



Contents lists available at SciVerse ScienceDirect

# Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: [www.elsevier.com/locate/jqsrt](http://www.elsevier.com/locate/jqsrt)

## Notes

# On one-dimensional velocity approximation for speed-dependent spectral line profiles



V.P. Kochanov\*

Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics, Siberian Branch, Russian Academy of Sciences, 1, Academician Zuev Square, 634021 Tomsk, Russia

## ARTICLE INFO

### Article history:

Received 26 November 2012

Received in revised form

8 February 2013

Accepted 11 February 2013

Available online 27 February 2013

### Keywords:

Speed-dependence

One-dimensional velocity approach

Approximate line profiles

## ABSTRACT

An application of one-dimensional velocity approach to calculation of speed-dependent spectral line profiles was considered. It was shown that a mean deviation of the line profile obtained within this approach from the line profile derived with integrating over three projections of an absorbing molecule's velocity does not exceed 1.1% at mass ratios of perturbing and absorbing molecules  $\leq 9$ . Analytical approximate expressions for speed-dependent line profiles, including spectral line narrowing and mixing, were obtained for one- and three-dimensional velocity approaches.

© 2013 Published by Elsevier Ltd.

## 1. Introduction

Quantitative spectroscopic data processing assumes the use of model line profiles including most essential physical factors of their forming. One of the conventional profiles is the speed-dependent line profile in the hard velocity-changing collisions model (e.g., see Refs. [1,2] and review of the problem therein). In this paper, we shall consider one of the aspects of a derivation of the speed-dependent line profiles on the basis of the one-dimensional velocity approach [3–9]. The essence of it is as follows.

Quantum kinetic equations for density matrix include three-dimensional (3D) velocity vectors, and the expression for a spectral line profile obtained from these equations implies averaging over velocities of light-absorbing molecules. In the case of speed-independent collision relaxation constants, this averaging reduces to the averaging over the only component of a velocity, which is parallel to a light wave vector. Thus, the problem becomes one-dimensional. In a general case of speed-dependent

relaxation constants, a line profile is more complicated due to the necessity to carry out the averaging over all three components of the velocity. This circumstance hampers analytical and especially numerical calculations of a line profile. To avoid this difficulty, the one-dimensional approach was proposed in Refs. [3–9] which consists in preliminary averaging of master equations over projections of a velocity perpendicular to a wave vector under supposition that the elements of a density matrix are products of two factors depending on longitudinal and transversal components of velocity. Of course, such approach encloses some systematic errors, at present being not quite definite. In particular, this approach was used in derivation of speed-dependent line profiles [10,11]. But the final expressions for the line profiles in Refs. [10,11] are obtained in a rough approximation where the averaging of relaxation constants over transversal components of velocity is neglected. This leads to distortion of manifestations of the wind effect (the dependence of relaxation constants on speed of absorbing molecules). Namely, calculations based on a further content of this paper show that maximal amplitude of the line profiles [10,11] exceeds a true one from 10% to 40% depending on the mass ratio of perturbing and absorbing molecules.

\* Fax: +7 3822 492086.

E-mail address: [koch@iao.ru](mailto:koch@iao.ru)

The goals of this paper are to derive a correct 3D-line profile; to improve the variant of 1D-approximation used in Refs. [10,11]; to estimate systematic errors inherent in the 1D-approach; and to develop analytical approximation for a 3D-line profile for the sake of its rapid computation.

## 2. 3D-line profile

The equation for density matrix in the hard velocity-changing collisions model, which determines a profile of a single spectral line, is [10]

$$[v(v) - i(\Omega - \mathbf{k}\mathbf{v})]R(\mathbf{v}) - \tilde{v}(v)W(v) \int R(\mathbf{v}')d\mathbf{v}' = iVn_0W(v);$$

$$\Omega = \omega - \omega_0, \quad W(v) = \exp(-v^2/\bar{v}^2)/(\pi^{3/2}\bar{v}^3), \quad \bar{v} = \sqrt{2k_B T/m_a}, \quad V = dE/(2\hbar). \quad (1)$$

Here  $R(\mathbf{v})$  is a constant part of a transition polarization (i.e., normalized light-induced dipole moment);  $v$  and  $\tilde{v}$  are the speed-dependent output and input frequencies of collision integral [3,4], respectively;  $\omega$  and  $\omega_0$  are the current frequency and the frequency of a line center, respectively;  $\mathbf{k}$  is the wave vector;  $\mathbf{v}$  is the velocity of an active molecule;  $V$  is the Rabi frequency;  $n_0$  is the equilibrium population difference;  $d$  is the matrix element of a dipole moment;  $E$  is the amplitude of the electric field of a light wave;  $k_B$  is the Boltzmann constant;  $T$  is the gas temperature;  $m_a$  is a mass of the absorbing molecule; and  $\hbar$  is the Planck constant. Radiative decay constants in Eq. (1) are omitted.

The absorption coefficient expresses via the solution of Eq. (1) as

$$K(\omega) = \frac{8\pi Nd\omega}{cE} \text{Im} \int R(\mathbf{v})d\mathbf{v}, \quad (2)$$

where  $N$  is the density of the active molecules and  $c$  is the light speed.

The commonly used dependence of collision relaxation constants on speed derived for the intermolecular interaction potential  $U(r) = -C/r^n$ , where  $r$  is the distance between colliding molecules and  $C$  is the constant of an intermolecular interaction, is [12,13,1,2,10]

$$v(v)/v_0 = \tilde{v}(v)/\tilde{v}_0 \equiv \varphi(s, \beta) = \Phi\left(-\frac{1}{2} + \frac{1}{n-1}, \frac{3}{2}, -\beta s\right);$$

$$s = v^2/\bar{v}^2, \quad \beta = m_b/m_a, \quad v_0 = v(0), \quad \tilde{v}_0 = \tilde{v}(0), \quad (3)$$

where  $m_b$  is the mass of a perturbing molecule and  $\Phi(a, b, z)$  is the confluent hypergeometric function [14]. The relationships of the output and input collision frequencies chosen in Eq. (3) as frequencies at zero speed with the respective frequencies averaged over velocity are the same as the relationship for homogeneous line half-widths  $\Gamma$  and  $\gamma$  [10,11]:  $\Gamma = (1 + \beta)^{-(1/2) + (1/n-1)}\gamma$ , where  $\Gamma$  is the half-width at  $v=0$  and  $\gamma$  is the respective quantity averaged over the velocity ( $\Gamma < \gamma$  for  $n > 3$ ).

Solution of Eq. (1) with integrating over the velocity carried out in the spherical coordinate system gives the sought for 3D-line profile

$$K(\Omega) = \frac{S}{\pi^{3/2}k\bar{v}} \text{Im} \frac{\mathcal{J}_1(\Omega, v_0, \beta)}{1 + i\tilde{v}_0\mathcal{J}_2(\Omega, v_0, \beta)/(\sqrt{\pi}k\bar{v})};$$

$$\mathcal{J}_1(\Omega, v_0, \beta) = \int_0^\infty e^{-s} \log\left(1 - \frac{2k\bar{v}\sqrt{s}}{\Omega + i\tilde{v}_0\varphi(s, \beta) + k\bar{v}\sqrt{s}}\right) ds,$$

$$\mathcal{J}_2(\Omega, v_0, \beta) = \int_0^\infty \varphi(s, \beta) e^{-s} \log\left(1 - \frac{2k\bar{v}\sqrt{s}}{\Omega + i\tilde{v}_0\varphi(s, \beta) + k\bar{v}\sqrt{s}}\right) ds;$$

$$S = 4\pi^2 N n_0 d^2 \omega / (c\hbar) \quad (4)$$

where  $S$  is the line intensity.

In the absence of collision line narrowing,  $\tilde{v}_0 = 0$ , the line profile  $K(\Omega)$  Eq. (4) reduces to the following expression:

$$K_{SDV}(\Omega) = \frac{S}{\pi^{3/2}k\bar{v}} \int_0^\infty e^{-s} \tan^{-1} \frac{2\sqrt{s}\Gamma'_\beta k\bar{v} ds;}{(\Omega - \Gamma'_\beta)^2 + \Gamma'_\beta{}^2 - s(k\bar{v})^2}$$

$$\Gamma'_\beta + i\Gamma''_\beta = (v_0 - \tilde{v}_0)\varphi(s, \beta), \quad (5)$$

which coincides with the speed-dependent Voigt profile [12], taking into account the relationships [14]

$$\log(x + iy) = \frac{1}{2} \log(x^2 + y^2) + i \tan^{-1}(y/x), \quad \tan^{-1}(y/x)$$

$$= \pi/2 - \tan^{-1}(x/y),$$

where  $\tan^{-1}(y/x)$  is defined in all the planes of variables  $x$  and  $y$ , i.e. it is understood as  $\arg(x + iy)$ .

From Eq. (4) it follows that the related integrals  $\mathcal{K}$  and  $\mathcal{L}$  in Refs. [10,11] must be replaced by  $-i\mathcal{J}_1/\pi$  and  $-i\mathcal{J}_2/\pi$ , respectively. That gives the transition to the 3D-approach. The alternative manner of improving line profiles [10,11] within the 1D-approach is described in Section 3.

In the case of  $M$  mixed lines the line profile can be obtained from Eq. (4) in the same manner that was used in Ref. [10] in the derivation of a general line profile (Eq. (22) in Ref. [10] and Eq. (1) in Ref. [11]):

$$K_M(\omega) = \frac{1}{\pi^{3/2}} \text{Im} \sum_{m=1}^M \frac{S_m}{k_m \bar{v}} U(\Omega_m, v_{m0}) / \left[ 1 + \frac{i}{\sqrt{\pi}} \sum_{\substack{l=1 \\ l \neq m}}^M \frac{\zeta_l}{k_l \bar{v}} U(\Omega_l, v_{l0}) \right];$$

$$U(\Omega_m, v_{m0}) = \frac{\mathcal{J}_1(\Omega_m, v_{m0})}{1 + i[\tilde{v}_{m0}\mathcal{J}_2(\Omega_m, v_{m0}) - \zeta_m \mathcal{J}_1(\Omega_m, v_{m0})]/(\sqrt{\pi}k_m \bar{v})},$$

$$\Omega_m = \omega - \omega_{m0}, \quad k_m \approx \omega_{m0}/c. \quad (6)$$

Here the indices  $m$  and  $l$  denote spectral lines,  $S_m$  and  $\omega_{m0}$  are the line intensities and centers, respectively, and  $\zeta_m$  are the cross-relaxation (line mixing) parameters defined in Ref. [10].

For dispersion intermolecular interaction with  $n=6$ , formulas for rapid approximate calculation of the integrals  $\mathcal{J}_1$  and  $\mathcal{J}_2$  and hence the line profiles Eqs. (4) and (6) are presented in Appendix A.

The relative mean quadratic deviation of the approximate line profile  $K_{appr}(\Omega)$  calculated with formulas given in Appendix A from the exact line profile Eq. (4),

$$\sigma = \sqrt{\sum_{j=1}^J [K(\Omega_j) - K_{appr}(\Omega_j)]^2 / (J-1) / K(\Omega)}, \quad (7)$$

is presented in Fig. 1. The time required for calculating  $K_{appr}(\Omega)$  is 6 times shorter than the time of calculating the approximate line profile [11].

Download English Version:

<https://daneshyari.com/en/article/5428726>

Download Persian Version:

<https://daneshyari.com/article/5428726>

[Daneshyari.com](https://daneshyari.com)