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978-0-521-11517-9 - Numerical Radiative Transfer
Edited by Wolfgang Kalkofen
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INTRODUCTION

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ABSTRACT: The papers in the two sections of this book address two topics: the efficient solution of radiative transfer problems by means of operator perturbation and related numerical methods, and the transfer equation for polarized radiation. This introduction provides synopses of the papers, assessing their specific importance and relevance within the broader context. The first section begins with a survey of numerical methods contained in this volume or forming their background; then the topics covered concern the use of diagonal operators, the acceleration of the convergence of the resulting equations, line transfer for a time-dependent two-level atom, the formulation of the transfer and statistical equilibrium equations for multi-level atoms in terms of equivalent two-level atoms, the construction of stellar atmospheres with non-LTE line blanketing, and the derivation of operator perturbation equations of low order from high-order equations. The second section, on polarized radiative transfer, also has its own introduction; the topics concern the use of the Feautrier equation, the derivation and solution of the transfer equation using real matrices, or complex matrices. The last two papers describe a discrete space technique and a generalization of the formal integral of the transfer equation to the case of an absorption *matrix* — methods that can be used also for line transfer with *partial redistribution*; apart from these two papers and a critical analysis in a paper in the first section of operator perturbation methods for partial redistribution, only *complete redistribution* is treated.

1. OPERATOR PERTURBATION

The task considered in the first section of this book is the solution of the equation of radiative transfer subject to constraints such as statistical equilibrium or radiative equilibrium. The mathematical problem can be stated in the form of a system of coupled differential equations in which the unknown functions are either the source function, or the intensity at all frequencies, angles, and depths, or, as in the construction of model atmospheres, the fundamental variables of the medium, such as temperature, pressure, and particle densities. Three numerical difficulties characterize typical transfer problems: The equations are non-linear, the system of equations has large order, and important characteristic length scales differ by many orders of magnitude — factors as large as 10^4 or 10^6 are not uncommon. The first section of this book deals with ways of overcoming two of these hurdles: it addresses the efficient solution of systems of stiff equations having very large order. Non-linearities may occur, but they are only incidental.

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The aim of the numerical methods described here is to solve the equations fast, yet accurately. The tool used is operator perturbation. The procedure is to separate a problem into two parts, the approximate calculation of corrections to a provisional solution, and the accurate calculation of the error made by the provisional solution in a conservation equation. The error becomes the driving term in the next cycle of correction calculations. Thus, this approach uses iterations to arrive at an accurate solution, even when the equations are linear.

In the error calculation, individual (*i.e.*, uncoupled) transfer equations are solved for known source function. This calculation treats only the short-range interactions of the radiation field, where the region of influence of the gas extends over a distance of the order of the mean-free-path of the respective photons. The long-range influence of scattering and the diffusion of photons in frequency must be contained in the correction calculation, where an approximate operator describes the radiative transfer. This places great emphasis on the construction of the approximate operator to ensure that it model the overall structure of the solution. It is therefore interesting to inquire into the design principles of operator perturbation methods with a view of learning how to construct approximate operators and how to modify or improve existing methods. This is the task considered in **Chapter 1** where I survey the basic ideas on which operator perturbation and related methods are built.

In **Chapter 2** Hamann describes a solution method for multi-level line transfer problems in extended atmospheres for the Sobolev limit of high differential velocity and applies it to a Wolf-Rayet atmosphere. To construct the approximate transfer operator he assumes that the photo-absorption rate is equal to the photo-emission rate except for photons that can escape in a single free flight. Thus the local intensity is equal to the local source function multiplied by a factor describing the fractional contribution by the line core to the absorption. The equations amount to a restatement of Rybicki's (1972) core saturation method; in the limiting case of a two-level atom without induced emission they are identical with the core saturation equations (*cf.* Rybicki 1985). The essential contribution of Hamann (and of Werner & Husfeld, 1985; *cf.* Chapter 3) is to have embedded the equations in the operator perturbation formalism. Since the resulting approximate transfer operator is diagonal, the solution of a line transfer

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problem is similar to Λ-iteration; it would be identical to Λ-iteration were it not for the leakage of photons in the wings of a line. This is the decisive difference. Hamann's equations converge whereas Λ-iteration fails, except in trivial cases. Of course, convergence is not spectacular. It is, in fact, no better than that of the core saturation method. But that does not seriously limit the usefulness of this method whose real strength is rooted in the fact that it separates the transfer equations from the equations of statistical equilibrium, which are now entirely local. The iterative solution process therefore alternates between the scalar transfer equations for the individual lines and the equations of statistical equilibrium. The method can be viewed as an accelerated Λ-iteration in which the amplification factor varies from being approximately equal to the inverse of the wing fraction of the absorption profile near the surface of the atmosphere, to the inverse of the scattering parameter ϵ at large depths. For strong lines this amplification can have enormous values far from the surface: a factor of several million is reached in one example.

The separation of the problem into the solution of the transfer equation and the equations of statistical equilibrium has two major advantages: It makes the order of the matrices occurring in this formulation for a given problem very small, thus allowing more ambitious problems to be attacked; and it makes programming the equations very simple. The drawback of the method is that it requires a relatively large number of iterations to solve a problem (*cf.* Chapter 4 for an acceleration method applied to these or similar equations). For small atomic systems, where the computer time is dominated by the solution of the transfer equations in the error calculation, this method is therefore not competitive with other operator perturbation methods.

Among interesting numerical questions discussed are: the calculation of the boundary between line core and line wings for a moving medium in the comoving frame formulation; the free parameter that defines the boundary between line core and wings and its effect on convergence; the formal solution in the error calculation treats individual frequencies but the equations are coupled over angle (or impact parameter) by the Thomson scattering term, a complication that is handled by means of the variable Eddington factor technique.

The formulation of the statistical equilibrium equations makes use of net radiative bracket expressions. A full discussion of these is given in Chapter 6. See Chapters 3 and 4 for similar operator perturbation methods.

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Werner's approach to radiative transfer in **Chapter 3** is similar to that described in Chapter 2, showing the same provenance from the group under Hunger in Kiel. The operator perturbation method is based on approximate Λ-operators that separate the transfer equation from the equations of statistical equilibrium, which then contain no explicit depth-coupling. In addition to the purely diagonal matrix used by Hamann, Werner also employs a triangular operator first suggested by Scharmer (1981, 1984); and for lines with an underlying continuum he investigates a different, but again diagonal, operator, with a larger probability for photon escape from the medium (*cf.* also Chapter 2); the free parameter defining this probability is chosen so as to improve the stability of the method.

In many instances the triangular operator is almost as convenient to use as the diagonal operator since at any given depth in the atmosphere the contribution of the lower layers to the radiation field is known; its speed advantage in the number of iterations over the diagonal operator can be as large as a factor of two, but more typically it is only slight. A possible disadvantage is that the equations of statistical equilibrium must be solved sequentially, and from the lower boundary in the outward direction, opposite from the direction in which the hydrostatic equilibrium equation is integrated. On parallel processors the purely diagonal operator is to be preferred since the calculations at the various depths are then independent of one another and can be carried out in parallel. This is also true in the construction of model atmospheres if the pressure is updated outside the Newton-Raphson iteration cycle.

Two types of problem are solved here with this method: multi-level line formation in atmospheres with given gross structure, and the construction of hydrogen line-blanketed model atmospheres in plane-parallel geometry, for effective temperatures between 30,000 and 100,000K. A problem is solved by the linearization of the conservation equations (*viz* radiative, hydrostatic, and statistical equilibrium; particle and charge conservation). The procedure is analogous to the complete linearization method of Auer & Mihalas (1969) except that the transfer operator is a diagonal or triangular matrix. In line transfer calculations for a given atmosphere the problem can often be simplified further by cancelling the core frequencies analytically; the statistical equilibrium equations resulting with the diagonal operator are then linear in the particle densities and no Newton-Raphson perturbation is necessary for their solution.

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The operator perturbation method is more convenient than the complete linearization method because of the smaller size of the matrices and because of ease of programming, and it allows much larger atomic systems to be attacked (*cf.* however Chapter 6 for expressing large problems in terms of equivalent two-level atoms). The author estimates that up to 100 non-LTE levels can be included in a calculation — the number of lines follows from the number of levels — whereas the complete linearization method is restricted to approximately 20 levels, the limits being set by the size of the largest matrices occurring in the formulations. The demonstration problems in the paper are for a hydrogen atom with five bound levels, and both line and continuum transitions are treated. Typical iteration numbers are 10 to 30 in the line formation calculations for given atmospheric structure, and 15 to 40 in model atmosphere constructions, the higher iteration numbers required at the lower temperatures; a maximum of 85 iterations is needed with the diagonal operator for a 30,000K model atmosphere. Werner presents detailed documentation of the properties of the method, including the tuning of the free parameter defining the separation of the line into core and wings and the effect on the rate of convergence and the stability. His experience with the two approximate operators suggests that the transfer in the wings, as implied by the triangular operator for example, may not have to be treated in line transfer problems but is important in the construction of model atmospheres, where wing transfer has a major impact on the rate of convergence.

While this method requires too many iterations to be competitive in the solution of small atomic systems with more efficient operator perturbation methods, such as Scharmer's (1981, 1984) or the one described in Chapter 5, the ease of formulation and programming and the small size of the matrices occurring in it make it ideal for many-level atoms.

In **Chapter 4** Auer offers a remedy for the relatively slow convergence of operator perturbation methods based on diagonal operators, reducing by a factor of at least two the number of iterations required to solve a problem. Any linearly convergent iteration scheme can be accelerated by this approach.

Unlike the Newton-Raphson equations, arising in complete linearization methods for example, operator perturbation equations have only linear convergence. The convergence rate is rapid in spite of that when the characteristics of the approximate operator match those of the exact operator, *i.e.*, when the

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maximal eigenvalue of the matrix in the perturbation expansion of the solution vector (*cf.* Kalkofen 1984, eq. 2.15) is *small* compared to unity. But diagonal approximate operators typically give eigenvalues *near* unity (*cf.* Olson, Auer & Buchler 1986, figs. 1-5), resulting in slow convergence when the new solution is based exclusively on the preceding solution (or in divergence for eigenvalues exceeding unity). To speed up convergence, information from earlier solutions must be used as well. Auer shows how this can be accomplished. He constrains the new solution by requiring that it be as close as possible in the least squares sense to an estimate of the converged solution of the equations. This requirement yields the coefficients for the extrapolation.

The method does not change the nature of the iterations, which remains linear. But it does drastically reduce the number of iterations necessary to satisfy a convergence criterion. Auer graphically depicts the improvement in the performance of solution methods that rely on diagonal approximate operators. He varies the number of preceding iterates he uses in the extrapolation and compares weighted and unweighted accelerations for approximate diagonal operators that are either obtained from estimates of the diagonal elements of the exact operator or constructed with the core saturation method. The improvement in his test cases is large. In one instance the number of iterations drops from more than 100 to about 20; weighting of the corrections by the inverse of the source function saves a few iterations. It is worth noting that the speed-up of convergence is obtained at almost no expense.

An important parameter in a line transfer problem is the thermalization length, the maximal distance over which features in the gross structure of an atmosphere are communicated by the line radiation to the gas. In a semi-infinite atmosphere this is also the depth to which the boundary influences the gas, and where the source function of a two-level atom saturates to the Planck function. Other parameters important for the general character of the solution are frequencies at which the atmosphere becomes transparent at points closer to the surface than the thermalization depth. The respective frequencies are located between line center and the frequency for which the monochromatic photon mean free path is of the order of the thermalization length. Frequencies further out in the wings are unimportant for the overall structure of the solution since the amount of energy escaping is too low to have an effect. Thus the broad features of

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the solution of a line transfer problem are defined by a small set of parameters. In **Chapter 5** I describe an operator perturbation method that makes use of this fact. The method employs two angle-frequency sets, a coarse set, typically consisting of a single angle point and a few well-chosen frequency points, and a dense set with many angle-frequency points. The coarse set is used to construct the approximate operator of the problem and the dense set to construct the exact operator.

The basic formulation is that of the integral equation method of Scharmer (*cf.* Scharmer & Nordlund 1982, Scharmer 1984), in which the driving term of the equation for computing corrections to a provisional solution is the error made by that solution in the equations of statistical equilibrium. But the integral equations are used merely as a device to derive a perturbation series. The actual numerical solution involves no integral equations. Instead, both the exact and the approximate integral equations are expressed in terms of their differential equation equivalents. This procedure of deriving the differential equations via intermediary integral equations insures that the perturbation series is equivalent to the exact equation and does not contain any extraneous terms (*cf.* Chapter 8). Thus, only systems of Feautrier equations are solved. In the case of the correction calculation the system is coupled but has very low order, which is given by the number of angle-frequency points in the sparse set; and in the case of the error calculation the system has high order, but the equations are uncoupled. As generally in these operator perturbation methods, the accuracy of the solution is given by the accuracy of the error calculation, which is second-order for the ordinary Feautrier equation and fourth-order with Auer's (1976, 1984) Hermite form.

Time-dependent problems in a moving medium are solved efficiently by using the converged solution at any time step as the starting solution at the subsequent time step and by perturbing the exact operator about the approximate operator that corresponds to the static medium. As a consequence, the profile function for the approximate operator is symmetric, halving the already low order of the system of equations for the correction calculation; in addition, the matrices need to be constructed and inverted only at the beginning of the computation, leading to substantial savings in computer effort. The drawback of this procedure is that the method is suitable only for problems in which the macroscopic flow velocity does not exceed a few times the speed of sound, a restriction that is typical, however, of formulations of transfer problems in the observer frame (*cf.* Chapter 7

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for a similarly restricted method, and Chapter 2 for the treatment of high differential velocities). This method assumes that a multi-level transfer problem is expressed as a sequence of equivalent two-level problems (*cf.* Chapter 6).

Two numerical examples are given in the paper. For line transfer in a model chromosphere with a velocity amplitude of three Doppler widths the exact problem is described with 4 angle points per hemisphere and 30 frequency points in the half profile, and the approximate operator is computed for a symmetric profile with a single angle point and 5 frequency points. This amounts to a reduction by a factor of about 50 of the order of the system of equations. Convergence is rapid. It is further accelerated by assuming that consecutive corrections at a given depth point define a geometric series, reducing the number of iterations required for the maximal error of the solution to drop below 1% to typically three or four, except for the first time step, where five or six iterations are necessary.

The typical line transfer problem in a stellar atmosphere consists of the equations of statistical equilibrium for an atomic model with several levels and the equations of radiative transfer for the corresponding lines and continua. One of the standard methods of solving these coupled equations is the complete linearization method of Auer & Mihalas (1969). This method accounts to first order for all the interactions of all the levels of the atom and at all optical depths. If the linearization is done fully consistently the resulting Newton-Raphson equations converge quadratically. This is a very satisfying property; but to achieve it one pays a high price in the order of the system of equations unless the number of lines is very small. A limit on the number of lines, and hence levels, that can be treated is soon reached. In the integral equation method the limit concerns primarily the number of levels rather than lines, but the result is the same. One way to increase the practical limit on the size of the atomic model has been described in Chapters 2 and 3, where the diagonal operator of the transfer equation permitted an exact solution of the coupling of all the interactions taking place within the model atom at any given optical depth, but at the expense of approximating the depth dependence of the transfer. Another way is to do just the opposite, to treat the depth dependence within each line exactly but to approximate the interactions among the various levels of the atom; since this approach treats the radiative transfer of a single line at any one time, the model is referred to as the *equivalent two-level atom.* In both cases, the numerical problem separates into

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one in which the order of the system of equations is given by the parameters of a single line, either the number of depth points or the number of angle-frequency points, and by the parameters of the model atom, such as the number of bound levels. How to set up the equations of the equivalent two-level atom is described in **Chapter 6** by Avrett & Loeser.

The paper addresses two main questions: how to write the equations of statistical equilibrium, whether in terms of individual photoexcitation and de-excitation rates or in terms of net radiative rates; and which level equations to single out of the equations of statistical equilibrium for deriving the source function of the equivalent two-level atom, whether the equations of only the upper and lower levels for the transition in question, or of all the levels.

When the statistical equations are written in terms of *single* upward and downward rates, the numerical results can be meaningless at large depths. This is especially true for the multiplet problem, discussed in the paper, in which the lower level is common and the upper levels are strongly coupled collisionally. On the other hand, when the equations are expressed in terms of *net* radiative rates, it can happen that the populations near the surface are negative, a result from which an iteration scheme might not recover. The best approach is to mix the two formulations, with the single and net rate expressions contributing each one half near the surface, and the net rates being used exclusively at large depths. All strong lines are treated the same way, the transition from one to the other formulation occurring in a particular layer in the atmosphere. The weak lines are frequently solved by a different procedure; since their source function is determined largely by the transfer in the strong lines, their radiation field can be obtained from a Λ-iteration. Avrett & Loeser describe both procedures for deriving the source function equation of an arbitrary model atom, *i.e.*, using either just the two combining levels, or all levels. No general prescription is given as to which procedure might be better, whether the former, which contains all the other unknown population ratios, or the latter, which contains all the other unknown radiation fields; in their numerical code the authors allow both procedures since they have found that different applications have different requirements. The two sets of source function equations are identical in the example given in the paper, that of a three-level atom.

Note that in spite of the symmetrical relation of the procedure described in this Chapter with the operator perturbation methods of Chapters 2

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and 3 concerning the separation of the equations into two blocks, one for the individual lines and the other for the atomic interactions, the equivalent two-level atom does not constitute an operator perturbation method. It may be used in conjunction with any approach to the solution of non-LTE problems, including operator perturbation methods (*cf.* Chapter 5), for which it extends the scope by removing the limits based on matrix size, leaving only the practical limit from managing large numbers of interactions. In this respect it resembles the methods based on diagonal operators. Note also that in any iteration the source function interaction coefficients (*i.e.*, ϵ and β) in the transfer equation of a particular line depend only on information from the preceding iteration; they do not (in this formulation) depend on the order in which the transfer equations are solved. Thus the transfer equations can be solved in parallel, an operation that could be carried out efficiently on parallel processors.

In **Chapter 7** Anderson describes a method for constructing line-blanketed model atmospheres in statistical equilibrium. In an ingenious way he uses the related, critical observations that the overall structure of an atmosphere depends mainly on the gross properties of the opacity and on the long-range communication between distant parts of the atmosphere. To exploit these features he groups the photons of the fine-grained frequency set needed for a full accounting of the opacity in a line-blanketed medium into coarse-grained frequency blocks in which all photons experience approximately the same interactions, *i.e.*, photons in a given frequency block have all nearly the same mean free path and probability of scattering into other layers. Thus, a block might consist of frequency points in the cores of the lowest resonance lines of some atom, or in the near or far wings, or of frequency points in subordinate lines of another atom. It follows that the frequencies in a block may be drawn from different, non-contiguous parts of the spectrum.

The transfer and conservation equations written for frequency blocks are treated in much the same way as the equations in the complete linearization method of Auer & Mihalas (1969). The main difference is that explicit reference to particle densities is eliminated. Therefore the order of the system of equations is independent of the number of energy levels in the equations of statistical equilibrium and is given essentially by the number of coarse-grained frequency blocks. In the example of this paper the number of block equations is on the order of 100,

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