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Research Note

Fast approximations for the R_{II-A} redistribution function

P. Gouttebroze

Laboratoire de Physique Stellaire et Planétaire, B.P. no. 10, F-91371 Verrières-Le-Buisson Cedex, France

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Summary. Approximations are proposed for the computation of the R_{II-A} redistribution function (which describes the redistribution of frequencies for photons scattered coherently in the atom's frame). These approximations are particularly efficient on vector computers. Precision and timing properties of the method are examined for a typical line formation problem (Lyα in the solar atmosphere).

Key words: lines: formation – lines: profile – numerical methods – radiation transfer

1. Introduction

The effects of partially coherent scattering on line formation are important in some astrophysical problems, such as that of the formation of strong resonance lines in stellar atmospheres. In this case, an accurate calculation of the line profiles requires the evaluation of the R_{II} redistribution function (which, according to Hummer's (1962) classification, corresponds to the case of scattering coherent in the atom's frame). Important differences may be found between partial and complete redistribution calculations, concerning the intensities in the line wings and the center-to-limb variations of the profiles. In addition, in the case of the modelling of a stellar upper atmosphere, the effects of partial redistribution in the Lyman-α line should be taken into account, since they can modify the statistical equilibrium of the hydrogen atom, and thus the electron density. The R_{II} function having rapid variations, it is generally necessary, in radiative transfer calculations, to evaluate it at a large number of frequency points. Accurate methods have been given, for instance, by Adams et al. (1971). Unfortunately, they are generally time-consuming and, on vector computers, it is difficult to adapt them to parallel processing in order to take advantage of the speed of the computer. As a consequence, the time needed to compute the redistribution matrices is generally much more important than that used to solve the radiative transfer equation, by the Feautrier method for instance. To overcome this problem, we propose here to replace the accurate, but complicated, formulae for the R_{II} redistribution function by approximate but simple ones, allowing parallel computations. In such a way, the time needed to compute redistribution functions may be decreased, on vector computers, by nearly two orders of magnitude.

2. Principle

Let v and v' be the reduced frequencies (i.e. the frequency distances from line center divided by the Doppler width) for the incoming and scattered photons, respectively. We are looking for some approximation of the redistribution function:

$$R_{II}(v,v') = \frac{1}{2\pi}\int_0^{\pi} \exp\left[-\left(\frac{v-v'}{2\sin\frac{\gamma}{2}}\right)^2\right] H\left(\frac{a}{\cos\frac{\gamma}{2}}, \frac{v+v'}{2\cos\frac{\gamma}{2}}\right) d\gamma \qquad (1)$$

where H is the Voigt function.

Following Jefferies (1968) notation, we set:

$$g_{II}(v,v') = \frac{R_{II}(v,v')}{\psi(v')} \qquad (2)$$

where ψ is the normalized absorption profile.

The symmetry properties of R_{II} and ψ, i.e. $R_{II}(-v,-v') = R_{II}(v,v')$ and $\psi(-v') = \psi(v')$, yield:

$$g_{II}(-v,-v') = g_{II}(v,v') \qquad (3)$$

which allows us to restrict the discussion to positive values of v'.

According to the value of v', the variation of $g_{II}(v,v')$ as a function of v has two principal forms. For $v'<2$, the curve is essentially symmetric around $v=0$. For $v'>4$, on the contrary, the curve is peaked at $v=v'$, and is approximately symmetric around this value. Thus, the discussion will be divided into three ranges of variation for v', a "core", a "wing" and a "transition" range, corresponding to three approximations for g_{II}, named g_c, g_w and g_t, respectively.

2.1. *The core region* ($v'<2$)

Here, the redistribution process is dominated by the Doppler effect, so that the R_{II} function is very similar to the R_I function corresponding to zero natural width:

$$R_{II}(v,v') \simeq R_I(v,v') = \frac{1}{2}\mathrm{erfc}[\max(|v|,|v'|)]$$

where erfc is the complementary error function:

$$\mathrm{erfc}(x) = (2/\sqrt{\pi})\int_x^{\infty} \exp(-t^2)\,dt$$

since $\psi(v') \simeq \pi^{-1/2}\exp(-v'^2)$, the "core" approximation will be:

$$g_c(v,v') = \exp(v'^2) \int_{\max(|v|,|v'|)}^{\infty} \exp(-t^2)\,dt$$

or, setting:

$$g_0(x) = \exp(x^2) \int_x^{\infty} \exp(-t^2)\,dt \tag{4}$$

$$g_c(v,v') = \begin{cases} g_0(v'), & \text{if } v \leqq v' \\ \exp(v'^2 - v^2)\, g_0(v), & \text{if } v > v' \end{cases} . \tag{5}$$

The function $g_0(x)$ is known as the Mills'ratio. For numerical purposes, it will be replaced by the approximation given by Pollack (1956):

$$g_0(x) \simeq 1/[x + (x^2 + 4/\pi)^{1/2}] . \tag{6}$$

This expression is in fact an upper bound for g_0. It gives the exact value for $x = 0$, and the relative error remains lower than 6% for all other values of x.

2.2. The wing region ($v' > 4$)

There, the g_{II} function becomes approximately symmetric around $v = v'$. It is tempting to replace R_{II} by its asymptotic value (Frisch, 1980):

$$R_{II}(v,v') \simeq \frac{a}{\pi\left[\frac{1}{2}(v+v')\right]^2} \operatorname{ierfc}\left(\frac{1}{2}|v'-v|\right)$$

with

$$\operatorname{ierfc}(x) = \int_x^{\infty} \operatorname{erfc}(t)\,dt .$$

The corresponding approximation for the absorption profile is:

$$\psi(v') \simeq a/(\pi v'^2)$$

which yields

$$g(v,v') \simeq \left(\frac{2v'}{v+v'}\right)^2 \operatorname{ierfc}\left(\frac{1}{2}|v-v'|\right) . \tag{7}$$

This expression, which represents correctly g_{II} in the neighbourhood of $v = v'$, has the disadvantage to be infinite for $v = -v'$. Since the ierfc(x) function decreases rapidly at large x, the useful range for v is limited to a few units around $v = v'$, so that it is possible to replace the first factor in (7) by a power series in $\varepsilon = (v/v') - 1$. Limiting this series to the terms of degree 0, 1 or 2, respectively, we obtain the following approximations:

$$g_w^{(0)}(v,v') = \operatorname{ierfc}\left(\frac{1}{2}|v-v'|\right) \tag{8a}$$

$$g_w^{(1)}(v,v') = \left(2 - \frac{v}{v'}\right)\operatorname{ierfc}\left(\frac{1}{2}|v-v'|\right) \tag{8b}$$

$$g_w^{(2)}(v,v') = \left(2.75 - 2.5\frac{v}{v'} + 0.75\frac{v^2}{v'^2}\right)\operatorname{ierfc}\left(\frac{1}{2}|v-v'|\right) . \tag{8c}$$

The functions ierfc and g_0 are related by:

$$\operatorname{ierfc}(x) = \pi^{-1/2}\exp(-x^2)[1 - 2x g_0(x)] \tag{9}$$

so that it is possible to use approximation (6) to compute ierfc economically.

2.3. The transition region ($2 \leqq v' \leqq 4$)

For these values of v', it is not possible to consider, as previously, that one of the two redistribution processes (Doppler or natural broadening) dominates the other. As the transition between the two regimes may be described by the ratio of Doppler and Lorentz profiles, we tried a simple combination of the core and wing redistribution functions:

$$g_t(v,v') = \frac{\psi_c(v')}{\psi_c(v') + \psi_w(v')} g_c(v,v') + \frac{\psi_w(v')}{\psi_c(v') + \psi_w(v')} g_w(v,v') \tag{10}$$

with:

$$\psi_c(v') = \pi^{-1/2}\exp(-v'^2)$$

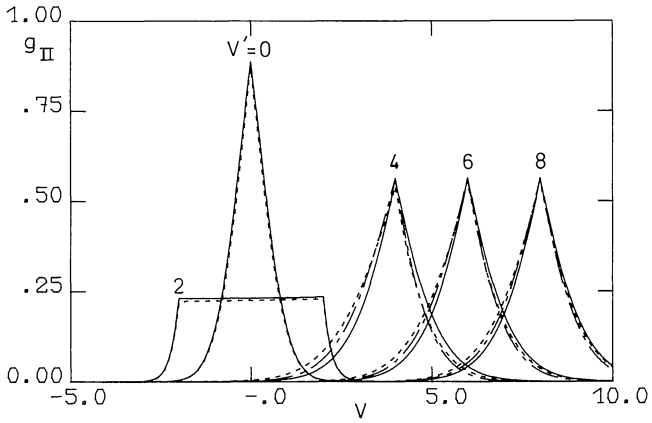

Fig. 1. Comparison of the function $g_{II-A}(v,v')$ (dotted line) with the present approximations, for $v' = 0, 2, 4, 6$ and 8; full line: APR(0); dot-dashed line: APR(1)

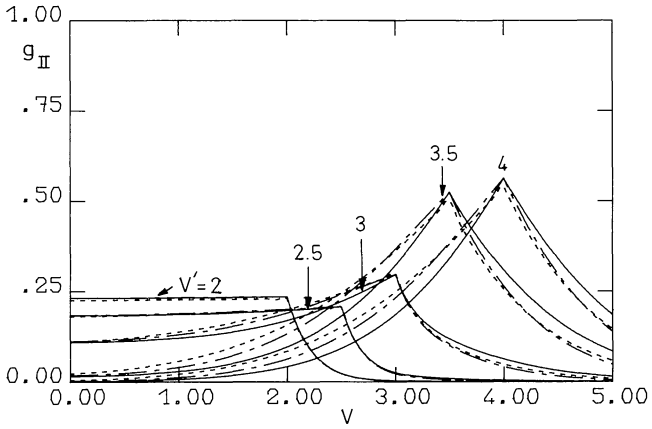

Fig. 2. Same as Fig. 1, but for $v' = 2, 2.5, 3, 3.5$ and 4

and:

$$\psi_w(v') = (a/\pi)/(a^2+v'^2)$$

and where g_w is one of the three formulae (8).

Empirically, these formulae are found to be sufficient. In particular, they reproduce satisfactorily the variation of the edge ($v=v'$) when v' varies (cf. Fig. 2).

In Figs. 1 and 2, we compare the present approximations, given by the formulae (5, 8, and 10), to an accurate evaluation of the g_{II-A} function, for a typical value of the damping constant ($a=10^{-3}$). Figure 1 gives a general insight on the approximation, while Fig. 2 details the transition region. The present approximations are referred to as APR (0) and APR (1), according as g_w is given by formula (8a) or (8b), respectively.

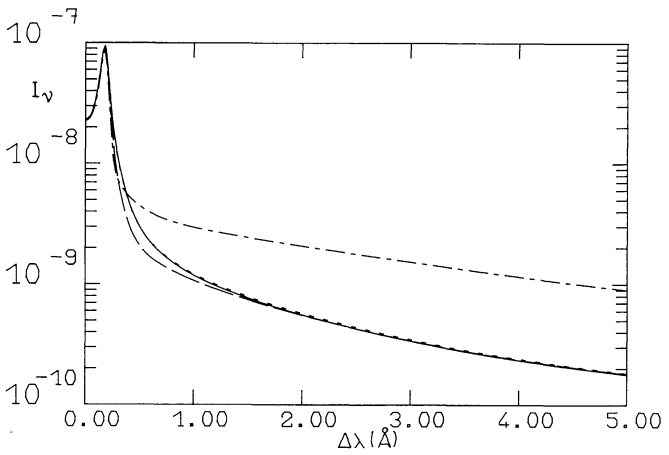

Fig. 3. Comparison of Lyman-α profiles calculated under 4 different assumptions: partial redistribution, (PR): full line, complete redistribution (CR): dot-dashed line, and the present approximation (APR) with two different formulae for the wings: APR (0): dashed line; APR (1): dotted line. PR and APR (1) are practically superimposed

3. Application

In a radiative transfer calculation with partial redistribution, it is in general necessary to compute a redistribution matrix for each depth in the atmosphere. One uses two frequency meshes: a coarse mesh with a number of points (N) equal to the order of the matrix, and a fine mesh (with M points) for the integration of the redistribution function. The matrices are computed column by column, each of these corresponding to a value of v'. To take advantage of the speed of a vector computer, the M values of $g(v,v')$ corresponding to the M values of v must be computed within a vector loop. In addition (but this is true for any type of computer), it is better to restrict the range of v values to those who are important. For instance, we use here the following ranges:

$$-4 \leqq v \leqq v'+5 \quad \text{if} \quad v' \leqq 4$$

$$v'-5 \leqq v \leqq v'+5 \quad \text{if} \quad v' > 4$$

eliminating the regions where $g(v,v')$ is lower than 10^{-3}.

The advantage of the present approximation lies principally in the fact that the formulae are simple enough to allow a parallel computation of all the values of the function related to the same value of v'. This is done in the subroutine given in the Appendix. The precision and timing properties of this routine were tested on a Cray-1 computer. The line under consideration was the Lyman-α line of hydrogen, and the atmospheric model was a solar-type one, including 99 depth points. The coarse frequency mesh had $N=20$ points, while the refined mesh had a number of points varying with altitude, determined by the criterion that the spacing between two successive points should be lower than 0.2 Doppler widths. On the whole, nearly $2\,10^6$ values of g_{II} were computed. The approximation was compared with a standard routine, relatively accurate but nonvectorized, using a 16-point angular quadrature formula in the core, and the series given by Adams et al. (1971) in the wings.

Figure 3 shows a comparison of Lyman-α profiles calculated with different redistribution functions: complete redistribution (CR), precise partial redistribution (PR), and the present approximations: APR (0) and APR (1). The CR approximation may overestimate the intensity in the wing by a factor of 5. The two APR are satisfactory in the core and in the wings. APR (0) gives too low intensities in the near wings, with a maximum departure of about 30% near $\Delta\lambda=0.5$ Å. The difference between APR (1) and PR intensities remains lower than 3%.

The times needed to compute the redistribution functions were 33, 0.45 and 0.46 seconds in the PR, APR (0) and APR (1) calculations, respectively. The time needed to solve the radiative transfer equation by the Feautrier method was 0.37 seconds. It should be noted that, in a line profile computation run, the redistribution functions are determined only once, while the radiative transfer routines are called a number of times in order to achieve convergence in the statistical equilibrium equations, so that APR calculations require approximately the same time than CR ones in practice.

In conclusion, the present approximations have the advantage of improving definitely the timing properties of non-LTE, partial redistribution codes using the standard Feautrier method, with only minor changes in the structure of the program. For the future, methods avoiding completely the calculation of redistribution functions, such as that proposed recently by Hubený (1985), seem very promising. But their use will certainly require much more important changes in the computer codes.

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Appendix

```
      SUBROUTINE APGII ( NV, A, V, VP, GII, AUX )
C
C              APGII COMPUTES AN APPROXIMATION FOR :
C                 GII(V,VP) = RII(V,VP) / PHI(VP)
C
      DIMENSION V(NV), GII(NV), AUX(NV)
C
C              APPROXIMATION FOR MILLS'RATIO
C
      GZERO(X) = 1.0 / ( ABS(X) + SQRT ( X**2 + 1.273239545 ) )
C
      DO 100 I = 1, NV
      GII(I) = 0.0
  100 CONTINUE
C
C              SELECT THE USEFUL RANGE FOR V
C
      VMIN = -4.0
```

```
      IF ( VP .GT. 4.0 ) VMIN = VP - 5.0
      VMAX = VP + 5.0
      DO 120 I = 1, NV
      AUX(I) = ABS ( V(I) - VMIN )
  120 CONTINUE
      I1 = ISMIN ( NV, AUX, 1 )
      DO 140 I = 1, NV
      AUX(I) = ABS ( V(I) - VMAX )
  140 CONTINUE
      I2 = ISMIN ( NV, AUX, 1 )
C
      IF ( VP .GT. 4.0 ) GO TO 200
      IF ( VP .GE. 2.0 ) GO TO 300
C
C             LINE CORE REGION
C
      GMAX = GZERO ( VP )
      DO 180 I = I1, I2
      GII(I) = CVMGT ( GMAX, EXP ( VP**2 - V(I)**2 ) * GZERO ( V(I) ),
     *         ABS(V(I)) .LE. VP )
  180 CONTINUE
      RETURN
  200 CONTINUE
C
C             LINE WING REGION
C        ( REMOVE 'C' IN FIRST COLUMN FOR FIRST, OR SECOND, ORDER
C          APPROXIMATION )
C
      DO 220 I = I1, I2
      AUX(I) = ABS ( 0.5*(V(I)-VP) )
      GII(I) = 0.5641895835 * EXP ( - AUX(I)**2 ) * ( 1.0 - 2.0 * AUX(I)
     1         * GZERO ( AUX(I) ) )
C    2         * ( 2.0 - V(I) / VP )
C    2         * ( 2.75 + ( -2.5 + 0.75 * V(I) / VP ) * V(I) / VP )
  220 CONTINUE
      RETURN
  300 CONTINUE
C
C             TRANSITION REGION
C
      PWING = 1.0 / ( 1.772453851 * ( A + VP**2 / A ) * EXP ( - VP**2 )
     *        + 1.0 )
      PCORE = 1.0 - PWING
      GMAX = GZERO ( VP )
      DO 320 I = I1, I2
      GII(I) = CVMGT ( GMAX, EXP ( VP**2 - V(I)**2 ) * GZERO ( V(I) ),
     1         ABS(V(I)) .LE. VP )
      AUX(I) = ABS ( 0.5*(V(I)-VP) )
      AUX(I) = 0.5641895835 * EXP ( - AUX(I)**2 ) * ( 1.0 - 2.0 * AUX(I)
     1         * GZERO ( AUX(I) ) )
C    2         * ( 2.0 - V(I) / VP )
C    2         * ( 2.75 + ( -2.5 + 0.75 * V(I) / VP ) * V(I) / VP )
      GII(I) = PCORE * GII(I) + PWING * AUX(I)
  320 CONTINUE
      RETURN
      END
```

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