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NOTE on the two possible formulations of the Hartmann-Tran line profile

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Abstract: This short note corrects an error made in the *errata* that followed the original papers presenting the so-called Hartmann-Tran profile and some software to compute it.

In 2013, the authors of this Note co-proposed a refined isolated-line shape [1] that goes beyond the Voigt profile by taking into account the effects of the speed dependences of the pressure broadening and shifting (within the quadratic model) and those of the collision-induced translational velocity changes (within the hard collision model) as well as that of the correlation between the changes of the rotational and translational motions. Due to its advantages [1], this model was recommended [2] as a reference line shape for high resolution spectroscopy. It is commonly called “Hartmann-Tran (HT)” profile and has been widely used recently, together with a software [3] for its calculation, (e.g. Sec. 4.1 of [4]). In early 2014, an *erratum* was made [5] to the model of Ref. [1], with an associated *erratum* [6] for the software described in [3]. The reason invoked for these *errata* was that we thought that the original formulation was wrong because the Fourier transform (FT) of the dipole auto-correlation function was made using $\exp(-i\omega t)$ instead of $\exp(+i\omega t)$. We recently found out that this statement is wrong, because choosing $\exp(-i\omega t)$ or $\exp(+i\omega t)$ is only a convention issue, and that an error was made in the *erratum* concerning the sign of the first order line-mixing contribution. The aim of this Note is to clarify the situation and to demonstrate that both Fourier transform choices lead to the same results if properly handled.

Original HTP model [1]: FT using $\exp(-i\omega t)$

For simplicity, let us disregard the Doppler effect, the pressure induced line-shift, the speed dependences of the collisional terms, and the changes of the molecule translational velocities (no Dicke effect). Within this frame, Eq. (A5) of [1] becomes:

$$G(\omega) = \frac{1}{i(\omega - \omega_0) + \Gamma} \quad \text{and} \quad H(\omega) = 0, \quad (1)$$

with ω_0 the line-center position and Γ the Lorentz HWHM. The area-normalized absorption coefficient given in Eq. (9) of [1] then becomes:

$$\alpha(\omega) = \frac{1}{\pi} \text{Re}[(1 + iY)G(\omega)], \quad (2)$$

where Y is the first order line-mixing coefficient introduced by Rosenkranz [7]. Assuming that Y is a real quantity, one has:

$$\alpha(\omega) = \frac{1}{\pi} \frac{[\Gamma + (\omega - \omega_0)Y]}{(\omega - \omega_0)^2 + \Gamma^2}. \quad (3)$$

which is identical to Eq. (2) of [7]. Let us now turn to the real part $n(\omega) - 1$ of the refractive index and define it as plus (+) the imaginary part of $(1 + iY)G(\omega)$. This leads to:

$$n(\omega) - 1 = \frac{1}{\pi} \text{Im}[(1 + iY)G(\omega)] = \frac{1}{\pi} \frac{[\omega_0 - \omega + Y\Gamma]}{(\omega - \omega_0)^2 + \Gamma^2}. \quad (4)$$

In the absence of line mixing ($Y=0$), $n(\omega) - 1$ is thus positive for $\omega < \omega_0$ and negative for $\omega > \omega_0$, as it should be (e.g. [8,9]).

HTP model after the *erratum* [5]: FT using $\exp(+i\omega t)$]

Within the assumptions made above, switching from using $\exp(-i\omega t)$ to using $\exp(+i\omega t)$ in the FT, and taking into account that the dipole auto-correlation function $\Phi(t)$ verifies $\Phi(-t) = \Phi(t)^*$, leads to replacing the transform and expressions derived from it with their complex conjugates. Equation (A5) of [1] and Eq. (1) above then become:

$$G(\omega) = \frac{1}{-i(\omega - \omega_0) + \Gamma} \quad \text{and} \quad H(\omega) = 0 . \quad (5)$$

By the same reasoning, Eq. (9) of [1] and Eq. (2) above become:

$$\alpha(\omega) = \frac{1}{\pi} \text{Re}[(1 - iY)G(\omega)], \quad (6)$$

i.e.:

$$\alpha(\omega) = \frac{1}{\pi} \frac{[\Gamma + (\omega - \omega_0)Y]}{(\omega - \omega_0)^2 + \Gamma^2}, \quad (7)$$

which is identical to Eq. (3) so that both FT approaches are consistent. Contrary to what was stated in [5], **$+i$ should be replaced by $-i$** also in Eq. (9) of [1] [i.e. as in Eq. (6) above].

For the dispersion term and real part $n(\omega) - 1$ of the refractive index, we now define it as minus ($-$) the imaginary part of $(1 - iY)G(\omega)$, which leads to:

$$n(\omega) - 1 = \frac{-1}{\pi} \text{Im}[(1 - iY)G(\omega)] = \frac{1}{\pi} \frac{[\omega_0 - \omega + Y\Gamma]}{(\omega - \omega_0)^2 + \Gamma^2}, \quad (8)$$

which is identical to Eq. (4).

Conclusion

Contrary to what was stated in the *erratum* [5]:

- (i) The equations given in the original HTP paper [1] are correct, provided that the absorption coefficient is computed from the real part of $[(1 + iY)G(\omega)]/[1 - H(\omega)]$ and the dispersion $n(\omega) - 1$ from plus the imaginary part of $[(1 + iY)G(\omega)]/[1 - H(\omega)]$ with Rosenkranz's definition of the Y coefficient [7].
- (ii) The statement made in the *erratum* [5] that the FT was made in [1] using $\exp(-i\omega t)$ was a wrong choice was not correct since either choice of FT can be made.
- (iii) The changes made in the *erratum* correspond to making a FT using $\exp(+i\omega t)$. Within this frame the absorption coefficient must be computed from the real part of $[(1 - iY)G(\omega)]/[1 - H(\omega)]$ **instead of** $[(1 + iY)G(\omega)]/[1 - H(\omega)]$, and the dispersion $n(\omega) - 1$ must be computed from minus the imaginary part of $[(1 - iY)G(\omega)]/[1 - H(\omega)]$, where the line-mixing coefficient Y is that given by Rosenkranz's definition. In other words, the statement made in [5] that "The complex number $i = \sqrt{-1}$ should not be replaced by $-i$ in Eq. (9) of [1]" was wrong.
- (iv) Provided that these elements are taken into account, both approaches (and the associated software of [3] and [6]) lead to exactly the same results.

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