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An adaptive gaussian quadrature for the Voigt function

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We evaluate an adaptive gaussian quadrature integration scheme that will be suitable for the numerical evaluation of generalized redistribution in frequency functions. The latter are indispensable ingredients for "full non–LTE" radiation transfer computations i.e., assuming potential deviations of the velocity distribution of massive particles from the usual Maxwell–Boltzmann distribution. A first validation is made with computations of the usual Voigt profile.

I. INTRODUCTION

Radiation transfer is, by essence, a difficult problem (e.g., Rutily & Chevallier 2006), as well as a question of very large relevance in astrophysics. It relies indeed on *complex* non-linear light–matter interactions (see e.g., Hubeny & Mihalas 2014, Rutten 2003).

At the very heart of the problem lays the issue of how photons may scatter on these *moving* massive particles constituting the atmosphere under study. The usual literature classify these processes as, either "complete" redistribution in frequency (CRD), or "partial" redistribution in frequency (PRD; see e.g., §10 of Hubeny & Mihalas 2014). The vast majority of astrophysical problems are solved, still, within the frame of CRD, for which further simplifications are the equality of emission and absorption profiles – the latter being also usually known *a priori* –, which also leads to the independence of the so-called source function vs. frequency.

Besides, and more generally, while non-equilibrium distributions of photons i.e., potential departures from the Planck law, have been routinely considered since the late 60's, a very limited number of studies tried to push further the description of the physical problem, by questioning *to what extent the most often assumed Maxwell–Boltzmann velocity distribution of the massive particles onto which photons scatter may remain valid* (see e.g., Oxenius & Simmonneau 1994, and references therein).

Non-maxwellian velocity distributions functions (hereafter vdf) have been studied (e.g., Scudder 1992 and further citations) or evidenced in *natural* plasma (see e.g., Jeffrey et al. 2017 for a recent study about solar flares). Such departures from Maxwell–Boltzmann vdf's have also been considered in the radiative modelling of spectral lines formed in neutral planetary exospheres (e.g., Chaufray & Leblanc 2013), where these authors introduced so-called κ vdf's into their photon scattering physical model.

However, such non-maxwellian vdf's are still known *ab initio* before solving the radiation transfer problem. The more general issue of computing *self-consistent* non-equilibrium distributions for both photons and massive particles – whose associated problem we coin "full non–LTE radiation transfer" – remains a quite open question in astrophysics, although a few studies have already been conducted in the past (see e.g., Borsenberger et al. 1986, 1987).

Hereafter, we provide a first numerical tool that will allow us to go further in this direction, enabling further computations of *generalized* redistribution functions. Moreover the numerical scheme we evaluated may also be of more general interest, for other topics of numerical (astro)physics.

II. REDISTRIBUTION IN FREQUENCY

As an illustrative but important example, we shall focus here on the case of coherent scattering in the *atomic* frame of reference, for a spectral line of central wavelength ν_0. We shall also assume that only "natural" broadening is at play for the upper energy level of, typically, a resonance line with an infinitely sharp lower level.

Therefore, we shall consider an elementary *frequency* redistribution function $r(\xi', \xi)$ such that:

$$r(\xi', \xi) = \varphi(\xi')\delta(\xi' - \xi)\,, \tag{1}$$

where ξ' and ξ are, respectively, the incoming and the outgoing frequencies of a photon, and δ is the usual Dirac distribution, together with:

$$\varphi(\xi') = \left(\frac{\Gamma}{\pi}\right) \frac{1}{(\xi' - \nu_0)^2 + \Gamma^2}\,. \tag{2}$$

The latter is a *Lorentzian* profile, with damping parameter Γ, resulting from the "natural width" of the upper atomic state of the transition at ν_0.

If we assume that the *angular* redistribution associated with the scattering event is *isotropic*, such a case of radiation damping and coherence in the atom's frame refers to the standard case "II-A" in the nomenclature of Hummer (1962; see also Hubeny & Mihalas 2014).

Once the elementary scaterring process have been defined in the atomic frame of reference, we have to consider for a further practical implementation into a radiative transfer problem, the collective effects induced by the agitation of a pool of massive particles populating the atmosphere. This is precisely in this "jump" to the observer's frame of reference, because of Doppler shifts such as:

$$\nu = \xi + \frac{\nu_0}{c}\vec{n}.\vec{v}\,, \tag{3}$$

where ν is the observed frequency, $\vec{n}$ may be either the incoming or the outgoing direction of a photon, and $\vec{v}$ the velocity of the massive particle onto which the scattering takes place, that some assumption has to be made about the vdf of the massive atoms (or molecules) present in an atmosphere, under given physical conditions.

Detailed derivations of R_{II-A} can be found in the classical literature about redistribution functions, from Henyey (1940)[5] to Hummer (1962). Standard redistribution functions have been first derived assuming that the vdf of the atoms scattering light is a Maxwell–Boltzmann distribution. Then, but more generally, any macroscopic redistribution function in the observer's frame suitable for implementation into the numerical radiative transfer problem will result from the further integration along each velocity components u_i (hereafter normalized to the most probable velocity $v_{\rm th.} = \sqrt{2kT/m}$) characterizing the movement of the scattering atoms and, therefore considering these changes of frequencies due to the associated Doppler shifts as expressed by Eq. (3). The latter phenomenon is usually refered to as Doppler, or *thermal* broadening.

III. THE NUMERICAL PROBLEM

We aim at generalizing computations of redistribution functions in order to be able to compute vdf's self-consistently with the radiation field. Therefore we need a *robust* numerical approach to repeatedly perform numerical integrations like:

$$H_1(x', x, \gamma) = \int_{-\infty}^{+\infty} \frac{f(u_1)du_1}{[(\frac{x+x'}{2})\sec(\gamma/2) - u_1]^2 + [\frac{a}{\Delta\nu_D}\sec(\gamma/2)]^2}\,, \tag{4}$$

where x' and x are the usual incoming and outgoing *reduced*[15] frequencies in the observer's frame, $\Delta\nu_D$ the Doppler width defined as $(\nu_0/c)v_{\rm th.}$, and γ the diffusion angle between incoming and outgoing directions in the plane defined by u_1 and u_2. For the Maxwell–Boltzmann case, we should indeed use:

$$f(u_1) = \frac{1}{\sqrt{\pi}}e^{-u_1^2}\,, \tag{5}$$

but we shall need to consider $f(u_1)$ to be $non-$analytic, and, at first, (slightly) departing from the maxwellian standard vdf. Indeed, physical conditions leading to small departures from a Gaussian vdf have already been identified and discussed by Oxenius (1986), and they would correspond to a non–LTE gas of moderate optical thickness. Note also that, for a preliminary study, we shall assume a self-consistent vdf solution of the problem that may still be decomposed as $f_1(u_1)f_2(u_2)f_3(u_3)$.

However, before exploring potential departures from gaussianity, we need to adopt a robust enough numerical strategy in order to numerically evaluate integrals such as Eq. (4), a task which is notoriously difficult even with Maxwell–Boltzmann fdv's. It is very easy to verify that, for instance a standard Gauss–Hermite (GH) quadrature, even at high rank k, fails at computing properly a somewhat simpler expression like the Voigt[20] function given in Eq. (13). We display in Fig. (1) the comparison between a GH integration and the new numerical scheme which is presented hereafter.

IV. ADAPTIVE GAUSSIAN QUADRATURE

We shall start following the scheme proposed by Liu & Pierce (1994), which is based on the classical Gauss–Hermite (GH) quadrature. The latter is indeed suitable for integrations of the kind:

$$I = \int_{-\infty}^{+\infty} f(y)e^{-y^2}dy\,. \tag{6}$$

Then the GH quadrature is such that:

$$\int_{-\infty}^{+\infty} f(y)e^{-y^2}dy \simeq \sum_{i=1}^{k} w_i f(y_i) \tag{7}$$

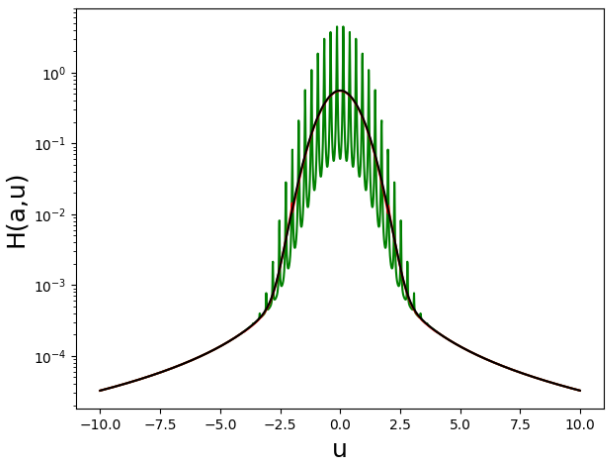

FIG. 1. The failure of a standard Gauss–Hermite quadrature of order $k = 70$ (green), as compared to the almost superimposed results from, respectively, the method using the Faddeeva complex function (dark) and our alternative double adaptive Gaussian quadrature scheme, for a normalized Voigt profile with $a = 10^{-2}$.

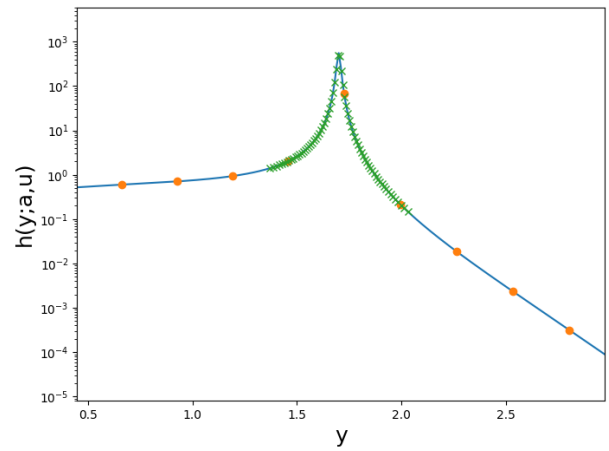

FIG. 2. Example of distribution of nodes for an initial Gauss-Hermite quadrature of order $k = 70$ (dots), and for our adaptive Gaussian quadrature centered at the Lorentzian peak (crosses).

where the nodes y_i are the zeros of the k-th order Hermite polynomial, and w_i the corresponding weights. Tabulated values of both nodes and weights can be found very easily, and they are also available for various programming language. We shall use `numpy`'s (Oliphant 2006) function `polynomial.hermite.hermgauss`, and a GH of order $k = 70$ for all results presented hereafter.

The main drawback of such a standard quadrature is that function f shall be scanned at the very nodes y_i *irrespectively from* the range where it may have its most significant variations.

However, Liu & Pierce (1994) proposed that, should a function g to be integrated, one may define:

$$h(y) = \frac{g(y)}{\mathcal{N}(y;\hat{\mu},\hat{\sigma})}\,, \tag{8}$$

where $\mathcal{N}$ is the usual Gaussian function:

$$\mathcal{N}(y;\hat{\mu},\hat{\sigma}) = \frac{1}{\hat{\sigma}\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{y-\hat{\mu}}{\hat{\sigma}}\right)^2}\,, \tag{9}$$

so that one can write:

$$\int_{-\infty}^{+\infty} g(y)dy = \int_{-\infty}^{+\infty} h(y)\mathcal{N}(y;\hat{\mu},\hat{\sigma})dy\,, \tag{10}$$

and, finally:

$$\int_{-\infty}^{+\infty} g(y)dy \simeq \sum_{i=1}^{k} \frac{w_i}{\sqrt{\pi}} h(\hat{\mu} + \sqrt{2}\hat{\sigma}y_i)\,. \tag{11}$$

This adaptive Gaussian quadrature scheme (AGQ) allows to use the original nodes and weights of the GH quadrature, but somewhat *zooms in* these domains where function g has its most significant variations.

The choice of $\hat{\mu}$ and $\hat{\sigma}$ is of importance. Liu & Pierce (1994) suggested to adopt $\hat{\mu}$ to be the mode of g, and $\hat{\sigma} = 1/\sqrt{j}$, where:

$$j = -\frac{\partial^2}{\partial y^2} \log g(\hat{\mu})\,. \tag{12}$$

We shall come back on this choice in the following section, and show that a somewhat larger $\hat{\sigma}$ value is more suitable for the special case of the Voigt profile.

V. AGQ TESTS WITH THE VOIGT FUNCTION

Let us consider the *normalized* Voigt function hereafter defined as:

$$H(a,u) = \frac{1}{\sqrt{\pi}}\left(\frac{a}{\pi}\right)\int_{-\infty}^{+\infty} \frac{e^{-y^2}dy}{(u-y)^2 + a^2}\,, \tag{13}$$

and which satisfies to:

$$\int_{-\infty}^{+\infty} H(a,u)du = 1\,. \tag{14}$$

Note that several authors use H for the Voigt profile normalized to $\sqrt{\pi}$, but U instead of our H normalized to unity though (see e.g., Hubeny & Mihalas 2014, their §8). We shall also use $h(y;a,u)$ for the integrand of Eq. (13).

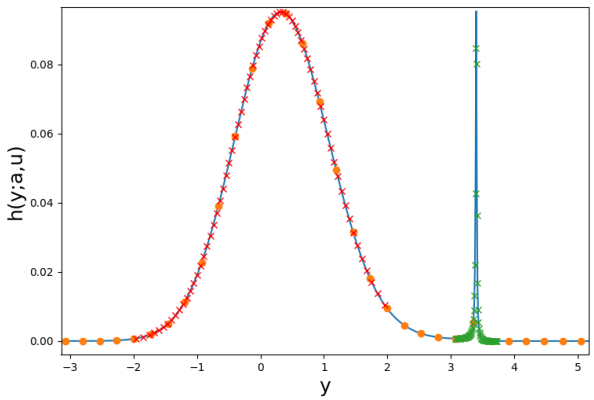

FIG. 3. Respective distributions of nodes, marked by crosses of different colors, from an initial Gauss-Hermite quadrature of order $k = 70$ when the Gaussian and Lorentzian peaks are of comparable amplitude, here for u around 3.

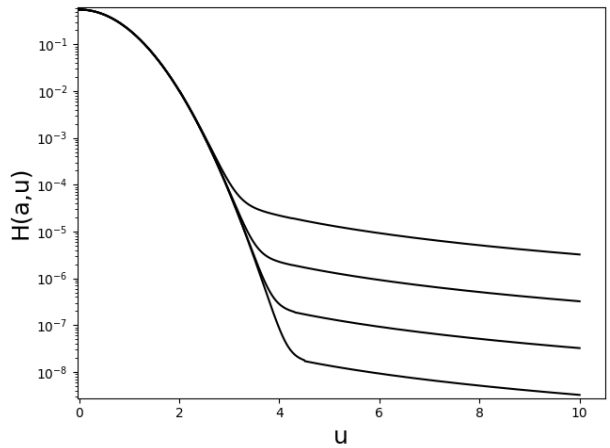

FIG. 4. Voigt profiles $H(a, u)$ computed with our double AGQ scheme for, respectively, $a = 0.001$, 10^{-4}, 10^{-5} and 10^{-6} (and decreasing wing values). Small discontinuities are still noticeable at the transitions values about 2 and 4. This should however not impair any standard scattering integral computation.

For this numerical integration, three main regimes should be considered, depending on the values of u i.e., according to the respective amplitudes of the Gaussian and the Lorentzian components of the integrand. For the line core region such that $|u| < 2$, we use a slightly modified AGQ, for which we use a value of $\hat{\sigma}$ larger than the one suggested in the original article of Liu & Pierce (1994). We display in Fig. (2) the new quadrature nodes, marked with crosses, centered at the Lorentzian peak located at $y \approx 1.7$, and using $3\hat{\sigma}$ instead of the value suggested in the original prescription of Liu & Pierce (1994). The nodes of the standard GH quadrature (at the *same* order) are displayed as dots. They extend too far away, clearly "miss" the large amplitude Lorentzian peak and therefore the dominant contribution to the integral.

Second, we perform a *double* AGQ scheme for the near wing regions such that $2 < |u| < 4$, and for which two discernable peaks of *comparable* amplitudes result from, respectively, the Lorentzian and the Gaussian components of the convolution (we shall hereafter refer to u_2 and u_4 for these two boundary values). In such a case, we use both the centering and integration range controls provided by the original AGQ for evaluating *separately* the contribution from each component of the integrand. For the Lorentzian component we therefore do as when $|u| < 2$, but *we add* to this part of the integral the contribution of the nearby Gaussian peak using *another* AGQ centered at 0, and of specific $\hat{\sigma}_G$ obviously adapted to the width of the known Gaussian component of the integrand (also, overlap with the nearby Lorentzian component should be avoided). The two distincts sets of nodes, based on the same original GH quadrature nodes, at same order, are displayed by crosses of different colors in Fig. (3).

Finally, for the far wing where $|u| > u_4$, and when the Lorentzian peaks fade out, the *usual* Gauss–Hermite quadrature is satisfactory.

Results using our double AGQ quadrature scheme are displayed in Fig. (4), for different values of a ranging from 0.01 to 10^{-4}, more likely regimes expected for our next computations. Maximum relative errors computations using the Faddeeva function method as a benchmark, and the `scipy.special.wofz` Python function, are at most of a few percents, as displayed in Fig. (5); note also that the latter was obtained using a u_4 value of 4.25, instead of the fiducial value of 4, indicating also in what direction a further fine-tuning could be worked out, if necessary, by considering u_2 and u_4 as slowly varying functions of a. Sometimes we can still notice small discontinuities at the changes of regimes, at u_2 and u_4. We believe however that, should our procedure be used for Voigt profile computations and radiative modelling, such small and very local discontinuities will not impair further computations of these scattering integrals entering the equations of the statistical equilibrium.

This new numerical scheme is particularly efficient for *small* values of a, typically lower than 0.01, where other schemes may fail (see for instance the discussion in Schreier 2018 about the implementation of `Voigt1D` in the `astropy` package in Python, using the McLean et al. 1994 method). But first of all, it is certainely suitable for our next applications of such a numerical integration scheme, and for physical conditions leading to very sharp Lorentzian peaks. We could also test the sensitivity of our scheme to the *order* of the initial Gauss–Hermite quadrature. For instance, for $a < 0.01$ we could go down to orders 40 to 50 without any significant loss of accuracy.

For larger values of a, typically more than 0.1, we noticed that *no* intermediate scheme between the original Liu & Pierce (1994) at line core, and the Gauss–Hermite

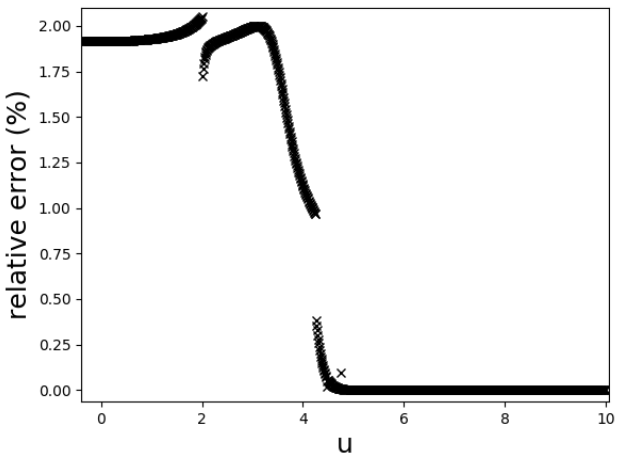

FIG. 5. Relative error between our computations with the double AGQ method, for $a = 10^{-4}$, and a reference computation using the Faddeeva complex function.

in the wings appears necessary. However the transition value between the two regimes should be adapted to the value of a, in a 2 to 4 range.

VI. CONCLUSION

We have tested a suitable numerical strategy for our first step towards "fully non-LTE" radiative transfer calculations, and the computation of generalized frequency redistribution functions. We modified the original strategy of Liu & Pierce (1994), but also applied it to a *non*-unimodal distribution.

Our numerical scheme does not pretend to compete with these numerical methods implemented for the *very* accurate computation of the Voigt function (see e.g., Schreier 2018 and references therein) since our aim is elsewhere, i.e. to explore departures from Gaussian vdf's. It is however providing very good results as compared to reference computations, such as the one using the Faddeeva complex function. Relative errors down to a few percent are systematically reported in the near wing region, and we believe that further fine tuning could be achieved for reaching an even better accuracy.

This is however not the scope of our study, which aims at computing generalized redistribution functions, after self–consistent computations of both massive particles and photons respective distributions under various physical conditions. In that respect, our main concern is well about a proper "capture" of the expected *very* sharp, and therefore very large amplitude Lorentzian peaks. And we believe that the principle of our numerical integration scheme should remain valid for the more easy to track contribution from the velocity distribution function, even for computed perturbations from a Gaussian shape.

As a final remark, we are also aware that computations with *non*-Gaussian functions convolved with a Lorentzian may also be doable, using a Fourier transform based method (e.g., Mendenhall 2007).

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