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Citation
Ivanov, V. V. (1967). Time variation of the profile of a Doppler broadened resonance line. *Bulletin Of The Astronomical Institutes Of The Netherlands*, *19*, 192. Retrieved from https://hdl.handle.net/1887/5900

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Note: To cite this publication please use the final published version (if applicable).

1967BAN....19..192I

1967, *Bull. Astr. Inst. Netherlands* **19** 192–196; *Communication from the Observatory at Leiden*

TIME VARIATION OF THE PROFILE OF A DOPPLER BROADENED RESONANCE LINE

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Received 9 February 1967

An infinite homogeneous dilute gas is initially excited at $t = 0$. The problem is solved under the assumption of complete redistribution in frequency. FIELD (1959) has solved the same problem using the exact redistribution function. Comparison of the results with those of Field shows that the leading terms of the asymptotic expansions of the solutions at $t \to \infty$ in both cases are the same. This result can be considered a justification of the approximation of complete redistribution.

1. Introduction

Much attention has been given in recent years to problems of line formation under non-LTE conditions (see, e.g., THOMAS and ATHAY, 1961; THOMAS, 1965; AVRETT and HUMMER, 1965). The standard problem is to find the radiation field in a frequency interval of one line only (two-level problem). The usual additional approximation is the assumption of complete redistribution in frequency. Coupled equations of statistical equilibrium and radiative transfer can then be easily solved numerically (AVRETT and HUMMER, 1965; AVRETT, 1965; HEARN, 1963). Sometimes even analytical solutions can be obtained (IVANOV, 1966; NAGIRNER and IVANOV, 1966).

There are three possibilities to check the accuracy of the assumption of complete redistribution. First, one can compare the redistribution functions themselves, as was done, e.g., by THOMAS (1957) and by JEFFERIES and WHITE (1960). Second, one can numerically solve some typical problems using exact and complete redistribution functions, and then compare the results. This approach was used by SOBOLEV (1955b, 1956), HEARN (1964) and most extensively by HUMMER (1964). There is still a third possibility which so far has not been used. One can compare exact analytical solutions found under the assumption of the complete redistribution with those corresponding to the exact redistribution functions. This is the approach used in the present note.

The most difficult point is, of course, to find an analytical solution of a problem of multiple scattering with the exact redistribution function. Fortunately there is such a solution. It was found several years ago by FIELD (1959). The assumptions used by Field are highly restrictive, but it is the price one has to pay to get an exact solution.

The same problem can also be easily solved under the assumption of complete redistribution. Comparison of the results with those of Field shows that the asymptotic expansions of the solutions in both cases have the same leading terms. This result is rather unexpected. Strictly speaking, it is directly applicable only to the particular problem under consideration. Nevertheless it can be useful as an additional justification for applying the approximation of complete redistribution to a much wider class of problems.

2. The problem

Let us consider an infinite homogeneous dilute gas composed of two-level atoms. The ground-state atoms are assumed to have a Maxwellian velocity distribution with temperature T. The only processes of excitation and de-excitation are photo-excitations $1 \to 2$ and downward spontaneous transitions $2 \to 1$. The density of the gas is so low that 1) collisional broadening of the line can be ignored, and 2) the mean free travel time of a quantum with the frequency of the centre of the line is

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large compared to the average life-time of the excited state (A_{21}^{-1}).

Initially all the atoms are in the ground state. At the moment $t = 0$, some part of them (the same at all points) are excited by some non-selective mechanism. Downward transitions $2 \rightarrow 1$ following this initial excitation build up the radiation field. The problem is to find the time variation of the intensity of radiation and of the degree of excitation of the atoms as well as the time evolution of the velocity distribution of the excited atoms.

Assuming the resonance line to have zero natural width, FIELD (1959) has shown that this problem is equivalent to the solution of the equation

$$\frac{\partial J(x, t)}{\partial t} = e^{-x^2} J(x, t) + \int_{-\infty}^{\infty} r(x', x) J(x', t)\, dx' \quad (1)$$

subject to the initial condition

$$J(x, 0) = e^{-x^2}. \quad (2)$$

Here x is the usual reduced frequency [$x = (\nu - \nu_0)/\Delta\nu_D$, where ν_0 is the central frequency of the line and $\Delta\nu_D$ is its Doppler width]; t is the time measured in units of mean free travel time of a quantum with frequency $x = 0$; $J(x, t)$ is the mean intensity of radiation and $r(x', x)$ is the frequency redistribution function. Because of the symmetry of the problem $J(x, t)$ and $r(x', x)$ are independent of position and angles.

Under the conditions specified above the exact redistribution function is (UNNO, 1952; SOBOLEV, 1955a, 1956)

$$r_e(x', x) = \int_{|\bar{x}|}^{\infty} e^{-v^2}\, dv;$$
$$|\bar{x}| = \text{greater of } |x|, |x'|. \quad (3)$$

The corresponding complete redistribution function is

$$r_c(x', x) = \frac{1}{\sqrt{\pi}} e^{-x'^2} e^{-x^2}. \quad (4)$$

Subscripts e and c will be used henceforth to denote quantities corresponding to the exact redistribution law (3) and the complete redistribution approximation (4), respectively.

3. Solution of the equations

Field noticed that the integral operator

$$\int_{-\infty}^{\infty} r_e(x', x) \ldots dx'$$

is the inverse of a differential one

$$\frac{\partial}{\partial x}\left[e^{x^2} \frac{\partial}{\partial x} r_e(x', x)\right] = -\delta(|x'| - |x|),$$

and used this fact to transform the integro-differential equation (1) for $J_e(x, t)$ into a differential equation which can be solved without major difficulties. The result is

$$J_e(x, t) = \frac{1 - \exp(-t\, e^{-x^2})}{t} + 2\int_0^{t\, e^{-x^2}} e^{-u} g\left(\frac{u}{t}\right) du, \quad (5)$$

where

$$g(u) = (\log u^{-1})^{-\frac{1}{2}} \int_0^{(\log u^{-1})^{\frac{1}{2}}} v^2 e^{-v^2}\, dv. \quad (6)$$

In the complete redistribution approximation the basic equation (1) reduces to

$$\frac{\partial J_c(x, t)}{\partial t} = e^{-x^2} J_c(x, t) + e^{-x^2} S_c(t) \quad (7)$$

with

$$S_c(t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2} J_c(x, t)\, dx. \quad (8)$$

The formal solution of (7) satisfying the initial condition (2) is

$$J_c(x, t) = e^{-x^2} \exp(-t\, e^{-x^2}) + $$
$$+ e^{-x^2} \int_0^t \exp[-e^{-x^2}(t - t')] S_c(t')\, dt'. \quad (9)$$

Combining (8) and (9) we obtain an integral equation for $S_c(t)$

$$S_c(t) = M(t) + \int_0^t S_c(t') M(t - t')\, dt', \quad (10)$$

where

$$M(t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-2x^2 - t\, e^{-x^2})\, dx. \quad (11)$$

Therefore, one has to solve integral equation (10) which is of the convolution type. Once $S_c(t)$ is known, the mean intensity $J_c(x, t)$ can be easily found from (9).

Denoting by $\bar{f}(k)$ the Laplace-transform of $f(t)$, we have from (10)

$$\bar{S}_c(k) = [1 - \bar{M}(k)]^{-1} - 1, \quad (12)$$

where

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$$\overline{M}(k) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-2x^2}\,dx}{e^{-x^2}+k} = \frac{1}{\sqrt{\pi}} \int_0^1 \frac{(\log y^{-1})^{-\frac{1}{2}} y\,dy}{y+k}. \tag{13}$$

The problem now is to find the inverse Laplace-transform of $\bar{S}_c(k)$, i.e.,

$$S_c(t) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} \left[\frac{1}{1-\overline{M}(k)} - 1\right] e^{tk}\,dk. \tag{14}$$

The function $[1-\overline{M}(k)]^{-1}-1$ is analytic in the whole complex k-plane cut along $[-1, 0]$. Using the Sohotskii-Plemelj formulae (see, e.g., MUSKHELISHVILI, 1951), we have for $k = -x \pm i0$ $(0 \leqslant x \leqslant 1)$

$$\int_0^1 \frac{(\log y^{-1})^{-\frac{1}{2}} y\,dy}{y+k} = \int_0^1 \frac{(\log y^{-1})^{-\frac{1}{2}} y\,dy}{y-x} \mp i\,\pi (\log x^{-1})^{-\frac{1}{2}} x. \tag{15}$$

The integral on the right-hand side is to be understood as the Cauchy principal value. Deforming the path of integration as shown in figure 1 and using (15) we have, after some algebra,

$$S_c(t) = \frac{1}{\sqrt{\pi}} \int_0^1 \frac{u(\log u^{-1})^{-\frac{1}{2}}}{[I(u)]^2 + \pi u^2 (\log u^{-1})^{-1}} e^{-ut}\,du, \tag{16}$$

where

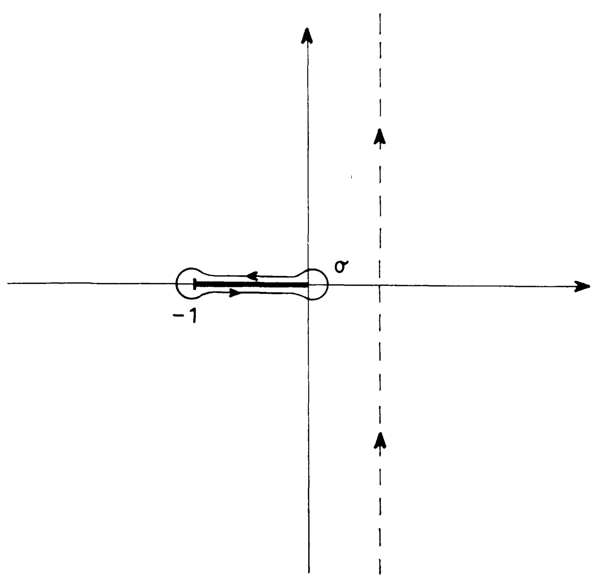

Figure 1. Deformation of integration path to evaluate the integral (14).

$$I(u) = \frac{u}{\sqrt{\pi}} \int_0^1 \frac{(\log y^{-1})^{-\frac{1}{2}}\,dy}{y-u}. \tag{17}$$

This is the final result. An explicit expression for the mean intensity $J_c(x, t)$ can immediately be found from (9). The resulting formula is rather complicated. There is no need to give it here as we shall not use it in the further discussion.

4. Asymptotic behaviour of the solutions

Let us now consider the asymptotic behaviour of the solutions at large t. It is more convenient to study first the complete redistribution case.

If $t \gg 1$, only the contribution of small u is important in the integrand of (16). The problem now is to find the asymptotic expansion of $I(u)$ for $u \to 0$. Using the technique developed by D. I. Nagirner (NAGIRNER and IVANOV, 1966), this can be done without any difficulties. The leading term of the expansion is given by

$$I(u) \sim \frac{2}{\sqrt{\pi}} u (\log u^{-1})^{\frac{1}{2}} \qquad (u \to 0). \tag{18}$$

This means that the second term in the denominator of the integrand of (16) at small u can be neglected. The result is that for $t \gg 1$

$$S_c(t) \sim \frac{\sqrt{\pi}}{4} \int_0^1 e^{-ut} u^{-1} (\log u^{-1})^{-\frac{3}{2}}\,du, \tag{19}$$

or, within the same accuracy,

$$S_c(t) \sim \frac{\sqrt{\pi}}{2} (\log t)^{-\frac{1}{2}} \qquad (t \gg 1). \tag{20}$$

Let us now turn to the mean intensity of the radiation. Following FIELD (1959), we introduce a critical frequency $x_0(t)$ such that

$$t\,e^{-x_0^2} = 1, \qquad x_0 = (\log t)^{\frac{1}{2}}. \tag{21}$$

The asymptotic behaviour of $J(x, t)$ is quite different for $x > x_0$ and for $x < x_0$. If $x > x_0$ one obtains from (9)

$$J_c(x, t) \sim e^{-x^2} \left[1 + \int_0^t S_c(t')\,dt'\right], \tag{22}$$

and, in particular, for large t

$$J_c(x, t) \sim e^{-x^2} \frac{\sqrt{\pi}}{2} t (\log t)^{-\frac{1}{2}} \qquad (t \gg 1, x > x_0). \tag{23}$$

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If $t \gg 1$ but $x < x_0$, one has, in virtue of (9) and (20),

$$J_c(x, t) \sim \frac{\sqrt{\pi}}{2} (\log t)^{-\frac{1}{2}} \qquad (t \gg 1, x < x_0). \quad (24)$$

The behaviour of $J_e(x, t)$ is essentially the same. If $t \gg 1$ and $x > x_0$, it is easy to show, using (5), that

$$J_e(x, t) \sim e^{-x^2} \frac{\sqrt{\pi}}{2 \mid x \mid} t. \quad (25)$$

As x is large, the intensity decreases with x quite steeply. Only the values of $\mid x \mid$ close to x_0 are of physical importance, and we can safely replace $\mid x \mid$ in the last formula by x_0. The result is

$$J_e(x, t) \sim e^{-x^2} \frac{\sqrt{\pi}}{2} t(\log t)^{-\frac{1}{2}}, \quad (26)$$

i.e. the same as (22). It was shown by Field that in the other limiting case ($x < x_0$)

$$J_e(x, t) \sim \frac{\sqrt{\pi}}{2} (\log t)^{-\frac{1}{2}}, \quad (27)$$

and this is again indistinguishable from the corresponding result for complete redistribution. Of course, there are some differences in asymptotic behaviour of $J_e(x, t)$ and $J_c(x, t)$, but the leading terms of the expansions are exactly the same.

The approach to asymptotics is clearly seen on the graphs given by Field which we reproduce here (figure 2).

The function

$$S_e(t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} r_e(x', x) J_e(x', t) \, dx' \quad (28)$$

has the same physical meaning as $S_c(t)$. It is easily seen from (3) that

$$\int_{-\infty}^{\infty} r_e(x', x) \, dx = e^{-x'^2}. \quad (29)$$

Therefore,

$$S_e(t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x'^2} J_e(x', t) \, dx'. \quad (30)$$

At large t only the region with $\mid x' \mid < x_0$ in the integrand is of importance. Using (26) we find

$$S_e(t) \sim \frac{\sqrt{\pi}}{2} (\log t)^{-\frac{1}{2}}. \quad (31)$$

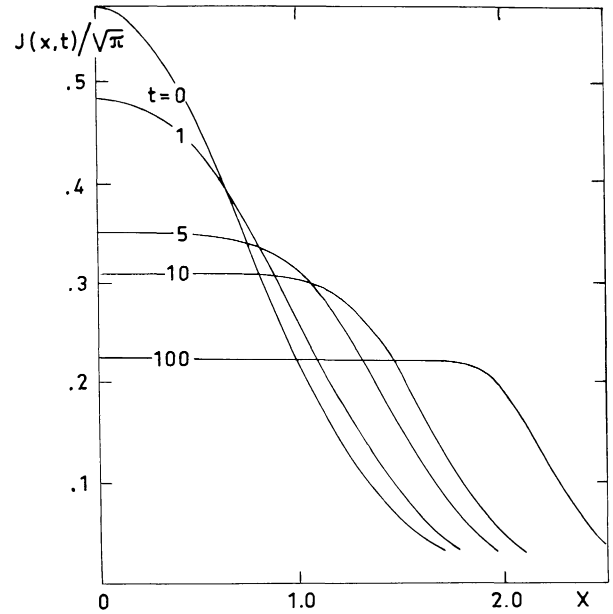

Figure 2. Time variation of the profile of the line (according to FIELD, 1959).

The leading term of the asymptotic expansion of $S_c(t)$ is the same as (31) so that $S_e(t) \approx S_c(t)$ for $t \gg 1$.

5. Physical interpretation of the results

To interpret the results in physical terms let us consider first the physical meaning of the redistribution functions.

Let an elementary gas volume be exposed to monochromatic radiation of frequency x', the intensity of which is independent of direction. The properties of the gas are those specified in section 2. As is well-known, the profile of the line emitted by such a volume element is proportional to $r(x', x)$ as a function of x. In the complete redistribution approximation the profile is of a Doppler type, while for the exact redistribution function (3) it is flat for $\mid x \mid < \mid x' \mid$ and steeply decreases for $\mid x \mid > \mid x' \mid$.

Under the assumptions made above, the profile of the emission line directly reflects the velocity distribution of excited atoms. The complete redistribution approximation is equivalent to the a priori assumption that this distribution is always Maxwellian. In our case it is a rather artificial assumption, as there is no physical mechanism (say, elastic collisions) to establish such a distribution.

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The exact redistribution function $r_e(x', x)$ as a function of x gives essentially the distribution of projected velocities of excited atoms on the line of sight. It can be shown that the corresponding distribution function of the velocities themselves is

$$dn_2 = \begin{cases} 0, & \text{if } \quad v < v', \\ n_2 \dfrac{m}{kT} \exp\left[-\dfrac{m(v^2 - v'^2)}{2kT}\right] v\,dv, & \text{if } \quad v > v', \end{cases} \quad (32)$$

with

$$v' = \frac{c}{\nu_0} \mid \nu' - \nu_0 \mid . \quad (33)$$

Here n_2 is the population of the upper level, dn_2 is the number of excited atoms with velocities $(v, v+dv)$ per cm^3, ν_0 is the central frequency of the line and ν' is the frequency of the exciting radiation ($\nu' = \nu_0 - x'\Delta\nu_D$). The reason why there are no atoms with $v < v'$ is quite clear: for low-velocity ground-state atoms Doppler shifts are too small to make these atoms capable of absorbing radiation of frequency ν'.

The velocity distribution (32) is quite different from a Maxwell distribution, i.e. the complete redistribution approximation seems to be rather crude. Nevertheless it works, and works really well, as we have seen in the preceding section.

The reason for this is evident. Strong deviations from a Maxwell distribution occur only if the frequency distribution of the exciting radiation is far from homogeneous. Indeed, if J were independent of frequency $[J(x, t) = J_0(t)]$, then

$$S_e(x, t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} r_e(x', x) J(x', t)\, dx' =$$

$$= J_0(t) \int_{-\infty}^{\infty} r_e(x', x)\, dx' = J_0(t)\, e^{-x^2}. \quad (34)$$

From the physical meaning of $r_e(x', x)$, the quantity $S_e(x, t)$ is proportional to the number of excited atoms with projected velocity $v_z = x(2kT/m)^{\frac{1}{2}}$. Hence (34) indicates that in this case excited atoms do have a Maxwell distribution.

The results of Field quoted above show that, as time goes on, the profile of the line becomes more and more flat. The flattening of the profile causes the velocity distribution of excited atoms to approach a Maxwell distribution. And this, in turn, justifies the assumption of complete redistribution.

The functions $S(t)$ are integrals of $S(x, t)$ over x, i.e. over v_z, and therefore are proportional to the population of the upper level. The physics behind equations (20) and (31) is that the profile of the line becomes wider as it evolves. This means that the ability of radiation to excite atoms becomes smaller, and this is the physical reason for the decrease in excitation.

The problem we have discussed is rather artificial. Nevertheless, as was shown by Field, the results obtained for time evolution of a radiation field can be applied (at least qualitatively) to much more realistic problems of multiple scattering in coordinate space.

Acknowledgements

The results reported here were obtained during the author's stay at Leiden in accordance with the program of cultural exchange between the Soviet Union and the Netherlands. I am indebted to the staff of the Leiden Observatory and, in particular, to Professors J. H. Oort and P. Th. Oosterhoff for their hospitality. Thanks are also due to Professor H. C. van de Hulst for stimulating discussion on radiative transfer problems and to Professor R. Gross for reading the manuscript.

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