text{lines}}} \frac{1}{2} \int_{\mu_*}^{1} I_c \, \frac{1 - e^{-\tau_S}}{\tau_S} \, (e^{-\Sigma \tau_B(\mu_B)}) \, \mu d\mu \qquad (7)$$

$$g_{Rad}^{ML} \sim \sum_{\substack{\text{all}\\\text{lines}}} \left\{ \frac{1}{2} \int_{\mu_*}^{1} I_c \, \frac{1 - e^{-\tau_S}}{\tau_S} \, (e^{-\sum \tau_B(\mu_B)}) \, \mu d\mu \right.$$

$$\left. + \frac{1}{2} \int_{-1}^{1} I_c \, \frac{1 - e^{-\tau_S}}{\tau_S} \left(\sum S_B (1 - e^{-\tau_B}) \, (e^{-\sum_{j=1}^{i} \tau_B^j (\mu_B)}) \right) \mu d\mu \right\} \tag{8}$$

where τ_B, S_B are the values of _interacting lines_ found at connected, blueward resonance zones (for a detailed discussion, see Puls, 1987). By definition, the first part of g_{Rad}(ML) is always smaller than g_{Rad}(SL). The second part of g_{Rad}(ML) consists firstly of the integration range −1...0 and is always negative, i.e. leads to a _force reduction_ by photons scattered back from above. Consequently, ML processes can lead to an increase compared to g_{Rad}(SL) _only_ if the integration range 0...1 becomes decisive and is (on the average) much larger than g_{Rad}(SL).

By inspection of the structure of the resonance zones (cf. Fig. 3), we find that this (in principle) can occur only for r $\gtrsim$ 2.5 R_*, because for smaller radii no connected resonance zones exist in this range (Fig. 3a). A further inspection of the second part of g_{Rad}(ML) then shows that this part is larger (on the average) than g_{Rad}(SL) only if $r_B^2 \, S_B/I_c \gg 1$, which means that the lines itselves _must not_ be pure scattering lines but have to contain a significant thermal contribution. Consequently, large line forces _by ML processes_ can only arise for r $\gtrsim$ 2.5 R_* and if the lines are not pure scattering lines, a fact which seems to

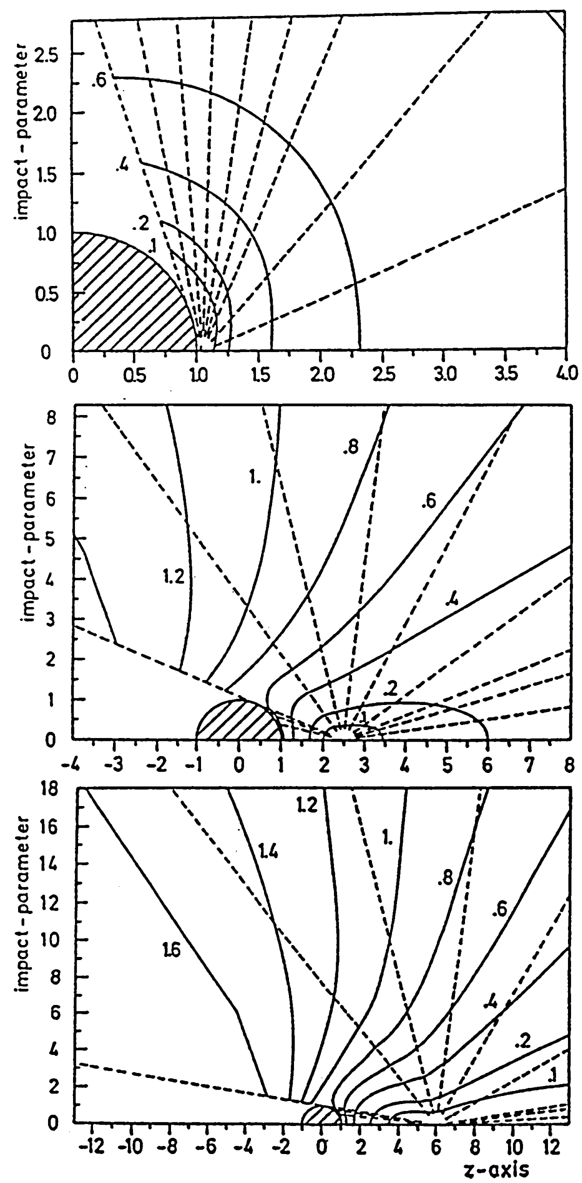

Fig.3 Resonance zones for the standard model of ζ Pup and r = 1.045 R_*(top), r = 2.5 R_* (middle) and r = 6 R_*(bottom)

be possible in the extermely dense winds of WR-stars. A (somewhat exaggerated) example of large line forces is shown by Puls (1987, Table 3a) where, assuming pure LTE-occupation, a ratio of $g_{Rad}(ML)/g_{Rad}(SL)$ of ~ 50 at r = 6 R_* and of 17,000 at r = 50 R_* is found. Until further investigation, it seems therefore to be probable that the final acceleration of WR star winds takes place far out in the wind. This hypothesis is strongly confirmed by newest observations (cf. the contribution by L.Auer and G.Koenigsberger, who found actually an acceleration of the wind of HD 90657 (WN4 + O4-6) at distances larger than 50 R_*) and by the analysis of HeI/II lines in HD 50896 (WN5) which in comparison with UV data revealed that "the velocity must undergo a substantial increase (i.e., from ~ 1700 km/s to > 2400 km/s) beyond 50 R_{core}" (Hillier, 1987 , and references therein).

A second remark should be made concerning the influence of ML-processes on $\bar{J}_L$ and therefore on the rate-equations. As shown by Puls (1987) , for strong (resonance) lines $\bar{J}(ML) \approx \bar{J}(SL)$, and large modifications are to be expected only for weak (subordinate) lines and $r \gtrsim 2\ R_*$, so that in the solution algorithm of the rate-equations a neglect of ML-processes is not of major importance.

2. SA *With* Continuum

In atmospheres where the continuum and the line forming layers overlap (WR-stars, continuum can be optically thick far beyond the sonic point for *all* wavelengths), the interaction of continuum and lines *in the interaction zone* has to be accounted for. The principle method is given by Hummer and Rybicki (1985), and model calculations have been performed by Puls and Hummer (1987). In this paper it was also shown that the *anisotropic* diffuse radiation field ~ $\mu dS_L/dr$ becomes decisive for the line acceleration in subsonic regions, which is shown in Fig.4. With respect to the interaction line/continuum, the ML approach has not been included so far.

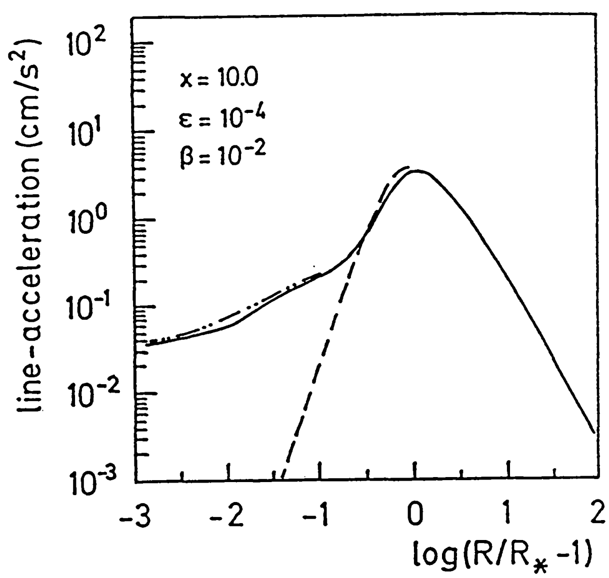

Fig.4 Line acceleration including line/continuum interaction (- - -), plus diffuse radiation field (-..-..) in comparison with "exact" CMF calculations (——).

B. Comoving Frame Method

Another method of specifying the radiation field is to solve the radiative transfer in the comoving frame, a frame *comoving with* *the interaction zone in question*. For details, see e.g. Mihalas (1979) and for the inclusion of ML processes Hamann (1979) and Puls (1987). With this approach then, the equation of radiative transfer can be solved for on a *fixed* grid, and no spatial microresolution is required, as we are moving now together with the resonance zone throughout the whole atmosphere. By transforming from the observer's into the comoving frame however, one obtains a *partial differential equation in space and frequency*. Replacing $\partial/\partial\nu$ by $1/\Delta\nu$ in the difference equation scheme, this requires at least $\sim$ 20 frequencies per line to obtain sufficient accuracy in terms of the Taylor expansion ($\Delta\nu_{Line} \sim 6*\Delta\nu_{Dop} \Rightarrow \Delta\nu_{grid}/\Delta\nu_{Dop} \approx 0.3$). For the most important 2,000 lines to be taken into account we end up with NF $\sim$ 40,000 frequencies to be calculated for a typical stellar wind problem. Including the interaction line/continuum, a factor of roughly two more points would have to be used.

A comparison of the results obtained with CMF and SA (including the diffuse radiation field) reveals that under almost general conditions these two methods are identical, as was shown by Puls (1987) with respect to ML-calculations and by Puls and Hummer concerning line/continuum processes (cf. Fig.4). Therefore, although the CMF method is espcecially valuable for test calculations of new effects to be investigated, the much faster SA approach (NF = 1 per line) should be preferred for practical purposes. Besides the large number of frequencies per line to be accounted for, a second disadvantage of CMF calculations should be mentioned: as the solution of the CMF equation yields the specific intensity in the CMF with respect to CMF-frequencies, only *angular- and frequency-integrated* quantities such as $\bar{J}$, $\bar{H}$, H_{tot} are (to order v/c) identical with observer's frame quantities. The calculation of frequency dependent quantities such as the emergent flux H_ν requires a separate treatment.

C. Monte-Carlo Methods

The Monte-Carlo (MC) simulation of a photon's path throughout the wind was developed by Abott and Lucy (1985) in order to calculate $\dot{M}$ for given velocity law including ML momentum transfer. Puls (1987) used the same method for test calculations of g_{Rad}(ML) for given $\dot{M}$ and velocity field. The MC simulation, by principle, is only economical if *pure scattering processes* (one photon absorbed $\Rightarrow$ one photon reemitted instantaneously) are investigated. This restriction prohibits a correct treatment of the *true* continuum in the wind — only e^- scattering can be considered — and leads to the treatment of all lines as *pure scattering lines*. which, in terms of the rate equations, is identical to assuming $S_L =: \bar{J}_L$ for all lines. As will be shown, this assumption is justified in most cases *if the converged NLTE occupation numbers are given*, where these numbers are calculated from radiative transfer methods mentioned above. Then,

i) the escape probabilities $e^{-\tau}$ used in MC are consistent with those following from the rate equations.

ii) the ratio $\bar{J}/S_L = (1 - \beta) + \beta_c I^{inc} / S_L$ (cf. eq.(5)) is actually of order unity for strong lines ($\beta\approx 0$) and $\beta_c I^{inc}/S_L \ll 1$, which is normally fulfilled O/B stars for those lines.

iii) for collisionally dominated lines, however, the assumption of $\bar{J} \approx S_L$ is totally inconsistent, as the occupation numbers then are driven much more by T_e rather than by T_{Rad}.

Under these restrictions, the MC simulation proves to be a useful and fast tool for the following types of calculations:
- investigation of different redistribution functions (spatial+frequential)
- calculation of emergent fluxes and albedos
- calculation of average quantities such as g_{Rad} and line blocking/blanketing (see the contribution of W.R. Schmutz), but *less quantitatively than other methods.*

The main and outstanding disadvantage of MC simulations, however, is given by the fact that they cannot be used for the simultaneous and self-consistent determination of occupation numbers, as the rate equations themselves are determined just by the deviation of $\bar{J}_L$ from S_L (net radiative brackets ~ $(1 - \bar{J}_L/S_L)$), so that an iteration cycle of rate-equations and MC radiative tranfer is absolutely inconsistent a priori.

Finally, Table 1 gives a brief summary and comparison of the discussed techniques to perform radiative transfer in stellar wind calculations.

Table 1

method	use	frequ.points	radial grid
1. observer's frame without lines: differential operator	pure continuum calculations	~1,000	40-60
2. observer's frame with lines: integral operator	continuum incl. line-blocking, emergent flux, albedo	2,000-2,500	micro-resolution 1,200... 1,800
3. observer's frame with lines: integral operator	as method 2., additionally $\bar{J}_L$, $\bar{H}_L$	micro-resolution ~700,000	micro-resolution 1,200... 1,800
4. Sobolev approach: analytical	$\bar{J}_L$, $\bar{H}_L$	one per line ⇒ 2,000	40-60
5. comoving frame: differential oper.	$\bar{J}_L$, $\bar{H}_L$	~ 20 per line ⇒ 40,000	40-60
6. Monte–Carlo simulation	emergent flux, albedo, g_{Rad}	~ 100,000 photons	

V. A UNIVERSAL OPERATOR TO SOLVE RADIATIVE TRANSFER IN EXPANDING ATMOSPHERES

From the considerations above and Table 1, it is evident that the *ideal* operator for detemining *all* aspects of the radiation field (as looked for in sect.2) should be some combination of method 2 and 4. Method 2 yields $I(\nu,\mu,r)$, $J(\nu,r)$, $H(\nu,r)$, $H(r)$, $g^{C}_{Rad}(r)$ including line-blocking on the predefined frequency grid, and the Sobolev approach gives $\bar{J}_L$, $\bar{H}_L$, g^{L}_{Rad} for specified incident intensity on each resonance zone $I^{inc}(\nu,\mu,r)$. A combination of these two methods has the big advantage of dealing only with a reasonable number of frequencies and *of including ML processes automatically*, whereas the major error arises only if the the profile functions overlap in the observer's frame, so that a treatment of one line per resonance zone is no longer justified. This error was considered by Puls (1987) and turned out to be of order 5%.
In the following we will work out some details of this newly developed operator which we will briefly call IOSA (integral operator plus Sobolev approach).

1. Integration of the Obervers's Frame Equation

As we are interested in the specific intensity $I(\nu,\mu,r)$ at *all* predefined spatial grid points, we have to integrate the equation of radiative transfer on each ray throughout the whole atmosphere. This means in the usual (p,z) geometry the integration (for positive angles $+\mu$) from $z_{max} = (R^2_{max} - p^2)^{1/2}$ to $z_{min} = (1 - p^2)^{1/2}$ (core rays) or $z_{min} = 0$ (non-core rays) and (for negative angles $-\mu$) from $z_{max} = -z_{min}(+\mu)$ to $z_{min} = -z_{max}(+\mu)$.
The actual problem of this integration — as everybody knows who has ever performed a formal solution in expanding atmospheres — is the definition of the integration variable Δz such that the appropriate $\Delta\tau$ is not too large (otherwise there is a big chance of missing some resonance zone in part or totally). The standard procedure is a sort of shooting method where, from an initial guess of Δz , $\Delta\tau$ is calculated and then, if $\Delta\tau > \Delta\tau_{max}$ (of order 0.1 or smaller), the value of Δz reduced by a factor so long until $\Delta\tau(\Delta z)$ is actually smaller than $\Delta\tau_{max}$. This procedure, especially if applied for thousands of frequencies and rays, is enormously time-consuming and makes an integral solution almost unfeasible. We therefore apply a simple *predictor* for Δz which has proven to be very useful and yields values of $\Delta\tau(\Delta z)$ nearly identical to the required $\Delta\tau_{max}$ (at least 5—sf). Following the linearization

$$\Delta\tau =: \Delta\tau_{max} = 0.5\ (\chi(z_i) + \chi(z_{i+1}))\ \Delta z$$

and the Taylor expansion

$$\chi(z_{i+1}) = \chi(z_i) + \frac{\partial\chi}{\partial z}\bigg|_{z_i}$$

Δz is found from the quadratic equation

$$\frac{1}{2} \frac{\partial \chi}{\partial z}\Big|_{z_i} \Delta z^2 + \chi(z_i)\ \Delta z - \Delta\tau_{max} = 0 \tag{11}$$

where the (total) opacity and its derivative are given by

$$\chi(z_i) = \chi^{cont}(z_i) + \sum_{\substack{\text{all}\\ \text{lines}}} \chi^i(z_i) * \Phi^i(\nu - \nu_A \mu V(z_i)/c) \tag{12}$$

$$\frac{\partial \chi}{\partial z}\Big|_{z_i} = \frac{\partial \chi^{cont}}{\partial z}(z_i) + \sum_{\substack{\text{all}\\ \text{lines}}} \left\{ \frac{\partial \chi^i}{\partial z}(z_i) * \Phi^i(z_i) - \chi^i(z_i) * \Phi'^{\,i}(z_i) \frac{\nu_A}{c} \frac{\partial \mu V}{\partial z}(z_i) \right\},$$

and the derivative of the profile function Φ' can be calculated analytically. Besides its ability of fast and accurate performance, the use of the above predictor has the additional advantages that one can use a rather large $\Delta\tau_{max}$ (0.3) and that one need no longer look for the beginning and end of resonance zones, at least as long one knows all opacity sources which can influence the considered observer's frame frequency ν.- Having determined I^+, I^-, a final angular integration yields all desired frequential quantities.

2. Calculation of $\bar{J}_L$, $\bar{H}_L$ for all Lines

To calculate the radiation field *in* the lines (including ML-processes, see eq.(4, 5)), we have to specify the incident intensity at each grid point (z,p) and appropriate observer's frame frequency $\nu_O^i = \nu_A^i/(1-\mu V/c)$. This can be done in two ways. Either, we can solve the equation of radiative transfer at just these frequencies (in dependence of ν_A^i, $\mu V(r)$) which requires an additional number of integrations proportional to N-line * number of radial grid points * number of rays , so that the total computing time is blown up by at least a factor of 2...3. In this case, it would be much faster (and almost equally accurate) to calculate I^{inc} in SA as was done by Puls (1987). The other possibility is to approximate I^{inc} which will be discussed now and gives (by comparison with "exact" CMF-calculations) only small errors on the %-level.
This method is based on the knowledge of $I(\mu,r)$ at two neighbouring observer's frame frequencies ν_n, ν_{n+1} found by the integral operator discussed above. In this frequency interval, we look for *all* lines with $\nu_n \geq \nu_A^i/(1-\mu V/c) \geq \nu_{n+1}$, i=1...k. For the first line then (cf. Fig 5) we have $I^{inc}(\nu_1) \approx I(\nu_n)$, which is almost exact. For the determination of the incident intensities on the following lines, two different approximations have been investigated.
The first one simply assumes that the intensity can be linearly interpolated between ν_1 and ν_{n+1} to yield the incident intensity for line i, i=2...k (Fig.5). This assumption is certainly justified for k=1 or k»1.
The second (and more elaborate) model applies if only a few lines are situated in the interval (cf. Fig. 6, where the case k=2 is

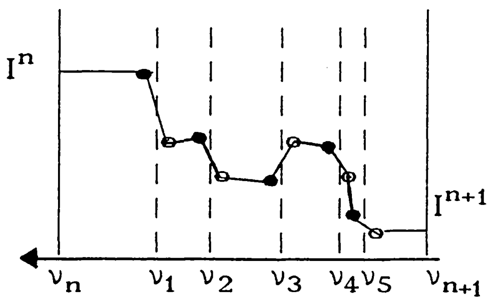

Fig. 5 (see text)
● incident intensity
o emergent intensity

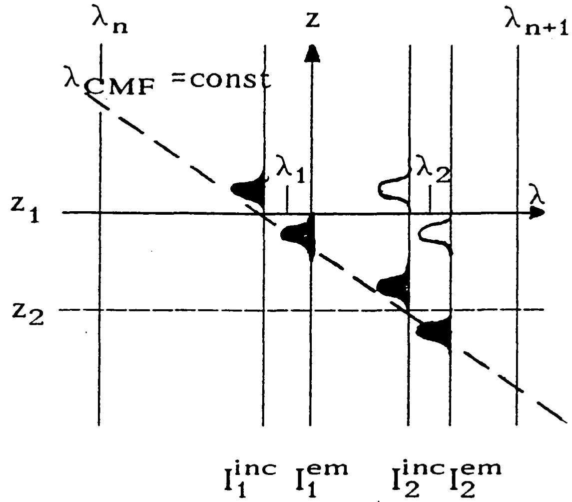

Fig.6 (see text)

shown). From the Sobolev approach, it follows that

$$I_1^{em}(z_1) \approx I(\nu_n)\, e^{-\tau_1(z_1)} + (1 - e^{-\tau_1(z_1)})\, S_1(z_1), \tag{13a}$$

where I_1^{em} is the specific intensity *emergent* from the resonance zone of the first line, situated at grid point z_1. For two *totally* overlapping lines ($\nu_A^1 = \nu_A^2$), the incident intensity on line 2 would be simply I_1^{em}. Due to the finite spacing in frequency and therefore in resonance zone ($z_2 \neq z_1$), we have instead

$$I_2^{inc}(z_1) \approx I(\nu_n)\, e^{-\tau_1(z_2)} + (1 - e^{-\tau_1(z_2)})\, S_1(z_2), \tag{13b}$$

which can be alternatively expressed

$$I_2^{inc}(z_1) = I_1^{em}(z_1) + \Delta I_1. \tag{13c}$$

Generally, we have

$$\begin{aligned} &I_i^{inc}(z_1) = I_{i-1}^{em}(z_1) + \Delta I_{i-1} \quad \text{with boundary conditions} \\ &I_1^{inc}(z_1) = I(\nu_n) \quad \text{and} \quad \Delta I_k + I_k^{em}(z_1) = I(\nu_{n+1}). \end{aligned} \tag{14}$$

So far, almost no approximation (up to the SA) was made. The only assumption in our elaborate model now is to postulate

$$\Delta I_1 = \Delta I_2 = \ldots = \Delta I_k =: \Delta I, \tag{15}$$

an assumption which results in a zero mean error with respect to I_i^{inc}, i= 2...k. Finally we have

$$\Delta I = \frac{I_k^{em}(z_1, \Delta I = 0) - I(\nu_{n+1})}{1 + \exp(-\sum_2^k \tau_i(z_1)) + \ldots + \exp(-\tau_k(z_1))} \tag{16}$$

where $I_k^{em}(z_1, \Delta I=0)$ is calculated in SA following the recipe $I_i^{inc}(z_1)$ =: $I_{i-1}^{em}(z_1)$ and can be found easily, as only local quantities at the considered grid point are involved. With this ΔI, all incident intensities can be recalculated and a final angular integration yields the desired quantities, corrected for line/continuum interaction and diffuse radiation field, if essential.

To summarize, our newly developed IOSA-operator has the major advantage that *all* aspects of the radiation field are solved for in *one single step*, under almost general conditions (line-blocking, ML-processes,...) and very rapidly (typical time scale of ca. 100 CRAY CPs for NF = 1500, N-line = 2000).

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