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Review

The Computation of Radiation Transport Using Feautrier Variables. II. Spectrum Line Formation in Moving Media

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This paper contains a review of methods for solving line transport problems in moving media in terms of the symmetric/antisymmetric radiation-field averages introduced by P. Feautrier. These techniques have proven to be popular and effective in a wide range of astrophysical applications, and may be useful in other areas of computational physics. We outline the physical motivation, formulation, and algorithms for both observer-frame and comoving-frame methods, each of which has distinctive advantages and disadvantages. We cite basic references to provide easy access to the astrophysical literature for workers in other fields.

I. INTRODUCTION

Analysis of the shapes and strengths of spectrum lines is the primary diagnostic tool used by astrophysicists to deduce the physical properties (density, temperature, etc.), and flow kinematics of the material in astrophysical objects ranging from the familiar (e.g., stars, interstellar clouds) to the exotic (pulsars, black holes, quasars). In addition, it is necessary to evaluate accurately the rate of radiant momentum (and energy) deposition in spectrum lines in order to understand the dynamics of many kinds of astrophysical flows. Hence the problem of spectrum line formation in

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moving media is a subject of central importance in modern astrophysics. More recently, there has been a heightened interest in this problem by laboratory physicists as it was appreciated that many of the phenomena encountered in, say, the blowoff from laser-fusion targets are virtually identical to the processes occurring in analogous astrophysical flows (e.g., radiatively driven stellar winds).

A wide range of techniques have been developed for treating line formation in moving media. One very important class of methods is based on the brilliant realization by Sobolev [70, 71] that in rapidly expanding media the whole problem of radiation *transport* can actually be evaded by reformulating both the photon transport equation and the rate equations determining the "chemical kinetics" (excitation-ionization state) of the material in terms of velocity-induced *escape probabilities*. This popular method, which is thoroughly described in [5, 12, 61, 72] and Section 14.2 of [46], has proven effective for carrying out simple, yet reasonably accurate, analyses of the spectrum from expanding stellar envelopes [13, 34, 74] and evaluating the radiative forces in them [73]. Indeed the power of the method has grown as some of its original limitations have been removed. It has now been generalized to include overlapping lines [60], flows with radiative coupling between two or more regions [45, 62], and three-dimensional media [63]; and recently a unification of the rapidly moving regime with the static limit [30], and inclusion of the effects of overlapping continuous opacity [31] has been achieved.

Nevertheless the Sobolev method is only approximate, and breaks down in regions where the flow goes subsonic, stagnates, and/or becomes optically thick in continua. Further it can lead to serious systematic errors in computed line profiles [18]. These, in turn, owing to the diffusive, nonlinear interactions which make the diagnostic problem quite ill-posed, can lead to unacceptably large errors in estimates of the physical state of the flow. Thus, in the end, numerical solution of the line transport problem, capable of high accuracy, are still required. Many such methods have been proposed, but in this paper we continue the developments of [50] (hereinafter referred to as "Paper I") and focus exclusively on differential-equation techniques using the symmetric-antisymmetric radiation-field averages first introduced by P. Feautrier. These methods have proven to be general, flexible, and computationally robust; just to provide perspective we mention that integral-equation analogs of some of them are described in [3].

We shall assume that the reader is familiar with Paper I, and to facilitate reference to that work we shall cite equation numbers from it with a prefix "I." As in Paper I we confine attention to one-dimensional planar or spherical geometry. We shall assume that the physical state (e.g., ρ, T) of the material, and the velocity field in the medium are given. Moreover, we shall ignore any explicit time-dependence of all quantities (including radiation) which implies that either the flow is *steady* or, more generally, flow speeds are so small compared to the speed of light, and radiative relaxation rates of the material are so fast, that the radiation field is *quasistationary*, i.e., adjusts essentially instantaneously to flow conditions as they evolve in time.

II. The Line Source Function

A. Static Media

Both to establish notation, and because it is impossible to understand why we must use certain numerical approaches without understanding some of the underlying physics, we first summarize some basic points about photon absorption, emission, and scattering in spectrum lines; for detailed discussion see [1, 32, 46]. To simplify the discussion consider first a static medium. Here it is useful to identify two frames: the *atom's frame*, in which we specify the absorption and emission properties of a single atom, and the *laboratory frame* where we deal with the macroscopic absorption and emission coefficients resulting from averaging over the (isotropic) microscopic random velocity distribution of all atoms. In the laboratory frame we write the *line opacity coefficient as*

$$\chi_l(\nu) = \chi_l \phi_\nu \tag{2.1}$$

where ϕ_ν is the *line absorption profile* (the convolution of the atom's frame absorption probability with the microscopic velocity distribution), normalized to

$$\int_0^\infty \phi_\nu \, d\nu = 1. \tag{2.2}$$

The laboratory frame *line emission coefficient* can be conveniently split into a *scattering term*

$$\eta_l^S(\mathbf{n}, \nu) = \sigma_l \oint (d\omega'/4\pi) \int_0^\infty d\nu' \, R(\mathbf{n}'; \nu'; \mathbf{n}, \nu) \, I(\mathbf{n}', \nu'), \tag{2.3}$$

which depends explicitly on the amount of radiation present locally, and a *thermal term*

$$\eta_l^t(\nu) = \kappa_l \phi_\nu B_\nu(T_{\text{exc}}), \tag{2.4}$$

which depends mainly on local material properties. Here σ_l and κ_l are the line scattering and absorption coefficients, $B_\nu(T_{\text{exc}})$ is the Planck function at some characteristic "excitation temperature" and $R(\mathbf{n}', \nu'; \mathbf{n}, \nu) d\nu' d\nu (d\omega'/4\pi)(d\omega/4\pi)$ is the *redistribution function* which gives the joint probability that, as seen by an observer in the laboratory frame, a photon is scattered from frequency range $(\nu', \nu' + d\nu')$ and direction $\mathbf{n}'$ in $d\omega'$ into $d\omega$ around direction $\mathbf{n}$ and frequency range $(\nu, \nu + d\nu)$. We take R to be normalized such that

$$(4\pi)^{-2} \oint d\omega' \int_0^\infty d\nu' \oint d\omega \int_0^\infty d\nu \, R(\mathbf{n}', \nu'; \mathbf{n}, \nu) = 1. \tag{2.5}$$

The analytical form of the redistribution function depends on the nature (i.e., degree of coherence) of the scattering process in the atom's frame. Expressions for a variety of important cases are given in [22, 24–28] and Chapter 13 of [46]; a useful review of computational methods of evaluation appears in [23]; and a quantum theoretical discussion of redistribution is given in [14].

Using the macroscopic quantities defined above we can write the line transfer equation as

$$dI(\mathbf{n}, \nu)/ds = -(\chi_c + \chi_l \phi_\nu)\, I(\mathbf{n}, \nu) + \chi_c S_c + \kappa_l \phi_\nu B_\nu(T_{\text{exc}}) + \sigma_l \oint (d\omega'/4\pi) \int_0^\infty d\nu'\, R(\mathbf{n}', \nu'; \mathbf{n}, \nu)\, I(\mathbf{n}', \nu') \tag{2.6}$$

or

$$\frac{dI(\mathbf{n}, \nu)}{d\tau_\nu} = I(\mathbf{n}, \nu) - \frac{\chi_c S_c + \chi_l \phi_\nu S_l(\mathbf{n}, \nu)}{\chi_c + \chi_l \phi_\nu} = I(\mathbf{n}, \nu) - a_\nu S_l(\mathbf{n}, \nu) - b_\nu, \tag{2.7}$$

where s and $d\tau_\nu \equiv -(\chi_c + \chi_l \phi_\nu) ds$ are respectively the pathlength and optical depth increment along a ray, and the *line source function* has the general form

$$S_l(\mathbf{n}, \nu) = (\alpha/\phi_\nu) \oint (d\omega'/4\pi) \int_0^\infty d\nu'\, R(\mathbf{n}', \nu'; \mathbf{n}, \nu)\, I(\mathbf{n}', \nu') + \beta. \tag{2.8}$$

Here we ignored continuum scattering and the (usually slow) frequency variation of some quantities across the (presumably narrow) width of the line. Equations (2.6)–(2.8) show explicitly the *integrodifferential* nature of the transfer equation. Moreover, as shown in Section II.A.(ii) of Paper I, it must be solved subject to two-point boundary conditions.

Expressions for the coefficients α and β in (2.8) can be derived from the *statistical equilibrium equations* governing the atomic level populations; see, e.g., [1, 32, 46]. (Note that the discussion of stimulated emission in Chap. 13 of [46] is wrong; corrected formulae are given in [4].) In general, α and β for the line $(i \leftrightarrow j)$ contain the collisional and *radiative* rates for all transitions connecting to either level i or level j, hence in general there is a radiative *interlocking* among *all* lines and continua in the complete transition array of the atom. This coupling poses a formidable nonlinear problem, which is discussed in [1, 32, 46] and the references cited therein; we shall return to this issue briefly in Section V, but for now we assume that all material coefficients, including α and β are *given* so we can deal only with the transfer problem.

For the trivial case of a two-level atom (only *one* line transition) one can show that $\alpha = (1 - \varepsilon)$ and $\beta = \varepsilon B_\nu\ (T_{\text{exc}})$, where ε is the *photon destruction probability*, by collisional deexcitation, per scattering. The absolutely critical point is that for resonance lines in rarefied astrophysical media ε is usually extremely small, perhaps 10^{-8} or even 10^{-10} (for a strong line), so that the transfer problem is almost *homogeneous*, with a solution that is extremely weakly coupled to local conditions.

Physically speaking the problem is that a line photon can scatter an enormous number of times before it is collisionally destroyed (at which point the transport process couples back into the local thermal structure of the material). Consequently, near an open surface there will exist a "*boundary*" layer—within which the radiation field can depart *markedly* (orders of magnitude) from its thermal value—that may penetrate a huge number of photon mean free paths into the medium. For coherent scattering, random-walk arguments show that the *thermalization depth* Λ (i.e., the optical depth at which the radiation field finally thermalizes) is of order $\varepsilon^{-1/2}$; for scattering with complete redistribution in a Doppler profile $\Lambda \sim 1/\varepsilon$, and in a Lorentz profile $\Lambda \sim 1/\varepsilon^2$! These immense values imply that any simple *iterative* evaluation of the scattering integral (starting from, say, a thermal value) is doomed to failure; the same remark applies to *shooting methods* and *eigenvalue methods* which admit exponentially growing parasites and hence fail catastrophically in optically thick scattering media (see Sections 6–1 and 6–2 of [46]). The difficulties just described perhaps explain the deep (almost obsessive) concern astrophysicists have about treating the scattering problem correctly, and their fondness for methods, such as those described in this paper, that allow an accurate solution, as a two-point boundary-value problem, of transfer equations in which the scattering integral appears explicitly. In dense laboratory plasmas ε is often much larger (perhaps 10^{-2} to 10^{-1}) and the problems described above are ameliorated; nevertheless they do not disappear entirely, and use of a good method still pays large dividends.

Equations (2.7) and (2.8) allow for the full angle and frequency dependence of the scattering kernel. In a static medium, after transformation to Feautrier variables and discretization as in (I.2.17) and (I.2.20) they can be solved by the Feautrier algorithm of Section II.C.(i) of Paper I. For a mesh containing D depths, M angles, and N frequencies the computational effort scales as cDM^3N^3.

Often we do not wish (or need) to deal with this much detail, so we invoke approximations. For example, if we can assume $I(\mathbf{n}', \nu')$ is nearly isotropic (as it will be at points where the optical depth exceeds unity at the relevant frequency) we can replace it in (2.8) by the mean intensity $J(\nu')$. We can then integrate over angles $\mathbf{n}'$, obtaining a line source function of the form

$$S_l(\nu) = (\alpha/\phi_\nu) \int_0^\infty R(\nu', \nu)\, J(\nu')\, d\nu' + \beta, \tag{2.9}$$

where the *angle-averaged redistribution function*

$$R(\nu', \nu) \equiv (4\pi)^{-1} \oint R(\mathbf{n}', \nu'; \mathbf{n}, \nu) d\omega' = (4\pi)^{-1} \oint R(\mathbf{n}', \nu'; \mathbf{n}, \nu) d\omega \tag{2.10}$$

gives the joint probability of photon scattering $(\nu', \nu' + d\nu')$ to $(\nu, \nu + d\nu)$, normalized to

$$\int_0^\infty d\nu' \int_0^\infty d\nu\, R(\nu', \nu) = \int_0^\infty \phi(\nu') d\nu' = 1. \tag{2.11}$$

The transfer problem (2.7) then simplifies to an equation of the form

$$dI(\mathbf{n}, \nu)/d\tau_\nu = I(\mathbf{n}, \nu) - a'_\nu \int_0^\infty R(\nu', \nu)\, J(\nu')d\nu - b'_\nu \tag{2.12}$$

which, when collapsed with variable Eddington factors, can be solved by the Feautrier algorithm as described as Sections II.C.(i), (ii) and III.C.(iii) of Paper I. The computational effort then scales as $I(cDMN + c'DN^3)$ and $I(c''D^2N + c'DN^3)$ in planar and spherical geometry respectively, where I is the number of iterations required to obtain convergence of the Eddington factors.

In many applications we can assume that as a result of collisional reshuffling in the atom's frame and/or Doppler reshuffling in the laboratory frame, the frequency ν at which a photon is emitted is totally uncorrelated with the frequency ν' at which it was absorbed. In this case of *complete redistribution*

$$R(\nu', \nu) = \phi(\nu')\, \phi(\nu), \tag{2.13}$$

hence the line source function becomes (essentially) *frequency independent*

$$S_l = \alpha \int_0^\infty \phi(\nu')\, J(\nu')d\nu' + \beta, \tag{2.14}$$

and we have a much simpler transfer problem of the form

$$dI(\mathbf{n}, \nu)/d\tau_\nu = I(\mathbf{n}, \nu) - c_\nu \bar{J} - d_\nu \tag{2.15}$$

where

$$\bar{J} \equiv \int_0^\infty \phi(\nu')\, J(\nu')d\nu'. \tag{2.16}$$

Equation (2.15) can be solved directly by the Rybicki technique described by Sections II.C.(iii) and III.C.(i) of Paper I; the computational effort scales as $cD^2MN + c'D^3$ and $c''D^3N$ in planar and spherical geometry, respectively. Two computational details requiring careful attention are: (1) For accuracy it is essential to choose a sufficiently fine frequency grid in quadrature-sum representations of (2.8), (2.9), or (2.14). For example, for a Doppler profile the spacing of the grid should be no more than half a Doppler width $\Delta\nu_D$. (2) It is imperative to renormalize quadrature weights to assure strict normalization of the discrete representations of the scattering integrals. When the photon destruction probability is very small, even small quadrature errors in the scattering integral can be disastrous because they can swamp the real thermal terms and produce a spurious solution.

B. Moving Media

Consider now moving media. Here we must discriminate three frames: (1) the atom's frame; (2) the *comoving frame*, actually a *set* of frames, each of which moves with the macroscopic flow velocity of the fluid element with which it is associated; and (3) the *observer's frame*, an inertial frame at rest, in which the fluid flows with a general velocity field $\mathbf{v}(\mathbf{r}, t)$. The line transfer problem can be solved in either the observer's (Sect. III) or the comoving frame (Sect. IV); as we shall see, each approach has distinctive advantages and disadvantages.

In the comoving frame the atoms have only their (isotropic) microscopic velocity distribution, hence all material properties (e.g., profiles and redistribution functions) are given by the same formulae, locally, as in the laboratory frame in a static medium. In particular the line opacity is *isotropic* in this frame, as is the line emissivity for complete redistribution and angle-averaged redistribution (but not general redistribution).

The description of material properties in the observer's frame is more complicated. Owing to Doppler shifts, at a point where the material moves with velocity $\mathbf{v}$ a photon having a frequency ν and moving in direction $\mathbf{n}$ in the observer's frame has a comoving-frame frequency

$$\nu' = \nu[1-(\mathbf{n}\cdot\mathbf{v}/c)]; \tag{2.17}$$

this is the frequency at which the photon can be absorbed (or was emitted) by the material. An obvious consequence of (2.17) is that material properties, specifically χ_l and η_l, become strongly *anisotropic* in the observer's frame even if they were isotropic in the comoving frame. In principle one should also account for *aberration* and *advection* effects, which are also $O(v/c)$. But in practice for spectrum lines these effects are negligible compared to Doppler shifts. The reason is that the radiation field, absorptivity, and emissivity in the line all vary markedly over a line width, which we can characterize adequately by the Doppler width $\Delta\nu_D = \nu_0 v_{\text{thermal}}/c$, where v_{thermal} is the rms line-of-sight speed of the atoms. Hence the effects of Doppler shifts are effectively amplified to $O(v/v_{\text{thermal}})$ and thus overwhelm all terms that are only $O(v/c)$. This rough argument is supported by detailed calculation [53]. For the (smooth) continuum even Doppler shifts are inconsequential, so we can treat continuum properties as if the medium were static.

In principle another complication is that in a moving medium we can no longer write the statistical equilibrium equations (I.2.62), but should instead use

$$(\partial n_i/\partial t) = -\nabla\cdot(n_i\mathbf{v}) + \sum_{j\neq i} n_j P_{ji} - n_i \sum_{j\neq i} P_{ij} \tag{2.18}$$

where the P's are total rates into and out of level i. Thus even for steady flow the rate equations contain a nonvanishing advective term, which couples the state of the material at one position to that at neighboring positions, and significantly complicates the analytical form of the coefficients (α, β) in the line source function [9], as well as changing the mathematical structure of the transfer problem. This advective coupling can be important, leading, for example, to a "freezing-in" of the ionization state in rapidly-expanding rarefied flows. But in this paper we shall assume that radiative and/or collision rates are sufficiently large to assure the rapid relaxation of the material to a quasi-steady state equilibrium, and will henceforth ignore the advective term in (2.18).

III. Observer-Frame Methods

A. Planar Geometry

(i) *Complete redistribution.* For computation it is convenient to measure frequency displacements from line center in units of a fiducial Doppler width $\Delta\nu_D^* \equiv \nu_0 v_{\text{thermal}}^*/c$, and to measure flow velocities in the same units, i.e. $V \equiv v/v_{\text{thermal}}^*$. Then the transformation (2.17) becomes

$$x' = x - \mu V \tag{3.1}$$

where $x \equiv (\nu - \nu_0)/\Delta\nu_D^*$ and similarly for x'. Here μ is the angle cosine of the direction of photon propagation $\mathbf{n}$ relative to the outward normal $\mathbf{k}$, $\mu = \mathbf{n} \cdot \mathbf{k}$. We thus write the material opacity and emissivity as

$$\chi(z, \mu, x) = \chi_c(z) + \chi_l(z)\, \phi(z, \mu, x) \tag{3.2}$$

and

$$\eta(z, \mu, x) = \eta_c(z) + \eta_l(z)\, \phi(z, \mu, x) \tag{3.3}$$

where

$$\phi(z, \mu, x) \equiv \phi[z; x - \mu V(z)], \tag{3.4}$$

normalized such that

$$\int_{-\infty}^{\infty} \phi(z, \mu, x) dx = 1. \tag{3.5}$$

For example, for a Doppler profile

$$\phi(z, \mu, x) = [\pi^{1/2}\delta(z)]^{-1} \exp\{-[x - \mu V(z)]^2/\delta^2(z)\} \tag{3.6}$$

where $\delta \equiv \Delta\nu_D(z)/\Delta\nu_D^*$. The total source function is therefore

$$S(z, \mu, x) = [\phi(z, \mu, x)\, S_l(z) + \gamma(z)\, S_c(z)]/[\phi(z, \mu, x) + \gamma(z)] \tag{3.7}$$

where $\gamma(z) \equiv \chi_c(z)/\chi_l(z)$, and, assuming complete redistribution,

$$S_l(z) = \tfrac{1}{2}\alpha(z) \int_{-\infty}^{\infty} dx \int_{-1}^{1} d\mu\phi(z, \mu, x)\, I(z, \mu, x) + \beta(z). \tag{3.8}$$

The transfer equation is then of the general form

$$\mu(\partial I_{\mu x}/\partial \tau_{\mu x}) = I_{\mu x} - S_{\mu x}. \tag{3.9}$$

Equations (3.4), (3.6), and (3.8) show explicitly the characteristic feature of observer-frame line-transfer calculations: there is an *inextricably tight coupling between the material properties and the angular and frequency variations of the radiation field.* As we shall shortly see it is this coupling that presents the greatest numerical difficulties to observer-frame computations.

Equation (3.9) can be cast into second-order form. Assuming the line profile is symmetric about line center, $\phi(x-\mu V)=\phi(-x+\mu V)$, which suggests that in constructing the Feautrier averages we group together the two pencils $I(z, +\mu, +x)$ and $I(z, -\mu, -x)$, for then $S(z, \mu, x)=S(z, -\mu, -x)$ and $d\tau(z, \mu, x)= d\tau(z, -\mu, -x)$. Thus replacing (I.2.2) and (I.2.3) with

$$j_{\mu x} \equiv \tfrac{1}{2}[I(z, +\mu, +x)+I(z, -\mu, -x)], \qquad (0 \leqslant \mu \leqslant 1) \tag{3.10}$$

and

$$h_{\mu x} \equiv \tfrac{1}{2}[I(z, +\mu, +x)-I(z, -\mu, -x)], \qquad (0 \leqslant \mu \leqslant 1) \tag{3.11}$$

we can manipulate (3.9) into the second-order form

$$\mu^2(\partial^2 j_{\mu x}/\partial \tau_{\mu x}^2) = j_{\mu x} - S_{\mu x}. \tag{3.12}$$

As in Paper I the upper boundary condition for zero incoming radiation is

$$\mu(\partial j_{\mu x}/\partial \tau_{\mu x})_0 = j_{\mu x}(0), \tag{3.13}$$

and in the diffusion limit the lower boundary condition is

$$(\partial j_{\mu x}/\partial \tau_{\mu x})_{\tau_{\max}} = -(1/\chi_{\mu x})(\partial B_\nu/\partial z)_{\tau_{\max}}. \tag{3.14}$$

For the diffusion approximation to apply, the Doppler shift over a photon mean free path must be negligible, i.e., $\chi_{\mu x}^{-1}\,|dV/dz| \ll 1$; otherwise (3.14) must be replaced by a more general expression (see [47]).

Equations (3.12)–(3.14) can be discretized exactly as in Section II.A.(iii) of Paper I, the discrete representation of $S_{\mu x}$ taking the form

$$S_{d+1/2,k} = a_{d+1/2,k} \sum_{k'=1}^{K} w_{k'} \phi_{d+1/2,k'} j_{d+1/2,k'} + b_{d+1/2,k} \equiv a_{d+1/2,k} \bar{J}_{d+1/2} + b_{d+1/2,k'} \tag{3.15}$$

where

$$\phi_{d+1/2,k} \equiv \phi(z_{d+1/2}; x_k - \mu_k V_{d+1/2}), \tag{3.16}$$

and the sum runs over an equal range of both positive and negative x's.

The quadrature sum in (3.15) is the Achilles' heel of the observer-frame method for two reasons: (1) As μ varies from -1 to $+1$ (recall that j couples $\pm\mu$), the frequency of line center shifts by $2|V|_{\max}$, where $|V|_{\max}$ is the maximum flow speed. Thus if $x_{\max}$ is the frequency displacement needed to assure $\chi_l \phi(x_{\max}) \ll \chi_c$, then the frequency quadrature must span a minimum bandwidth $\pm X$ where $X = x_{\max} + |V|_{\max}$. Moreover the frequency grid should have a spacing $\Delta x \lesssim \frac{1}{2}$ for accuracy. These requirements are not severe for subsonic flows, where $|V|_{\max} \lesssim 1$. But they become onerous for supersonic flows (e.g., a stellar wind or laser-pellet blowoff), where v/c may approach 10^{-2}, hence $2v_0 v/c\Delta v_D^* \sim 200$, which implies that we may need $N \sim 400$ frequency-quadrature points in (3.15). (2) The requirements on the angle quadrature are equally severe. From (3.4) it is obvious that if we can tolerate only some maximum $\Delta x_{\max}$ in the frequency quadrature, then the maximum tolerable angle increment (even if the radiation field is isotropic!) is $\Delta\mu_{\max} \sim \Delta x_{\max}/|V|_{\max}$. Thus the number of angle-quadrature points M may have to be comparable to the number of frequency-quadrature points, and in high-velocity flows the size of the system ($K = M \cdot N$) becomes unmanageable.

Strategies can be suggested to reduce the computational burden (e.g., argue for isotropy of $j_{\mu\nu}$, represent it by a coarse linear spline in μ, and perform the angular integration *analytically*—feasible for a Doppler profile), but they inevitably become questionable in the region of most interest (the observable boundary surface where *transport* occurs) and must be validated by mesh refinement, thus defeating the attempt at economy. As we shall see in Section IV these problems are better overcome by using comoving-frame methods in high-velocity flows, when possible.

Given the need for a large number K of angle-frequency quadrature points, one invariably chooses the Rybicki algorithm of Section I.C.(iii) of Paper I to solve the discretized observer-frame system because the computational effort scales $cKD^2 + c'D^3$, i.e., linearly in K, whereas the scaling of the Feautrier algorithm is unfavorable, cDK^3. Moreover notice that a loophole open to us in static media, namely collapsing the size of the system by using variable Eddington factors, is now closed because the scattering integral explicitly contains the angle-frequency dependent variable $j_{\mu\nu}$, not just the mean intensity J_ν. In short there is generally no choice but to use the Rybicki algorithm. On the other hand, one must also be careful to resolve the velocity variation on the *spatial* mesh (ideally $\Delta V \lesssim \frac{1}{2}$ between grid points) to assure accurate optical depth increments $\Delta\tau_{\mu\nu}$ (recall $\chi_{\mu\nu}$ contains $\phi_{\mu\nu}$). Hence for large $|V|_{\max}$ we can get hurt even with the Rybicki method because the number of depth-points D must be $\sim 2|V|_{\max}$ and the computational effort rises as D^2 or D^3.

(ii) *Partial redistribution.* An observer-frame computation of line transport with partial redistribution in a moving fluid is particularly vexing, and comes equipped with pitfalls. The suggestion [29] that it might be possible to use redistribution functions angle-averaged over both the microscopic velocity distribution and the macroscopic flow velocity in an observer's frame calculation [11, 75] turns out to be a bad one that leads to spurious results [21, 44, 55, 76]. One is thus forced to solve the full angle-frequency dependent problem (2.6)–(2.8). Forming averages as in (3.10) and (3.11) we have

$$\mu(\partial h_{\mu x}/\partial \tau_{\mu x}) = j_{\mu x} - \tfrac{1}{2}[S(\mu, x) + S(-\mu, -x)] \tag{3.17}$$

and

$$\mu(\partial j_{\mu x}/\partial \tau_{\mu x}) = h_{\mu x} - \tfrac{1}{2}[S(\mu, x) - S(-\mu, -x)], \tag{3.18}$$

or, using (2.7) and (2.8), equations of the general form

$$\mu(\partial h_{\mu x}/\partial \tau_{\mu x}) = j_{\mu x} - c_x \mathscr{S}^S_{\mu x} - d_x \tag{3.19}$$

and

$$\mu(\partial j_{\mu x}/\partial \tau_{\mu x}) = h_{\mu x} - c_x \mathscr{S}^a_{\mu x}. \tag{3.20}$$

By use of the symmetry relations for redistribution functions (see [28] or pp. 420–422 of [46]), one can show [56] the symmetric and antisymmetric scattering integrals in (3.19) and (3.20) are

$$\mathscr{S}^S_{\mu x} = \tfrac{1}{2} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} d\mu' [R(\mu', x' - \mu' V; \mu, x - \mu V) + R(-\mu', -x' + \mu' V; \mu, x - \mu V)]\, j_{\mu x} \tag{3.21}$$

and

$$\mathscr{S}^a_{\mu x} = \tfrac{1}{2} \int_{-\infty}^{\infty} dx' \int_{0}^{1} d\mu' [R(\mu', x' - \mu' V; \mu, x - \mu V) - R(-\mu', -x' + \mu' V; \mu, x - \mu V)]\, h_{\mu x} \tag{3.22}$$

so there is a clean cleavage of the right-hand sides of (3.19) and (3.20) into terms containing only $j_{\mu x}$ or $h_{\mu x}$. Methods of generating quadrature weights for discrete representations of (3.21) and (3.22) are discussed in [56].

Some important redistribution functions satisfy the symmetry relation

$$R(-\mu', -x'; \mu, x) = R(\mu', x'; \mu, x). \tag{3.23}$$

For these $S^a_{\mu x} \equiv 0$, and (3.19)–(3.22) can be cast into the standard second-order form (3.12) and solved by the Feautrier algorithm in Section II.C.(i) of Paper I. The Rybicki algorithm is, of course, unavailable because the integral is explicitly frequency-dependent rather than containing a single variable $\bar{J}$. Other important redistribution functions do not obey (3.23); for these we must solve the coupled first-order equations (3.19)–(3.22). Grouping all angle-frequency components of $j_{\mu x}$ and $h_{\mu x}$ at a given depth point (cell center or interface) into vectors as in (I.2.29) we obtain a system of the same form as (I.3.15)–(I.3.16), which can be solved by the algorithm in (I.3.17)–(I.3.22). In either case the computational effort scales as $cDK^3 = cDM^3N^3$, where M and N are the number of angle and frequency points in the quadrature. This quadrature is at least as difficult to perform as in the case of complete redistribution (for the same reasons); for large velocities (which imply large values of K) the computation becomes costly, and is better performed in the comoving frame when possible (Sect. IV).

B. Spherical Geometry

Line formation in moving spherical media can also be treated by observer-frame methods [39]; in the astrophysical literature the greatest emphasis has been given to *expanding* flows (velocity increasing monotonically outward). Using the tangent-ray geometry shown in Fig. 2 of Paper I we write the transfer equation as

$$\pm[\partial I(s,p,x)/\partial s] = \chi[r(s,p),x]\,\{S[r(s,p),x] - I(s,p,x)\} \tag{3.24}$$

where $r(s,p) \equiv (s^2+p^2)^{1/2}$. Defining

$$j(s,p,x) \equiv \tfrac{1}{2}[I^+(s,p,x) + I^-(s,p,-x)] \tag{3.25}$$

and

$$h(s,p,x) \equiv \tfrac{1}{2}[I^+(s,p,x) - I^-(s,p,-x)], \tag{3.26}$$

and assuming complete redistribution so that

$$S[r(s,p),x] = a[r(s,p),x]\,\bar{J}[r(s,p)] + b[r(s,p),x], \tag{3.27}$$

we can manipulate (3.24) into the second-order form

$$(\partial^2 j_{px}/\partial\tau_{px}^2) = j_{px} - S_{px} \tag{3.28}$$

where $d\tau_{px} \equiv -\chi[r(s,p),x]ds$, and we have economized the notation in an obvious way. In (3.27),

$$\bar{J}[r(s,p)] \equiv \int_{-x_{\max}}^{x_{\max}} dx \int_0^1 d\mu\, \phi[r; x-\mu V(r)]\, j[s(r,\mu), p(r,\mu), x] \tag{3.29}$$

where $\mu \equiv s/(s^2+p^2)^{1/2}$.

Unlike the static case discussed in Section III.B.(i) of Paper I, in this case we cannot pose a useful boundary condition on the plane $s=0$ because $I^+(0,p,+x) \neq I^-(0,p,-x)$, hence $h(0,p,x) \neq 0$. We circumvent this difficulty by following each tangent ray (outside the core) for its *entire* length $\pm s(p,R)$, using zero incident-intensity boundary conditions

$$(\partial j_{px}/\partial\tau_{px})|_{s=\pm s(p,R)} = \pm j_{px}|_{s=\pm s(p,R)} \tag{3.30}$$

at each of the rays.

Discretizing (3.27)–(3.30) as in Paper I we obtain systems of the form

$$\mathbf{T}_{ln}\mathbf{j}_{ln} = \mathbf{U}_{ln}\bar{\mathbf{J}} + \mathbf{V}_{ln} \qquad (l = 1,..., L; n = 1,..., \pm N) \tag{3.31}$$

where $\bar{\mathbf{J}}$ and $\mathbf{j}_{ln}$ contain the spatial variations of $\bar{J}$ and $j(s, p_l, x_n)$ along the ray specified by p_l. If there are G_l grid points along the entire ray, then $\mathbf{T}_{ln}$ is a $(G_l \times G_l)$ tridiagonal matrix, and $\mathbf{j}_{ln}$ and $\mathbf{V}_{ln}$ are vectors of length G_l. But because of spherical symmetry $\bar{J}(-s, p_l) \equiv \bar{J}(s, p_l)$, hence we can cut the length of $\bar{\mathbf{J}}$ to $g_l = \frac{1}{2}(G_l + 1)$ and $\mathbf{U}_{ln}$ is then a rectangular $(G_l \times g_l)$ chevron matrix (see [39]). Solving (3.31) we obtain an expression of the form

$$\mathbf{j}_{ln} = \mathbf{A}_{ln} - \mathbf{B}_{ln}\bar{\mathbf{J}}, \tag{3.32}$$

where $\mathbf{A}_{ln}$ is of length G_l and $\mathbf{B}_{ln}$ is $(G_l \times g_l)$. Now (3.29) when discretized becomes

$$\bar{J}(r_{d+1/2}) = \sum_{n=-N}^{N} w_n \sum_{l=1}^{L_d} \omega_{d+1/2,l}\phi[r_{d+1/2}; x_n - \mu(r_{d+1/2}, p_l)\, V(r_{d+1/2})] \times j[s(r_{d+1/2}, p_l), p_l, x_n] \tag{3.33}$$

where L_d is the number of rays intersecting the sphere $r = r_{d+1/2}$, and the w's and ω's are quadrature weights. But by exploiting symmetry we can economize the calculation because $I^{\pm}(s, p, x) = I^{\mp}(-s, p, x)$. Hence $j(s, p, -x) \equiv j(-s, p, x)$ and $h(s, p, -x) \equiv -h(-s, p, x)$; we can therefore eliminate the j's at negative x and positive s in (3.33) in favor of those at positive x and negative s:

$$\bar{J}(r_{d+1/2}) = \sum_{n=1}^{N} w_n \sum_{l=1}^{L_d} \omega_{d+1/2,l}\{\phi[r_{d+1/2}; x_n - \mu_{d+1/2,l}V_{d+1/2}]\, j_{d+1/2,ln} + \phi[r_{d+1/2}; x_n - \mu_{d+1/2,l}V_{d+1/2}]\, j_{d'+1/2,ln}\} \tag{3.34}$$

where $d' \equiv G_l + l - d$. Thus even though we are forced to solve along the full length of each ray, we need consider only half of the line profile in frequency. Equation (3.34) can be rewritten as

$$\mathbf{J} = \sum_{l,n} \mathbf{Q}_{ln}\mathbf{j}_{ln} \tag{3.35}$$

where $\mathbf{Q}_{ln}$ is a $(g_l \times G_l)$ rectangular chevron matrix containing profile functions and quadrature weights. Using (3.32) in (3.35) we can develop the $(D \times D)$ system $\mathbf{C}\bar{\mathbf{J}} = \mathbf{D}$, which we solve for $\bar{\mathbf{J}}$, thus obtaining the source function. The computational effort scales as $cND^3 + c'D^3$.

For observer-frame calculations in spherical geometry, the Rybicki elimination scheme just described is used exclusively because a Feautrier elimination scheme would be very cumbersome to implement, since the number of tangent rays intersecting each radial shell changes with depth. (This difficulty would not hinder a discrete-space method similar to that described in Sect. III.B.(ii) of Paper I.)

Moreover, as was true for planar geometry, we can not eliminate the angular variable by using moment equations because $\bar{J}$ contains $j_{\mu x}$ explicitly, not just J_x. This impracticality of using a Feautrier elimination scheme also explains why *observer-frame* partial-redistribution calculations in spherical geometry have never been carried out using Feautrier variables.

Observer-frame line transport calculations in spherical geometry work well only for low-velocity flows. The basic reason is that the variation of the projected velocity along each ray induces a scan in comoving-frame frequency through the line profile. In order to get meaningful optical depth increments along a ray we must therefore resolve the *resonances* (i.e., neighborhoods where photons can interact with the line profile near line center) on the ray. These occur at different positions on different rays for a given observer-frame frequency, and for different observer-frame frequencies on a given ray. Hence in practice we must try to resolve the *projected* velocity field (i.e., projected $\Delta V \lesssim \frac{1}{2}$ between adjacent grid points) along the entire length of all rays, which turns out to be difficult to do owing to a peculiarity of the geometry.

Specifically, the projected velocity (of a radial flow) will always be identically zero on the symmetry plane defined by the points of tangency of parallel rays to a set of radial shells (see Fig. 2 of Paper I). But if successive radial shells are spaced by Δr, the angle cosine of a ray at the first grid point away from the symmetry plane is

$$\mu_0 \approx (2\Delta r/r)^{1/2}. \tag{3.36}$$

Hence even if we use a very fine radial mesh (say $r_{d+1}/r_d = 1.03$), μ_0 will still be substantial ($\mu_0 \approx 0.25$ in this case), so the projected velocity jumps from zero to a substantial fraction of the *full* radial velocity of the shell in a single step along the ray. Thus zoning that provides overkill for resolving the *radial* variation of the velocity field (and other physical variables) is still much too coarse along the tangent rays unless the maximum flow amplitudes are, at most, only mildly supersonic. This problem does not arise in comoving-frame calculations, where only the *gradient* of the velocity, not the amplitude, enters.

A scheme for mapping from the "coarse" radial mesh to much finer tangent-ray mesh, and back, as described in [49]. This trick gives satisfactory results and allows one to solve problems inaccessible to comoving-frame calculations; but it is clumsy, and is (marginally) viable only when vectorized.

C. Formal Solution

Having finally obtained the line source function, whether by observer-frame or comoving-frame methods, one is in a position to perform a formal solution for the emergent radiation field. This calculation is always performed in the observer's frame by solving the tridiagonal systems (I.2.28) for each angle and frequency of interest. If only the *emergent* radiation is wanted, one can solve these systems from bottom to top, obtaining the emergent intensity at the end of the forward-elimination step; no back-substitution is necessary.

As in any observer-frame calculation, the only critical issue is to resolve all resonances on the rays selected. In planar geometry this matter can be disposed of almost trivially because it is sufficient to guarantee that the velocity field is resolved ($\Delta V \lesssim \frac{1}{2}$ between grid points) along the outward normal ($\mu = 1$) to the medium, for then the increment of projected velocity, $\mu \Delta V$, is resolved as well. Hence one can choose, once and for all, a single refined mesh on which $V(z)$ is adequately resolved, and interpolate all basic physical variables (e.g., χ_c, χ_l, V, $\bar{J}$, etc.) which are generally slowly varying, by a suitable scheme (e.g., cubic splines). Then for each choice of (μ, ν) the profile function $\phi(z, \mu, \nu)$ is calculated directly from the interpolated values of the underlying variables (specifically μV) at each point of the refined mesh. The calculation is easily vectorized over frequency on each ray. The total computational effort scales as $cD'MN$ (which is irreducible), where D' is the number of depth points on the refined mesh and M and N are the numbers of angles and frequencies. In practice N may have to be large because one must span the whole line profile including velocity shifts. M can be any number desired, with the caveat that if one wishes to evaluate angle-integrated quantities such as the emergent *flux*, then one must choose M large enough to resolve the angular variation of $I_{\mu\nu}$, which can be dramatic even for unimpressive depth-variations of the underlying physical variables (see, e.g., Fig. 5 of [47]).

In spherical geometry the formal solution becomes a tedious chore because, as mentioned earlier, the resonance positions are different along different tangent rays for a fixed observer-frame frequency, and of course also different for different frequencies. In addition we must cope with the pathology of the large geometry-induced projected-velocity jump at the first grid point away from the symmetry plane. The upshot is that no one radial mesh refinement will suffice for all resonances, as it did in planar geometry, and one has little choice but to *search* for resonances for each (p, ν) choice, and custom-tailor a refined mesh for each one. For simple expanding flows there will be only *one* resonance for each (p, ν) and the search procedure can be partially systematized; but for general (i.e., nonmonotonic) velocity fields there can be several resonances, and the search must be done by brute force. Needless to say, this computation is essentially unvectorizeable, and can become quite time-consuming, despite the fact the computational effort is linear in the number of tangent rays and frequencies, because the overhead is immense.

D. *Remark*

Lest the reader be misled, let us remark that although we have emphasized that observer-frame methods tend to be difficult (or unsatisfactory) for high-velocity flows, for the important case of complete redistribution they are reliable, easy to implement (particularly in planar geometry), and cheap when the total velocity amplitude in the medium is only a few line widths. They thus play a very important role in astrophysics, for example, in the study of the radiative signatures of wave motions or low-amplitude stellar oscillations. Moreover, they have one outstanding virtue, namely they work for *arbitrary* (i.e., nonmonotonic) velocity fields. As we shall see below, the situation is essentially reversed for comoving-frame methods, which work well for large velocities, and are the easiest and most natural to use for partial redistribution problems, but are easy (if at all!) to implement only for monotonic expansion of the medium.

IV. Comoving-Frame Methods

The idea of solving line transport problems in the comoving frame was first suggested by McCrae and Mitra [43] almost 50 years ago. Although they were able, even then, to explore a few highly idealized examples by astute analytical methods, practical application of the method was not feasible until substantial computational power became available in the last decade. The approach is now fairly well developed, and has been used to produce very realistic simulations of spectra from stellar winds [17, 19, 20, 35–37, 40–42, 69].

Before outlining algorithms, it is well to mention some of the advantages and disadvantages of the method. The first step is to develop a transfer equation in which *all* quantities (material properties, radiation field, angles, frequencies) are measured in the comoving frame; in practical application one needs an equation accurate only to $O(v/c)$. In this frame we enjoy the following advantages: (1) The material properties are *isotropic*; in particular the flow velocity does not appear in the argument of the line profile function as it does in observer-frame formulations. Thus it is now relatively easy to compute optical depth increments and the quadrature in the scattering integral. Indeed, in the latter, unless we specifically wish to treat general (i.e., angle-dependent) redistribution problems, we can integrate over angle directly and use (comoving-frame) *moments* of the radiation field. (2) The comoving frame is the natural frame in which to evaluate redistribution functions, and in this frame we can validly perform angle averages and use angle-averaged redistribution functions. (3) Because we now use frequencies measured in frames moving with the fluid, to calculate an accurate scattering integral we can work with just the (narrow) bandwidth needed to cover the *static* line profile *independent of the flow speed* (provided the flow is monotonic—see below). Relative to an observer-frame computation we thus obtain an enormous reduction in the required number of frequency points in high velocity flows. (4) Only *gradients* of projected velocities along rays appear in the equation. These are relatively easy to resolve on the computational mesh, and do not suffer the abrupt geometry-induced jumps suffered by the flow-velocity itself in spherical geometry.

These advantages must be balanced against two disadvantages: (1) The differential operator is more complicated: a frequency-derivative term now appears, which accounts for the differential Doppler shift a photon (whose observer-frame frequency is, of course, fixed) experiences as it moves along a ray through different fluid elements moving *differentially* with respect to one another. We must therefore now solve an (integro) *partial* differential equation instead of an (integro) *ordinary* differential equation as in the observer's frame. The equation is fundamentally hyperbolic and poses an initial boundary-value problem. (2) Because of the need to provide a well-posed initial condition, the problem is easy to solve only for a monotonic velocity variation. Happily this case is important physically (stellar winds, blowoffs, explosions).

Algorithms have been developed for both planar [21, 47, 55, 57, 59] and spherical [18, 52, 54] geometry. In the interest of brevity we shall discuss only spherical geometry because the algorithms are similar (cf. [52, 47]), and the spherical case is more important in actual applications.

A. Formulation

The form of comoving-frame equation can be understood easily by noticing that when we calculate the derivative ($\partial I_\nu/\partial s$) of the specific intensity with respect to pathlength in the observer's frame, we are assuming that the *observer's* frame frequency is held constant. But from (2.17) it immediately follows that in a differentially moving medium the corresponding comoving-frame frequency varies along the ray. Thus if we measure I' and ν' in the comoving frame, we expect

$$\left.\frac{\partial I_\nu}{\partial s}\right|_\nu \rightarrow \left.\frac{\partial I'_{\nu'}}{\partial s}\right|_{\nu'} + \frac{d\nu'}{ds}\frac{\partial I'_{\nu'}}{\partial \nu'} = \frac{\partial I'_{\nu'}}{\partial s} + \frac{\nu_0}{c}\frac{dv}{ds}\frac{\partial I'_{\nu'}}{\partial \nu'}. \tag{4.1}$$

With the understanding that *all* quantities are measured in the comoving frame in the remainder of this section, we henceforth drop primes.

A rigorous derivation leads to the following comoving-frame transfer equation in spherical symmetry:

$$\mu\frac{\partial I(r,\mu,\nu)}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial I(r,\mu,\nu)}{\partial \mu} - \frac{\nu_0 v(r)}{cr}\left[1-\mu^2+\mu^2\frac{d\ln v(r)}{d\ln r}\right]\frac{\partial I(r,\mu,\nu)}{\partial \nu}$$
$$= \eta(r,\nu) - \chi(r,\nu)\, I(r,\mu,\nu). \tag{4.2}$$

Here we tacitly assumed the emissivity is isotropic (e.g., complete redistribution or angle-averaged partial redistribution). Only Doppler-shift terms have been included in (4.2) for the reasons discussed in Section II.B above (see also [53]). Along a tangent ray (4.2) becomes

$$\pm\frac{\partial I_{sp\nu}}{\partial s} - \gamma(s,p)\frac{\partial I^{\pm}_{sp\nu}}{\partial \nu} = \eta(r,\nu) - \chi(r,\nu) I^{\pm}_{sp\nu} \tag{4.3}$$

where $r \equiv (p^2+s^2)^{1/2}$ and $\mu \equiv s/r$. Writing $d\tau_{sp\nu} \equiv -\chi(s,p,\nu)ds$ and defining the Feautrier variables

$$j_{sp\nu} \equiv \tfrac{1}{2}[I^+(s,p,\nu) + I^-(s,p,\nu)] \tag{4.4}$$

and

$$h_{sp\nu} \equiv \tfrac{1}{2}[I^+(s, p, \nu) - I^-(s, p, \nu)] \tag{4.5}$$

we can replace (4.3) by the system

$$\frac{\partial j_{sp\nu}}{\partial \tau_{sp\nu}} + \gamma_{sp\nu} \frac{\partial h_{sp\nu}}{\partial \nu} = h_{sp\nu} \tag{4.6}$$

and

$$\frac{\partial h_{sp\nu}}{\partial \tau_{sp\nu}} + \gamma_{sp\nu} \frac{\partial j_{sp\nu}}{\partial \nu} = j_{sp\nu} - S_{sp\nu}. \tag{4.7}$$

Note that we do not need to mix frequencies on both sides of the line core in (4.4) and (4.5), as we did in the observer frame (cf. (3.25) and (3.26)) because we are now always locally at rest with respect to the line profile.

To solve the system (4.6) and (4.7) we need two spatial boundary conditions at each end of the ray, and an "initial" condition in frequency; those used to dealing with hydrodynamics problems can regard τ as our "space" variable and frequency as our "time" variable. For zero incident radiation at the outer boundary $r = R$ we have

$$\left.\frac{\partial j_{sp\nu}}{\partial \tau_{sp\nu}}\right|_{s_{\max}} + \gamma(s_{\max}, p, \nu) \left.\frac{\partial j_{sp\nu}}{\partial \nu}\right|_{s_{\max}} = j_{sp\nu}|_{s_{\max}}. \tag{4.8}$$

On the symmetry plane we can now write $h(0, p, \nu) \equiv 0$ because we have not mixed frequencies together, hence for rays not intersecting the core

$$(\partial j_{sp\nu}/\partial \tau_{sp\nu})_{s=0} = 0. \tag{4.9}$$

For rays intersecting the core we replace (4.9) with the diffusion approximation or an imposed radiation condition (see [52] or Chap. 14 of [46], for details). To pose the "initial" condition we simply notice that *in an expanding medium* photons received locally by any observer have always been *redshifted* relative to their frequencies at their points of origin. Hence the highest-frequency edge of the line profile cannot intercept *line* photons from any other point in the medium, but only *continuum* radiation blueward of the line; we regard the latter as given (obtained from a separate calculation) and take

$$j(s, p, \nu_{\max}) = j_{\text{continuum}}. \tag{4.10}$$

B. Complete Redistribution

For complete redistribution we can solve (4.6)–(4.10) by a modified Rybicki algorithm. In this case the source function has the form

$$S(s, p, \nu) = \alpha(r, \nu)\, \bar{J}(r) + \beta(r) \tag{4.11}$$

where $r = r(s, p)$ and

$$\bar{J}(r) \equiv \int_{\nu_{\min}}^{\nu_{\max}} d\nu\, \phi(\nu) \int_0^1 d\mu\, j[s(r, \mu), p(r, \mu), \nu]. \tag{4.12}$$

Notice the enormous simplification of (4.12) relative to (3.29) because ϕ depends only on ν, not on μ.

The system is now discretized by choosing grids $\{r_d\}$, $\{p_i\}$, and an induced grid $\{s_{d_i}\}$, and a frequency grid $\{\nu_n\}$ with $\nu_{\max} = \nu_1 > \nu_2 > \cdots > \nu_N = \nu_{\min}$, and is solved as a marching problem in frequency. Thus we discretize (4.12) as

$$\bar{J}(r_{d+1/2}) = \sum_{n=1}^{N} w_n \sum_{i=1}^{I_d} \omega_{d+1/2,i} \phi(r_{d+1/2}, \nu_n) j[s(r_{d+1/2}, p_i), p_i, \nu_n]. \tag{4.13}$$

In writing difference equations for (4.6) and (4.7) one must of course assure stability. Two options that give unconditional stability are (1) fully implicit (backward Euler) [52], or (2) Crank–Nicholson ([18, 59], and Addendum in [52]) differencing. In constructing the Crank–Nicholson scheme one must take products of averages in terms containing χj or χh on the right-hand side rather than averages of products. Formally Crank–Nicholson offers a better truncation error, and is less dissipative than backward Euler. But it is more complicated to code, and does not reduce to the correct diffusion approximation frequency-by-frequency in the deepest layers where the flow velocity vanishes. In fact, in several trial calculations with optically thick envelopes and exponentially vanishing velocities inward (realistic in a star) we found the Crank–Nicholson scheme could blow up, basically because in this limit the effective "signal speed" $(1/\gamma)$ becomes infinite, the time derivative drops out of the equations, and we are left with a set of linearly dependent equations. In our own work we have therefore always used backward Euler, and will continue to do so here. Test calculations have shown that it gives excellent results even with surprisingly coarse frequency meshes [52], essentially because velocity-induced escapes dominate everything else in the transport process.

Thus adopting a backward Euler scheme we replace (4.6) and (4.7) with

$$(j_{d+1/2,in} - j_{d-1/2,in})/\Delta\tau_{din} = h_{din} + \delta_{di,n-1/2}(h_{din} - h_{di,n-1}) \tag{4.14}$$

and

$$(h_{d+1,in} - h_{din})/\Delta\tau_{d+1/2,in} = j_{d+1/2,in} - S_{d+1/2,in} + \delta_{d+1/2,i,n-1/2}(j_{d+1/2,in} - j_{d+1/2,i,n-1}). \tag{4.15}$$

Solving (4.14) analytically for h_{din},

$$h_{din} = \{[(j_{d+1/2,in} - j_{d-1/2,in})/\Delta\tau_{din}] + \delta_{di,n-1/2} h_{di,n-1}\}/(1 + \delta_{di,n-1/2}), \tag{4.16}$$

We eliminate h from (4.15) to obtain a second-order system containing only j's at the current frequency ν_n and (known) j's and h's at ν_{n-1}. Representing the variation of j and h along a ray by the vectors

$$\mathbf{j}_{in} = (j_{3/2in}, ..., j_{d+1/2,in}, ..., j_{D+1/2,in}) \tag{4.17}$$

and

$$\mathbf{h}_{in} = (h_{1in}, ..., h_{din}, ..., h_{D+1,in}) \tag{4.18}$$

we find that the discretized differential equations and boundary conditions yield a system of the form

$$\mathbf{T}_{in}\mathbf{j}_{in} + \mathbf{U}_{in}\mathbf{j}_{i,n-1} + \mathbf{V}_{in}\mathbf{h}_{i,n-1} + \mathbf{W}_{in}\bar{\mathbf{J}} = \mathbf{X}_{in} \tag{4.19}$$

and

$$\mathbf{h}_{in} = \mathbf{G}_{in} + \mathbf{H}_{in}\mathbf{h}_{i,n-1}. \tag{4.20}$$

Here $\mathbf{T}_{in}$ is tridiagonal; $\mathbf{G}_{in}$ and $\mathbf{V}_{in}$ are bidiagonal; $\mathbf{H}_{in}$, $\mathbf{U}_{in}$, and $\mathbf{W}_{in}$ are diagonal; and $\mathbf{X}_{in}$ is a vector.

To solve the system, we choose a ray, and carry out a frequency-by-frequency elimination, noting that $\mathbf{U}_{i1}$, $\mathbf{V}_{i1}$, and $\mathbf{H}_{i1}$ are all zero. We thus find

$$\mathbf{j}_{in} = \mathbf{A}_{in} - \mathbf{B}_{in}\bar{\mathbf{J}} \tag{4.21}$$

and

$$\mathbf{h}_{in} = \mathbf{C}_{in} - \mathbf{D}_{in}\bar{\mathbf{J}} \tag{4.22}$$

where

$$\mathbf{A}_{in} = \mathbf{T}_{in}^{-1}(\mathbf{X}_{in} - \mathbf{U}_{in}\mathbf{A}_{i,n-1} - \mathbf{V}_{in}\mathbf{C}_{i,n-1}) \tag{4.23}$$

$$\mathbf{B}_{in} = \mathbf{T}_{in}^{-1}(\mathbf{W}_{in} - \mathbf{U}_{in}\mathbf{B}_{i,n-1} - \mathbf{V}_{in}\mathbf{D}_{i,n-1}) \tag{4.24}$$

$$\mathbf{C}_{in} = \mathbf{G}_{in}\mathbf{A}_{in} + \mathbf{H}_{in}\mathbf{C}_{i,n-1} \tag{4.25}$$

and

$$\mathbf{D}_{in} = \mathbf{G}_{in}\mathbf{B}_{in} + \mathbf{H}_{in}\mathbf{D}_{i,n-1}. \tag{4.26}$$

Then using (4.21) and (4.13) we develop a final system of the form

$$\left(\mathbf{I} + \sum_{i,n} \mathbf{F}_{in}\mathbf{B}_{in}\right)\bar{\mathbf{J}} = \sum_{i,n} \mathbf{F}_{in}\mathbf{A}_{in}, \tag{4.27}$$

which we solve for $\bar{\mathbf{J}}$, hence the source function S. For D radial shells and N frequencies the computational effort (which can be intensively vectorized) scales as $cD^3N + c'D^3$, which is the same as for the observer-frame method. But because in the comoving frame the frequency quadrature need cover only the range $\pm x_{\max}$ required to describe the static line profile, rather than $\pm(x_{\max} + |V|_{\max})$ as in the observer frame, the comoving-frame calculation can be markedly cheaper for high-velocity flows (provided, of course, that suitable initial conditions can be posed so that it can be used at all).

C. Partial Redistribution

The simplifications afforded by solving the line transfer equation in the comoving frame become perhaps most evident in the case of partial redistribution. The essential point is that the material properties are all locally isotropic in the comoving frame, and in contrast to the situation in the observer's frame [see (3.21) and (3.22)] velocity-induced Doppler shifts (with their angle-frequency coupling) do not appear explicitly in the arguments of R (they are accounted for in the differential operator). Hence it is mathematically possible to average over angles, and it makes physical sense to do so if the radiation field is fairly isotropic locally. We can then use the line source function given by (2.9), which implies a total source function (line plus continuum) of the form

$$S(r, \nu)=\zeta(r, \nu)\int_0^\infty R(r; \nu', \nu)\, J(r, \nu')d\nu' + \varepsilon(r, \nu). \tag{4.28}$$

Actual calculations [21, 55] have verified that this approach gives physically reasonable results.

Adopting (4.28) and taking the zeroth and first angular moments of (4.2) we have, in spherical geometry,

$$\frac{1}{r^2}\frac{\partial(r^2H_\nu)}{\partial r} - \alpha\left[\frac{\partial}{\partial\nu}(1-f_\nu)J_\nu + \beta\frac{\partial}{\partial\nu}(f_\nu J_\nu)\right] = \chi_\nu(S_\nu - J_\nu) \tag{4.29}$$

and

$$\frac{\partial(f_\nu J_\nu)}{\partial r} + \frac{(3f_\nu - 1)J_\nu}{r} - \alpha\left[\frac{\partial}{\partial\nu}(1-g_\nu)H_\nu + \beta\frac{\partial(g_\nu H_\nu)}{\partial\nu}\right] = -\chi_\nu H_\nu, \tag{4.30}$$

where for brevity $\alpha \equiv \nu_0 v/cr$ and $\beta \equiv d\ln v/d\ln r$. Notice that we now require *two* variable Eddington factors, $f_\nu \equiv K_\nu/J_\nu$ as in (I.2.37) and

$$g_\nu = N_\nu/H_\nu \tag{4.31}$$

where

$$\{J_\nu, H_\nu, K_\nu, N_\nu\} \equiv \tfrac{1}{2}\int_{-1}^{1} I(\mu, \nu)\{1, \mu, \mu^2, \mu^3\}d\mu. \tag{4.32}$$

Then using the sphericity factor q_ν defined by (I.3.27) we can rewrite (4.29) and (4.30) as

$$q_\nu\frac{\partial(r^2H_\nu)}{\partial X_\nu} + \gamma_\nu\left[\frac{\partial}{\partial\nu}(1-f_\nu)r^2J_\nu + \beta\frac{\partial}{\partial\nu}(r^2f_\nu J_\nu)\right] = r^2(J_\nu - S_\nu) \tag{4.33}$$

and

$$\frac{\partial(f_\nu q_\nu r^2 J_\nu)}{\partial X_\nu} + \gamma_\nu \left[\frac{\partial}{\partial \nu}(1-g_\nu) r^2 H_\nu + \beta \frac{\partial}{\partial \nu}(r^2 g_\nu H_\nu) \right] = r^2 H_\nu. \tag{4.34}$$

The basic computational strategy for solving (4.33) and (4.34) is the same as described in Section II.C.(ii) of Paper I: given estimates of the Eddington factors f_ν and g_ν we solve the moment equations for H_ν and J_ν, hence S_ν; then using the current estimate of S_ν we update f_ν and g_ν from a formal solution, and iterate to convergence. We shall give only the barest sketch of the algorithm; see [54] for complete details.

Discretizing in both space and frequency as in Section IV.B above (again adopting a backward Euler scheme) we have two equations of the form

$$\begin{aligned} &\frac{q_{d+1/2,n}}{\Delta X_{d+1/2,n}}(r_{d+1}^2 H_{d+1,n} - r_d^2 H_{dn}) \\ &\quad + \frac{\gamma_{d+1/2,n-1/2} r_{d+1/2}^2}{\Delta \nu_{n-1/2}} \Big[(1 - f_{d+1/2,n-1} + \beta_{d+1/2} f_{d+1/2,n-1}) J_{d+1/2,n-1} \\ &\quad - (1 - f_{d+1/2,n} + \beta_{d+1/2} f_{d+1/2,n}) J_{d+1/2,n} \Big] \\ &= r_{d+1/2}^2 \Big(J_{d+1/2,n} - \zeta_{d+1/2,n} \sum_{n'} \mathscr{R}_{d+1/2,n'n} J_{d+1/2,n'} - \varepsilon_{d+1/2,n} \Big) \end{aligned} \tag{4.35}$$

and

$$\begin{aligned} &\frac{1}{\Delta X_{dn}}(f_{d+1/2,n} q_{d+1/2,n} r_{d+1/2}^2 J_{d+1/2,n} - f_{d-1/2,n} q_{d-1/2,n} r_{d-1/2}^2 J_{d-1/2,n}) \\ &\quad + \frac{\gamma_{d,n-1/2} r_d^2}{\Delta \nu_{n-1/2}} [(1 - g_{d,n-1} + \beta_d g_{d,n-1}) H_{d,n-1} - (1 - g_{dn} + \beta_d g_{dn}) H_{dn}] = r_d^2 H_{dn}, \end{aligned} \tag{4.36}$$

where $\gamma \equiv \alpha/\chi$. Equation (4.36) can be solved analytically to give an explicit expression for H_{dn} in terms of $J_{d+1/2,n}$, $J_{d-1/2,n}$, and $H_{d,n-1}$. Then by invoking an "initial" condition $(\partial I/\partial \nu) = 0$ because the continuum radiation intercepted by the blue wing of the line is (assumed) frequency independent, we can solve recursively in n to obtain

$$\begin{aligned} r_d^2 H_{dn} = \sum_{n'=1}^{n} \psi_{dnn'} (&f_{d+1/2,n'} q_{d+1/2,n'} r_{d+1/2}^2 \\ &\times J_{d+1/2,n'} - f_{d-1/2,n'} q_{d-1/2,n'} r_{d-1/2}^2 J_{d-1/2,n'}) / \Delta X_{dn'} \end{aligned} \tag{4.37}$$

where

$$\psi_{dnn'} \equiv \frac{1}{1+\omega_{dnn}} \prod_{l=n'+1}^{n} \frac{\omega_{dl,l-1}}{1+\omega_{dll}} \tag{4.38}$$

and

$$\omega_{dkl} \equiv \gamma_{d,k-1/2}(1 - g_{dl} + \beta_d g_{dl})/\Delta\nu_{k-1/2}. \tag{4.39}$$

Using (4.37) in (4.35) and applying spatial boundary conditions (see [54]) we end up with a set of equations for J_ν of the standard Feautrier form

$$-\mathbf{A}_{d+1/2}\mathbf{J}_{d-1/2} + \mathbf{B}_{d+1/2}\mathbf{J}_{d+1/2} - \mathbf{C}_{d+1/2}\mathbf{J}_{d+3/2} = \mathbf{L}_{d+1/2} \tag{4.40}$$

where $\mathbf{J}_{d+1/2}$ is a vector of length N containing the frequency variation of J_ν at $r_{d+1/2}$. These are solved by the Feautrier elimination scheme in Section II.C.(i) of Paper I. The total computational effort scales as $I(cDN^3 + c'D^2N)$, where I is the number of iteration cycles required to converge the Eddington factors (usually 3 or 4). We emphasize again that the frequency bandwith need only be large enough to cover the *static* line profile, hence N is not large.

Thus by working in the comoving frame we can solve partial redistribution problems in expanding spherical media; recall that in Section III.B we showed that there is no convenient method for solving such problems in the observer's frame. In planar geometry we can either use the scheme sketched above, or work directly in terms of angle-frequency components $j_{\mu\nu}$ (still assuming angle-averaged redistribution) [55]. In the latter case the computational effort scales as cDM^3N^3, which is still much more favorable than the corresponding observer-frame calculation because the latter requires much larger values of M and N to span the line profile including flow-velocity shifts, and to assure accuracy of the (difficult) quadratures in (3.21) and (3.22). But it is still probably cheaper to use variable Eddington factors.

Finally we mention that a method for solving angle-frequency dependent partial redistribution problems in expanding spherical flows has been outlined in [48], but has never been implemented, so its effectiveness is unknown.

D. Formal Solution

Given the comoving-frame source function, the normal solution for the emergent radiation field (and/or Eddington factors) is carried out in the observer's frame just as described in Section III.C.

E. Remarks

The comoving frame method begins to lose its attractiveness for nonmonotonic velocity fields [55, 58] for two reasons. (1) It becomes much more difficult to pose an "initial" condition in frequency because line wing photons can now, in general, interact with the line absorption profile in more than one location in the flow. Moreover one must be careful to pose the condition at the correct side of the line (blue or red) in order to track the characteristics of the PDE correctly [55]. (2) The bandwidth of the problem increases as we are forced to go to ever-higher (or lower) frequencies in order to pose a clean "initial" condition.

The method can still be used for low-velocity flows in planar geometry, but as the velocity *fluctuation* away from monotonic variation increases, the approach becomes more cumbersome than the observer-frame method (though it may still be easier to evaluate the scattering integral in the comoving frame because of isotropy of the material properties). For low-amplitude arbitrary velocity fields it is probably best to use the observer-frame method from the outset.

V. Critique

In this paper we have considered only the transfer problem in a *single* spectrum line. The general machinery required to handle multilevel atoms with interlocked transitions is quite elaborate; see [1, 2, 32, 46]. An extremely simplified iteration scheme for treating multilevel problems in expanding media with comoving-frame methods is described in [38, 51]. This so-called "equivalent two-level atom" iteration is not particularly robust for *static* media, but works surprisingly well in moving media, mainly because velocity-induced escapes dominate the problem, and overwhelm the subtle couplings among transitions that might otherwise arise.

We have also discussed only *direct* solutions, which are, of course, often costly, though certainly more viable than ever on vector computers. But a whole class of clever iterative techniques based on Cannon's "quadrature perturbation" techniques—better known to numerical analysts as the method of deferred correction—have been suggested [6, 7, 8, 10, 15, 16, 33]. In our opinion these methods hold great promise, and need to be explored and developed more thoroughly. Perhaps the most promising new scheme is the approach developed by Scharmer and his associates [64, 65, 68] which uses an *approximate* inverse of the integral-operator representation of the transfer equation (in the observer's frame) to develop a strongly convergent iteration scheme; the underlying philosophy is strongly reminiscent of preconditioning schemes (such as ICCG and ILUCG) which are proving so effective in a diverse range of applications. A multilevel version of this scheme has also recently been developed [66, 67].

Looking beyond current efforts, the future appears very interesting, though unpredictable (at least by us!). As large-memory multi-processor machines become available, many problems that are intractable or clumsy (say because of intensive I/O) today will become easy "tommorrow" even with current algorithms. And we cannot even hazard a guess what will happen when truly parallel processors with a variety of different architectures and logical topologies arrive. Perhaps we will then simulate transport in a network of processors in direct mimicry of the way it actually happens in nature. Perhaps we will junk our deterministic methods and go entirely to Monte Carlo. Perhaps it is best to stop here and simply say that we hope that clever people interested in computational physics will continue to work hard at developing *new* methods to solve the problems we have discussed, and thus make this article totally obsolete in a few years.

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