Voigt Profile Fitting to Quasar Absorption Lines: An Analytic Approximation to the Voigt-Hjerting Function

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ABSTRACT

The Voigt-Hjerting function is fundamental in order to correctly model the profiles of absorption lines imprinted in the spectra of bright background sources by intervening absorbing systems. In this work we present a simple analytic approximation to this function in the context of absorption line profiles of intergalactic HI absorbers. Using basic calculus tools, we derive an analytic expression for the Voigt-Hjerting function that contains only fourth order polynomial and Gaussian functions. In connection with the absorption coefficient of intergalactic neutral hydrogen, this approximation is suitable for modeling Voigt profiles with an accuracy of $10^{-4}$ or better for an arbitrary wavelength baseline, for column densities up to $N_{\text{HI}} = 10^{22}$ cm$^{-2}$, and for damping parameters $a \lesssim 10^{-4}$, i.e. the entire range of parameters characteristic to all Lyman transitions arising in a variety of HI absorbing systems such as Ly$\alpha$ Forest clouds, Lyman Limit systems and Damped Ly$\alpha$ systems. We hence present an approximation to the Voigt-Hjerting function that is both accurate and flexible to implement in various types of programming languages and machines, and with which Voigt profiles can be calculated in a reliable and very simple manner.

Key words: methods: analytic, quasars: absorption lines, line: formation, line: profiles, line: identification

1 INTRODUCTION

Absorption processes and their signatures (absorption lines) imprinted on the spectra of bright background sources (quasars, Gamma-ray bursts, etc.) are one of the main sources of information about the physical and chemical properties of intervening systems. It is well known that information about their temperature, density, chemical abundances, and kinematics can be extracted from the analysis of these absorption lines. For instance, a detailed insight into the physical state of the intergalactic medium (IGM) is provided by the analysis of the absorption lines found in the spectra of distant quasars (QSOs) (see e.g. Hu et al. 1995, Kim et al. 1997, 2001, 2002). These lines are due mainly to absorption by neutral hydrogen (HI) present in a class of low column density absorbers generally known as Ly$\alpha$ Forest, and due to other elements in low ionisation stages (CII, CIV, SiII, MgII, FeII, OII, etc.), which arise in higher column densities absorbing systems associated with galaxies, such as the Lyman Limit Systems (LLSs) and Damped Ly$\alpha$ Absorbers (DLAs). A wealth of information about the distribution, density, temperature, metal content, etc. of these systems is now available as a result of exhaustive and extensive studies of QSO absorption lines (see e.g. Rausch 1998, Rao 2005 for a review on Ly$\alpha$ absorbers, and on metal systems and DLAs, respectively).

In this type of analysis, and within the realm of a given cosmological model, the number and observed central wavelength of the absorption lines provide information on the spatial distribution of the absorbing systems. Furthermore, knowledge about the actual physical state of these systems can be obtained basically from the line profiles. Both line counting and line profile measurement are tricky tasks though, since the accuracy with which they can be performed highly depends on the resolution of the observed spectra. For instance, depending on the spatial distribution of the absorbing systems, lines can appear very close to each other or even superpose (line blending), and a low spectral resolution may lead to the misidentification of the resulting composite profile as being a single, complex one. Because of this same reason, the determination of the exact shape of each individual absorption profile is far from being trivial, and misidentified profiles may lead to wrong conclusions about the properties of the absorbing systems.

If one assumes that the physical state of the absorbing medium is uniquely defined by its temperature and column density, single absorption line profiles are ideally described by Voigt profiles. Mathematically, a Voigt profile is given in terms of the convolution of a Gaussian and a Lorentzian distribution function, known as Voigt-Hjerting function (Hjerting 1938), and a constant factor that contains information about the relevant physical properties of
the absorbing medium (cf. Sect. 2.1). Any departure from a pure Voigt profile in the observed lines is expected to yield information about the kinematic properties (non-thermal broadening, rotational or turbulent macroscopic motions), as well as spatial information (clustering) of the absorbing systems.

The Voigt-Hjerting function has long been known and, consequently, various numerical methods to estimate and tabulate this function have been developed and presented (Hjerting 1935; Harris 1948; Finn & Mugglestone 1965). Also, a great effort has been done in order to derive a semi-analytic approximation to this function that reproduces its behavior with high accuracy (see e.g. Whiting 1968; Kielkopf 1974; Monaghan 1971), being the latter by far the one with the highest accuracy. With the help of these methods, computational subroutines have been developed that make it nowadays possible to numerically integrate this function for a wide parameter space (see e.g. Humfressed 1983).

The aim of this work is to make a further contribution to the practical handling of the Voigt-Hjerting function in order to compute Voigt profiles. Starting with an exact expression for this function in terms of Harris’ infinite series, we argue why this series may not be truncated to first order in \( \alpha \), and consequently various numerical methods to estimate and tabulate this function have been developed and presented (Hjerting 1938; Whiting 1968; Kielkopf 1974; Monaghan 1971), being the latter by far the one with the highest accuracy. With the help of these methods, computational subroutines have been developed that make it nowadays possible to numerically integrate this function for a wide parameter space (see e.g. Humfressed 1983).

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2 THE VOIGT-HJERTING FUNCTION IN THE CONTEXT OF HI ABSORPTION LINES

2.1 The Absorption Coefficient

The probability of a photon with an energy \( E = h\nu / \lambda \) to be absorbed within a gas with column density \( N \) and kinetic temperature \( T \), also known as absorption coefficient, is given by

\[
\tau_\nu(\lambda) = (C_i \cdot N \cdot a) \cdot H(a, x(\lambda)),
\]

where

\[
C_i = \frac{4 \sqrt{\pi} \cdot e^2 \cdot f_0}{m_e \cdot c \cdot \Gamma_i}
\]

is a constant for the \( i \)th electronic transition caused by the photon absorption. Here \( m_e \) is the electron mass, \( f_0 \) is the oscillator strength, and \( \Gamma_i \) the damping constant or reciprocal of the mean lifetime of the transition. The function \( H \) is the so-called Voigt-Hjerting function and is given by

\[
H(a, x) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-x^2}}{x^2 + a^2} \, dy.
\]

Let \( \lambda_i = h\nu / e_i \) be the resonant wavelength of the corresponding transition, and \( \Delta \nu_{i,j} = \frac{\lambda_i}{\lambda_j} \) the thermal or Doppler broadening, which defines a Doppler unit. Here, the Doppler parameter \( b \) is related to the kinetic temperature of the gas via \( b = \sqrt{2kT / m_p} \), where \( k \) is the Boltzmann constant and \( m_p \) is the proton mass. It follows from these definitions that the damping parameter

\[
a = \frac{\Delta \nu_{i,j}}{4\pi \cdot \Delta \nu_{i,d}}
\]

quantifies the relative strength of damping broadening to thermal broadening, and that the variables \( x \equiv \frac{(\lambda - \lambda_i)}{\Delta \nu_{i,j}} \) and \( y \equiv \frac{x}{\pi} \) are just the wavelength difference relative to the resonant wavelength in Doppler units, and the particle velocity in units of the Doppler parameter, respectively.

The particular form of the absorption coefficient \( \tau_\nu \) induces a characteristic absorption feature known as Voigt profile. Hence, the Voigt profile, and consequently the Voigt-Hjerting function, naturally arise in the process of absorption-line formation, when one assumes that the physical state of the absorbing medium is uniquely defined by its density and kinetic temperature. Generally speaking, it is the physical conditions that determines the shape of the absorbing features, i.e. the line profiles. Conversely, it is true that line profiles give information about the physical state of the absorbing medium. In particular, line profiles other than Voigt profiles give information about the departure of the physical conditions assumed here.

The class of HI absorbers present in the IGM (Lyα Forest Clouds) and associated with galaxies and larger structures (LLSs, DLAs) can be characterised by their column density \( N_{\text{HI}} \) and kinetic temperature, and consequently their absorption features obtained on e.g. QSO spectra are well described by Voigt profiles. Their observed column densities span a range of ten orders of magnitude, approximately from \( 10^{12} \) to \( 10^{22} \) cm\(^{-2} \), and have temperatures that correspond to Doppler parameters approximately in the range \( 10 \) to \( 100 \) km s\(^{-1} \), with a median value around \( 36 \) km s\(^{-1} \), that decreases with redshift (Kim et al. 1997). For such a range in \( b \), the damping parameter \( a \) for the Lyman transitions of intergalactic HI spans a range of \( 9.3 \cdot 10^{-9} \) to \( 6.05 \cdot 10^{-4} \). In this case, high values of \( a \) correspond to Lyα, while lower values are typical for higher order Lyman transitions. Transitions of other elements, such as C, Si, Mg, Fe, O, etc., and their various ionisation stages, are also typically found on QSO spectra, and their damping parameters cover a range which strongly overlaps with that of HI. This can be seen in Figure where we show the distribution of \( a \) for different elements (including HI) in different ionisation stages, for a Doppler parameter \( b_{\text{HI}} = 36 \) km s\(^{-1} \) for HI, and assuming that the doppler parameter for other elements is related to \( b_{\text{HI}} \) via \( b_x = b_{\text{HI}} \cdot \sqrt{m_{\text{HI}} / m_x} \), where \( m_x \) is the mass of element X. For clarity, we have grouped all different ionisation stages of a given element under a single label. The values of the atomic constants (central wavelength of the transition
and Γ-value) have been taken from Morton (2003). The shaded area contains the values of a above the range characteristic to intergalactic HI for which our approximation to the Voigt-Hjerting function—derived in the next sections—cannot be applied or should be applied with caution. Note, however, that the region spanned by a for intergalactic HI, i.e. the region underneath the shaded area, contains most of the a-ranges spanned by all other elements, especially those corresponding to C, O, Mg, and Fe. For other elements, such as Cr or Zn, the damping parameter has values right at the upper limit of this range. For this reason and for the sake of simplicity, in the following we will constrain our discussion to the Lyman absorption lines of intergalactic HI, but the reader shall bear in mind that the discussion and method to synthesise Voigt profiles presented in this work can be directly applied to the transitions of other elements associated with HI absorbing systems, according to Figure 1.

2.2 The Absorption Coefficient of HI at Low Column Densities

Following Harris (1948), it is true that for a < 1, i.e. when Doppler broadening dominates over damping broadening, the Voigt-Hjerting function \( \delta H_0 \) can be expressed as

\[
H(a, x) = \sum_{n=0}^{\infty} H_n(x) a^n,
\]

where the functions \( H_n(x) \) are defined by

\[
H_n(x) = \frac{(-1)^n}{\sqrt{\pi} n!} \int_0^{\infty} v^n e^{-v^2/2} \cos(xv) dv.
\]

These functions are bounded with respect to n and x, and they have values of the order of unity. Indeed, taking the absolute value of the integral, neglecting the cosine, which takes values of the order of unity, and computing the resulting integral one can show that

\[
|H_n(x)| \leq \frac{2}{\sqrt{\pi}} \approx 1.132,
\]

for all n ∈ \( \{0, 1, 2, \ldots\} \) and x ∈ \( \mathbb{R} \). From this it follows that if a ≪ 1, the Voigt-Hjerting function can very well be approximated to zeroth order in a by the first term of the series \( \delta H_0 \), i.e. \( H(a, x) \approx H_0(x) \), as first noted by Walshaw (1953). Note that this result is exact in the limit a → 0. Taking the definition \( \delta H_0 \), it follows that

\[
H_0(x) = e^{-x^2},
\]

and thus \( H(a, x) \approx e^{-a^2x^2} \), for a ≪ 1. We call this the Voigt-Hjerting function to zeroth order.

But what actually means that the condition a ≪ 1 be satisfied, so that this zeroth order approximation can be safely used to model absorption line profiles? In order to address this, we compute for the extreme values of a for intergalactic HI, a ≈ 10^{-8} and a ≈ 10^{-4}, the departure of the Voigt-Hjerting function from a pure Gaussian function. This is shown in Figure 2 as the logarithmic difference between \( \delta H_0 \) and \( H_0 \) relative to H as a function of x, i.e. the quantity \( \delta H_0 \equiv 1 - H_0/H \). Note how the zeroth order approximation completely differs from the actual Voigt-Hjerting function at x ≥ 3.5 for a = 10^{-8}, and at x ≥ 4.5 for a = 10^{-4}. Thus, even a value of a as small as 10^{-8} is not a sufficient condition for the zeroth order term to be a good approximation of H for an arbitrary range in x.

In the context of the HI absorption coefficient, the condition on a for which the approximation to zeroth order of the Voigt-Hjerting function is valid, translates into a restriction on N_{HI}, and more specifically on the quantity C_J · a · N_{HI}. This can be seen by taking a glance at equation \( \delta H_0 \): Despite the fact that the condition a ≪ 1 holds, the product C_J · a · N_{HI} can be very large for high

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1 A list containing the values of the damping parameters for the elements and their different ionisation stages shown in Figure 1 is available in plain-text format at www.astro.physik.uni-goettingen.de/~tepper/hjerting/damping.dat. Please consult this list in order to know the exact value of a for a given element in a given ionisation stage.

2 The values of the Voigt-Hjerting function were computed numerically using a routine based on Monaghan’s algorithm in Murphy (2002) (cf. Section 5).
enough\(^3\) column densities, and since the functions \(H_n\) are of the order of unity, such terms can have a significant contribution to the absorption coefficient. Along this line of reasoning, and taking into consideration that the constant \(C_1\) in equation (4) is of the order of \(10^{-11}\) cm\(^{-2}\) for all Lyman transitions, it is clear that the departure of the Voigt-Hjerting function from its zeroth order approximation becomes significant in the wavelength ranges \(x \gtrsim 3.5\) and \(x \gtrsim 4.5\) (in Doppler units) at column densities \(N_{\mathrm{HI}} \gtrsim 10^{19}\) cm\(^{-2}\) for a damping parameter \(a = 10^{-8}\), and at column densities \(N_{\mathrm{HI}} \gtrsim 10^{19}\) cm\(^{-2}\) for \(a = 10^{-4}\). Since intervening HI absorbers typically have column densities in the range \(10^{12} - 10^{22}\) cm\(^{-2}\), a Gaussian approximation to \(H\) for modeling intergalactic HI absorption line profiles is only suitable for the low end of the column density range.

In addition to the factor \(C_1 \cdot a \cdot N_{\mathrm{HI}}\) being large and even more decisive for the uselessness of the zeroth order approximation for an arbitrary range in \(x\), is the fact that the zeroth order term, \(e^{-x^2}\), rapidly decreases for large values of \(x\) and is therefore overwhelmed by higher order terms in Harris' expansion, which hence dominate the behavior of the absorption coefficient, as already seen in Figure 2. To shed some light on this, consider the following numerical example: Out to \(x \approx 4\) (in Doppler units), and for \(a = 10^{-4}\), the Voigt-Hjerting function is of the order of \(4.2 \cdot 10^{-6}\). The zeroth order term in the series (4) satisfies \(H_0 (x = 4) \approx 1.1 \cdot 10^{-7}\), whereas the first order term \((a \cdot H_1) (x = 4) \approx 3.9 \cdot 10^{-6}\). Thus, at large enough \(x\), the behaviour of \(\tau\) is evidently governed by the terms of order \(n \geq 1\) in the series (5).

2.3 Higher Column Densities and First Order Term

Due to the arguments stated above, and even though the damping parameter satisfies \(a \ll 1\), it is clear that the absorption coefficient of intergalactic HI cannot simply be approximated by a constant times \(e^{-x^2}\) for an arbitrary wavelength range and column densities greater than \(10^{15}\) cm\(^{-2}\). One actually has to take into account terms of higher order in the series (4), at least to first order in \(a\), i.e. \(H(a, x) \approx (H_0 + a \cdot H_1) (x)\). In fact, one should take into account all terms up to \(n\)th order for values of \((C_1 \cdot a \cdot N_{\mathrm{HI}})^{-1}\) that are nearly equal or greater than the absolute difference between the sum \(\sum_{n=0}^{\infty} H_n (x) a^n\), and the exact Voigt-Hjerting function. However, as we shall show next, the approximation to first order in \(a\) in Harris' expansion is enough to model absorption line profiles with moderate to high accuracy for the range of parameters \((a, N_{\mathrm{HI}}, C_1)\) characteristic to intervening HI absorbers.

In order to prove the above statement, we look at the relative contribution of the zeroth and first order terms to the Voigt-Hjerting function for \(a \in (10^{-8}, 10^{-4})\) and an arbitrary range in \(x\). This is achieved, for example, by computing the logarithm of the quantity \(\delta H_1 \equiv (H_0 + a \cdot H_1)/H\) as a function of \(x\) for the two extreme values of \(a\), as shown in Figure 3. Here we have advanced the function \(H_1\) which is being handled in the next section. Note that the greater the contribution from the zeroth and first order term to \(H\), the smaller the quantity \(\delta H_1\). In this case, as can clearly be seen, \(\delta H_1\) takes on values of the order of \(10^{-7}\) or less over the whole wavelength range shown here and for the whole range in \(a\) for intergalactic HI.

If one takes into account that \(H(x) \ll 1\) for all \(x\), it is obvious that the relative difference is equal or greater than the absolute difference, i.e. \(\delta H_1 \equiv |H - (H_0 + a \cdot H_1)|\). Thus, in the case of \(a \approx 10^{-4}\) and \(\delta H_1 \approx 10^{-7}\), the departure of \(H\) from its first order approximation becomes significant at column densities \(N_{\mathrm{HI}} > (a \cdot H_1 / C_1)^{-1} = 10^{22}\) cm\(^{-2}\), and at even larger \(N_{\mathrm{HI}}\) for \(a < 10^{-8}\) and/or smaller \(\delta H_1\). Hence, the first two terms of Harris' expansion dominate the behaviour of \(H\) over the whole wavelength range shown here, with an accuracy of \(10^{-7}\) or greater, for the range in \(a\) characteristic to intergalactic HI. On this basis, we consider that an approximation to first order in \(a\) of the Voigt-Hjerting function in terms of the functions \(H_0\) and \(H_1\) is suitable to model Voigt profiles. Since the function \(H_0\) is known and simple \textit{per se}, we now turn to the task of finding an approximation to the function \(H_1\) in terms of a simple, analytic expression.

3 THE DAWSON FUNCTION REVISITED

According to definition (3) we have

\[
H_1(x) = \frac{-4}{\sqrt{\pi}} \int_0^x v e^{-v^2} \cos(2ux) \, dv.
\]

Integrating this equation partially, and computing the resulting Si-nus transform of a Gaussian it follows (Mihalas 1970)

\[
H_1(x) = \frac{2}{\sqrt{\pi}} \left[1 - 2x F(x)\right],
\]

where we adopt the notation first introduced by Miller & Gordon (1933)

\[
F(x) \equiv e^{-x^2} \int_0^\infty e^{2uv} \, dv.
\]

\(F\) is known as the Dawson function (Dawson 1955).

It is evident that finding an approximation for \(H_1\) translates into the same problem for \(F\). We thus want to show that a simple analytic expression can be found which approximates the Dawson function, and hence the function \(H_1\), accurately enough, in order for an approximation of the Voigt-Hjerting function in terms of these functions to be useful for synthesising Voigt profiles.
3.1 Properties of the Dawson Function

We briefly want to state some important properties of the Dawson Function. First, this function is antisymmetric, i.e. \( F(-x) = -F(x) \) for all \( x \in \mathbb{R} \). Because of this, from now on we restrict our analysis to \( x \geq 0 \). Besides, it has no roots in the positive semi-axis, and \( F(0) = 0 \), as can easily be seen from its definition (Fundamental Theorem of Calculus). Furthermore, \( F \) is bounded, since \( H_1 \) is bounded itself (cf. Sect. 2). Indeed, differentiation with respect to \( x \) gives

\[
\frac{d}{dx} F(x) = 1 - 2x F(x). 
\] (10)

Hence, the upper bound is given by \( F(x_0) = (2x_0)^{-1} \), where \( x_0 \) is defined by equaling \( F \)’s derivative to zero and solving for \( x \). Actually, \( F \) has its maximum at \( x_0 = 0.92413 \) with \( F(0.92413) = 0.54104 \). From this last equation it follows also that equation (8) can be rewritten as

\[
H_1(x) = \frac{-2}{\sqrt{\pi}} \frac{d}{dx} F(x). 
\] (11)

We want to know how the function \( F \) behaves asymptotically, i.e. for \( x \ll 1 \) as well as for \( x \gg 1 \). Using the power series of the exponential we get

\[
F(x) = e^{-x^2} \sum_{n=0}^{\infty} \frac{1}{n!} x^{2n} = e^{-x^2} \sum_{n=0}^{\infty} \frac{1}{n!} x^{2n+1}.
\] (12)

In this case, the sum and the integral operator commute, since the term \( e^{-x^2} \) by its corresponding power series and rearranging this last equation reads in explicit form

\[
F(x) = x \left( 1 - \frac{2}{3} x^2 + \frac{1}{15} x^4 + \cdots \right). 
\] (13)

Thus, for \( x \ll 1 \) the Dawson function behaves asymptotically up to third order as

\[
F(x) \approx x \cdot \left( 1 - \frac{2}{3} x^2 \right), \quad x \ll 1. 
\] (14)

In order to investigate how \( F \) behaves for \( x \gg 1 \), we first rewrite the function \( F \) with the replacement \( v' = x - v \) and the aid of the power series of the exponential as

\[
F(x) = \sum_{n=0}^{\infty} \frac{1}{n!} I_n(x), 
\] (15)

with the definition

\[
I_n(x) = \int_0^\infty v^{2n} e^{-v^2} dv. 
\] (16)

It is not hard to see that every term of the series (15) is separately bounded with respect to \( x \) as well as \( n \). Making the replacement \( v' = 2v \) in eq. (16), and integrating for \( x \neq 0 \) we get for \( n \in \mathbb{N}_0 \)

\[
I_n(x) = \frac{1}{(2x)^{n+1}} (2n)! \left( 1 - e^{-2x^2} \right) - e^{-x^2} R_n(x), 
\] (17)

where \( R_n(x) \) is a rather cumbersome polynomial function. Now, for \( x \gg 1 \), we may drop all terms which contain an exponential factor and in this way we get the asymptotic form

\[
F(x) \approx \sum_{n=0}^{\infty} \frac{1}{(2x)^{2n+1}} (2n)! \left( 1 - e^{-2x^2} \right), \quad x \gg 1. 
\] (18)

It can be seen from this expression that \( F \) vanishes as \( (2x^2)^{-1} \) for \( x \to \infty \), and that the first derivative \( F' \), and thus the function \( H_1 \), also vanish in this limit as \( (2x^2)^{-1} \). From equation (10) it is also true that \( F' \) converges to unity for \( x \to 0 \) and that \( H_1 \) converges to \( (-2 / \sqrt{\pi}) \) in this limit. Since we want our approximation to \( F \), and consequently to \( H_1 \) and \( H_2 \), to be valid in the whole range \( x \in [0, \infty) \), we require it to fulfill both these conditions as well.

4 THE ANALYTIC APPROXIMATION \( D_1 \)

Equation (15), together with eq. (16), represent indeed an exact expression for the Dawson function. However, these expression are not suitable for practical computation. We therefore explore the possibility of finding an analytic expression which is easy to handle and which can be used to compute the value of \( F(x) \) for \( x \in [0, \infty) \). In particular, we shall see if it is possible to truncate the series (15) in order to find an approximation to \( F \), which has all its properties (antisymmetry, boundedness, etc.), which converges for \( x \to \infty \) as well as for \( x \to 0 \), and which is well defined in the whole range \([0, \infty)\). For instance, equations (15) and (19) do not fulfill these requirements. Nevertheless, they show us how our desired function has to behave asymptotically.

Let us define

\[
D_n(x) \equiv \sum_{n=0}^{N} \frac{1}{n!} I_n(x),
\] (19)

where the \( I_n \)’s are given by eq. (16). Using this definition we get

\[
D_1(x) = \left( 1 - e^{-2x^2} \right) \cdot \left[ 1 + \frac{1}{2x} \right] e^{-2x^2} \cdot \left[ 1 + \frac{1}{2x} \right]
\] (20)

It is easy to show that this function behaves qualitatively in the same way as \( F \) does, i.e. it is antisymmetric, bounded, and has no roots in the positive semi-axis. Furthermore, both these functions have the same asymptotic behavior. Indeed, up to third order we have for \( x \ll 1 \)

\[
D_1(x) \approx x \cdot \left( 1 - \frac{2}{3} x^2 \right), \quad x \ll 1.
\] (21)

as can be shown by expanding the exponentials in eq. (20) in terms of their power series. A glance at eq. (14) makes the similarity between \( F \) and \( D_1 \) evident in this limit. For \( x \gg 1 \) we get from eq. (20), neglecting the exponentials,

\[
D_1(x) \approx \frac{1}{2x} + \frac{1}{2x}, \quad x \gg 1.
\] (22)

that is the same as for \( F \) (see eq. 15). Furthermore, the first derivative of \( D_1 \) with respect to \( x \) is unity at \( x = 0 \) and vanishes as \( (2x^2)^{-1} \) for \( x \to \infty \). However, the maximum of \( D_1 \) is at \( x = 0.87269 \) with \( D_1(0.87269) = 0.52212 \), i.e. at slightly different values from those of \( F \).

The magnitude and range of the error in approximating the Dawson function by the function \( D_1 \) can be estimated, at least qualitatively, in the following way: From equations (15) and (19) it follows that

\[
F(x) = D_1(x) + \sum_{n=2}^{\infty} \frac{1}{n!} I_n(x).
\] (22)

The sum in this last equation, i.e. the absolute error in our approximation \( F(x) \approx D_1(x) \), is a positive semi-definite quantity, since each term of the sum has this property. Hence, it is true that \( 0 < D_1(x) \ll F(x) \) for \( x \in [0, \infty) \). Furthermore, since both \( F \) and \( D_1 \) converge to zero for \( x \to 0 \) as well as for \( x \to \infty \), and both these functions are bounded, it follows from eq. (22), that the error also vanishes for \( x \to 0 \) as well as for \( x \to \infty \), that
it is also bounded, and that its maximum value is less equal than max \( F(x) - D_1(x) \). From this, and since their respective maxima are slightly shifted with respect to each other, one is led to the conclusion, that the error is constrained to a narrow range in \( x \) and that the maximum error in our approximation to \( F \) occurs near the maxima of these functions, i.e. in the vicinity of \( x = 1 \).

We want further try to quantify the actual error in our approximation to \( F \). It shall be enough to know, for our purposes of finding an approximation to the Voigt-Hjerting function, that the error in the approximation \( F(x) \approx D_1(x) \) is bounded and constrained to a narrow wavelength interval around \( x = 1 \). Besides, we will indirectly estimate the error in this approximation when quantifying the error in our approximation to \( H \) in Section 5.

### 4.1 The Voigt-Hjerting function to First Order

Once we have found an approximation to the Dawson function, we can use it to give the desired expression for the Voigt-Hjerting function using Harris’ expansion to first order in \( a \). Replacing in equation 11 the function \( F \) by our approximation \( D_1 \) (eq. 20), taking the corresponding derivative, and rearranging terms we get

\[
H_1(x) \approx \frac{2}{\sqrt{\pi}} K(x) e^{-x^2},
\]

where we have defined

\[
K(x) = \frac{1}{2x^2} \left[ (4x^2 + 3)(x^2 + 1) e^{-x^2} - \frac{1}{2} (2x^2 + 3) \sinh x^2 \right].
\]

We want to highlight the fact that equation 23 is well defined, i.e. it has no singularities in the whole interval \([0, \infty)\). Furthermore, it converges to the correct value in the limits \( x \to 0 \) and \( x \to \infty \). Indeed, it is easy to show that \( \lim_{x \to 0} H_1(x) = \frac{2}{\sqrt{\pi}} \), and \( \lim_{x \to \infty} H_1(x) = 0 \), whether one uses for \( H_1 \) the exact expression 8 or the approximation 23. In contrast, in approximations to the Voigt-Hjerting function to model Voigt profiles often used in the literature (see e.g. Spitzer 1973; Zhang et al. 1997) and given in the form \( c_1 \cdot e^{-x^2} + c_2 \cdot x \), where the \( c_i \)'s are constants, the second term which represents the Lorentzian damping clearly diverges for \( x \to 0 \), and one has to artificially define the wavelength range in which this second term is used. It is customary to neglect this term for low column densities and in the vicinity of \( x = 0 \), but how to exactly choose the radius of the vicinity is not clear and completely arbitrary. However, with an expression like equation 23 at hand, no such assumptions have to be made.

Taking into account that \( a \ll 1 \) in order to neglect terms of order \( a^2 \) in the series 8, we get, using the expressions for \( H_0 \) (eq. 6) and \( H_1 \) (eq. 23), that the Voigt-Hjerting function to first order in \( a \) is given by

\[
H(a, x) \approx e^{-x^2} \left[ 1 - a \frac{2}{\sqrt{\pi}} K(x) \right].
\]

This expression is symmetric in \( x \), as it should be, and thus it is valid for \( x \in \mathbb{R} \) and \( a \ll 1 \). According to this equation, the Voigt-Hjerting function can be regarded as a “corrected” Gaussian function, where the correction term depends on the parameter \( a \). In the context of the absorption coefficient of HI, this correction term also depends on the column density \( N_{\text{HI}} \), of course, via the quantity \( a \cdot N_{\text{HI}} \).

### 5 ANALYSIS

In order to quantify the quality of our approximation to \( H \), we perform a test on speed as well as on precision, comparing a numerical method to compute \( H \), based on our approximation, to other standard, available methods to numerically compute this function. For this purpose, we use the approach and corresponding computational routine developed by Murphy (2002), which consists of the numerical implementation in FORTRAN of four different methods to compute \( H \): Harris’ \( H_1 \) and \( H_2 \), Humlíček’s, and Monaghan’s. In Murphy’s notation, Harris’ \( H_1 \) and \( H_2 \) correspond to the Voigt-Hjerting function approximated by the first three and five terms of the series expansion 4, respectively. Humlíček’s optimized algorithm and Monaghan’s differential approach to approximate \( H \) are explained in detail in Humlíček (1985) and Monaghan (1971), respectively. Our method to compute \( H \) consists simply in the numerical implementation in FORTRAN of equations 22 and 25.

#### 5.1 Speed

Following Murphy’s approach, the relative speed of all five methods is determined by calculating the time that a routine based on each method requires to compute the Voigt-Hjerting function for \( x \in [0, 10] \) and damping parameters \( a \) in the range \( 10^{-6} - 10^{-4} \) for a total of \( 1.5 \cdot 10^7 \) runs. In this way, we get that the relative speed\(^4 \) of each method in the order \( H_1 : (this \ work) : Humlíček : H_2 : Monaghan \) corresponds to \( 1 : 4.2 : 5.8 : 6.8 : 66.6 \), independent of \( a \). According to this result, our method is second fastest.

#### 5.2 Precision

The precision of our method relative to the other methods mentioned above is determined in the following way: First, the values of the Voigt-Hjerting function computed using Monaghan’s algorithm for \( x \in [0, 10] \) and \( a \in [10^{-6}, 10^{-4}] \) are taken as fiducial. Then, the value of \( H \) for the same range in \( x \) and \( a \) is computed using each of these methods, and the logarithmic difference between each method and its fiducial value, i.e. the quantity \( \log_{10} \delta H \) with \( \delta H \equiv 1 - H_{\text{method}}/H_{\text{Mon}} \), is calculated as a function of \( x \) for each different \( a \). The result is shown in Figure 4. It can be seen from this figure that Harris’ \( H_2 \) is the second most precise method to compute \( H \), if one takes Monaghan’s algorithm as fiducial, but is six times slower than Harris’ \( H_1 \), and one-and-a-half times slower than our method, as stated in the previous section. Our method has a precision of \( 10^{-4} \) or better for \( x \leq 4 \). For all values of \( a \), the precision differs around \( x = 4 \) to a value of the order of 0.01, and the precision increases again for values of \( x > 4 \). The precision is better for smaller \( a \), as expected, since the zeroth order term gains in importance in our approximation for decreasing \( a \). For \( a \leq 10^{-6} \) and \( x < 1.5 \), our method is more precise than Harris’ \( H_1 \) or Humlíček’s, and, as seen above, 1.5 times faster than the latter.

\(^4\) The rearrangement of equations 22 and 25 that leads to the smallest number of operations reads, in code syntax,

\[
H(a, x) = H_0 - a / \sqrt{\pi} / x^2 \cdot \left[ H_0, H_0, (4 \cdot x^2 + 7 \cdot x^2 + 4 + Q) - Q - 1 \right],
\]

where the terms \( x^2 \), \( H_0 \equiv e^{-x^2} \) and \( Q \equiv 1.5 \cdot x^2 \) have to be computed just once.

\(^5\) This calculations were performed on an Intel Xeon 3.2 GHz processor.
5.3 Modeling of HI absorption profiles

We now turn to analyse how accurate is our method in order to model HI absorption profiles. Taking the whole range in column density $\log N_{\text{HI}} \in [12.0, 22.0]$ dex and Doppler parameters $b \in [10.0, 100.0] \text{ km s}^{-1}$ characteristic to intergalactic HI, we synthesise for each pair $(N_{\text{HI}}, b)$ (with a resolution of $\Delta \log N_{\text{HI}} = 0.05$ dex, and $\Delta b = 0.5 \text{ km s}^{-1}$) a single Lyα absorption profile in the range $\lambda \in [100, 2300] \text{ Å}$ with a resolution of $\Delta \lambda = 0.01 \text{ Å}$. The absorption profile is synthesised according to equations (1) and (2), using both our method and Monaghan's to compute $H$. We then compute for each pair $(N_{\text{HI}}, b)$ the absolute value of the difference between the profiles generated using these two methods relative to Monaghan's, i.e. $\delta V \equiv |1 - e^{-\Delta \tau}|$, with $\Delta \tau \equiv \tau_{\text{our}} - \tau_{\text{Mon}}$, as a function of wavelength for the whole wavelength range, and pick the maximum value of this difference in the entire range. We choose to do so in order to pick up the worst cases possible, i.e. those with the lowest accuracy, and put in this way a stringent lower limit to the accuracy of our method. The result is shown as a contrast diagram on the $(\log N_{\text{HI}}, b)$-plane in Figure 5. Note that, in this case, it is not the logarithmic, but the linear difference which is shown. The highest precision is of the order of $10^{-16}$ or even better. However, for the sake of simplicity, any value below $10^{-4}$ has been coded as zero. The largest discrepancy between both methods, i.e. the lower limit in the precision of our method if one takes Monaghan's as fiducial, amounts to 0.01, in agreement with the result shown in Figure 4.

As can clearly be seen, the (lower limit in the) precision of our method depends both on $b$ and $N_{\text{HI}}$. While the dependence on $b$ extends to the whole range $10.0 - 100.0 \text{ km s}^{-1}$, the dependence on $N_{\text{HI}}$ is limited to the range $\log N_{\text{HI}} = 16 - 20$ dex. For a fixed $b$, there is a regime of values around 0.01 with a width of nearly 2 dex,
The origin of any inaccuracy in our method is obviously the fact that terms of order \( n \geq 2 \) have been neglected in the series \( \delta V \), and furthermore, that the second term is this series has been approximated as well. In particular, the origin of the 'low-accuracy' stripe on the \((\log N_{\text{HI}}, b)\)-plane can qualitatively be understood in terms of the functional dependence of \( \delta V \) on \( b \) and \( N_{\text{HI}} \). Considering that both our method and Monaghan’s take the zeroth order term exactly into account, it is legitimate to state that the quantity \( \Delta H = H_{\text{our}} - H_{\text{Mon}} \) has at least a dependence of first order on \( a \), i.e. \( \Delta H(a, x) = a \cdot h(a, x) \) where \( h \) is a function that may be of zeroth order in \( a \). Hence, using equation (1) and this last expression, it follows that

\[
\Delta \tau(\lambda) = C'_i \cdot \frac{N_{\text{HI}}}{b^2} \cdot h(a, x), \quad \text{with} \quad C'_i = \frac{e^2}{4 \sqrt{\pi m_e c}^2} \Gamma_i.
\]

As can be seen, \( \tau \) strongly depends on the ratio \( \frac{N_{\text{HI}}}{b^2} \). Therefore, an increase in \( b \) of one order of magnitude (from 10 to 100 km s\(^{-1}\)) is nearly compensated (in the sense that the value of \( \tau \) remains nearly constant) by an increase in \( N_{\text{HI}} \) of two orders of magnitude, which accounts for the stripe of 2 dex in column density seen on the \((\log N_{\text{HI}}, b)\)-plane. Why this happens precisely between \( \log N_{\text{HI}} = 16 \approx 20 \text{ dex} \), as well as the shape of this stripe, is nontrivially related to the exact value of the constant \( C'_i \), the fact that \( h \) may depend also on \( b \) through the damping parameter \( a \), and the fact that the \( \Delta V \) dependence effectively not on \( \Delta \tau \), but on \( e^{-\Delta \tau} \).

It is worth mentioning that, for higher-order Lyman transitions, the precision of our method to compute Voigt profile has the same behaviour on the \((\log N_{\text{HI}}, b)\)-plane, and is the same as or even better than the precision of the Ly\( \alpha \) transition shown here. The reasons for this are, first of all, that the functional form of the absorption coefficient is obviously the same, irrespective of the transition. In addition, the lowest precision possible of 0.01 is the same for the whole range in \( a \) spanned by the Lyman transitions, according to Figure 5. Furthermore, higher transitions have lower damping parameters and our approximation is better the lower \( a \), as already mentioned. Finally, since the constant \( C'_i \) is smaller the higher the order of the transition, the critical range of lowest precision is shifted to higher column densities and higher Doppler parameters. Since the ranges in \( N_{\text{HI}} \) and \( b \) are fixed for intergalactic \( \text{HI} \), this has the net effect of increasing the high-precision region on the \((\log N_{\text{HI}}, b)\)-plane—i.e. the region to the left of the stripe—for higher order transitions. In other words, the precision of our method improves from \( \text{Ly} \alpha \) to higher Lyman transitions.

Even though a discrepancy of the order of 0.01 when using our method to model Voigt profiles may seem large, we want to emphasise again that this is merely an lower limit for the precision in the entire wavelength range \( \lambda \in [100, 2300] \) Å, in the case of \( \text{Ly} \alpha \). It turns out that the range in wavelength for which the accuracy is lowest is negligible for practical purposes. In order to show this, we first choose three points on the \((\log N_{\text{HI}}, b)\)-plane along the stripe of lowest precision, i.e. for which the maximum difference is largest. Using these parameters, we synthesise \( \text{Ly} \alpha \) absorption profile using our method and Monaghan’s, and compute again for each of these "worst scenarios" the quantity \( \delta V \) for the whole wavelength range. The result is shown in Figure 6. Each row corresponds, from top to bottom, to the parameter pairs \((\log N_{\text{HI}}, b) = (17.0, 10.0), (18.0, 20.0), \) and \((19.0, 70.0) \) chosen along the low-precision stripe. The upper panel of each row shows the \( \text{Ly} \alpha \) absorption profile synthesised using our method, and the corresponding lower panel gives the logarithmic difference \( \Delta \log_{\text{our}} \delta V \) between our method and Monaghan’s as a function of wavelength. As can be seen, the smallest discrepancies are given at the line cores, as expected, since in
this regime the zeroth order term dominates and both our approach and Monaghan’s exactly take this term into account. The largest discrepancies, of the order of 0.01, are present in an extremely narrow range of $\Delta \lambda \approx 0.06 \, \AA$ for $(\log N_{\text{HI}}, b) = (17.0, 10.0)$, of $\Delta \lambda \approx 0.17 \, \AA$ for $(\log N_{\text{HI}}, b) = (18.0, 20.0)$, and of $\Delta \lambda \approx 0.53 \, \AA$ for $(\log N_{\text{HI}}, b) = (17.0, 20.0)$. This discrepancies are found at the boundaries between Gaussian core and Lorentzian wings, due to the fact that our method neglects terms of order $b^2$, which dominate the behaviour of $H$ in that regime. Note, however, that the difference rapidly drops with increasing distance (in $\AA$) from the line center to values of the order of $10^{-10}$ at a distance $\Delta \lambda \approx 5 \, \AA$ for the first two rows, and $\Delta \lambda \approx 15 \, \AA$ for last row. Hence, the effective accuracy of our method is far better than 0.01 in the wavelength range shown here. For the same reason mentioned in the last paragraph, the precision for higher order Lyman transitions is of the same order as or even better than for the Ly$\alpha$ transition shown here.

6 APPLICATION

As a further test of the quality of our approximation to model Voigt profiles, and to show its accuracy in a less academic situation as in the last section, we consider fitting a synthetic spectrum to a real quasar absorption spectrum with a population of intergalactic HI absorbers spanning a representative range in $b$ and $N_{\text{HI}}$ along a random line-of-sight. For this purpose we use the observed spectrum of the quasistellar source QSO J2233-606, a relatively bright ($B = 17.5$) quasar at an intermediate redshift $z_{\text{em}} = 2.238$.

The spectrum of the source QSO J2233-606, centered at the HDF-S, was obtained during the Commissioning of the UVES instrument at the VLT Kueyen Telescope and reduced at the Space Telescope European Coordinating Facility. The high-resolution spectroscopy ($R \approx 45000$) was carried out with the VLT UV-Visual Echelle Spectrograph (UVES). The data were reduced in the ECHELLE/UVES context available in MIDAS. The final combined spectrum has constant pixel size of 0.05 $\AA$ and covers the wavelength range 3050-10000 $\AA$. The S/N ratio of the final spectrum is about 30 per resolution element at 4000 $\AA$, 90 at 5000 $\AA$, 80 at 6000 $\AA$, 40 at 8000 $\AA$. The data used here are publicly available and were retrieved from www.stecf.org/hstprogrammes/J22/J22.html, in its version of November 23, 2005.

With help of the MIDAS package FITLYMAN [Fontana & Ballester 1995], which performs line fitting through $\chi^2$ minimization of Voigt profiles, Cristiani & D’Odorico (2000) determined the redshifts, column densities, and Doppler widths of the identified absorption features imprinted in the spectra of QSO J2233-606. In this way, they found that the line of sight to QSO J2233-606 intersects a total of 270 Ly$\alpha$ Forest clouds, and identified other 24 absorption systems containing metal lines. The Ly$\alpha$ absorbers span a range in column density of $10^{12.20} - 10^{17.10}$ cm$^{-2}$, and a range in Doppler parameters of $1.0 - 111.0$ km s$^{-1}$. The distribution of the parameter pairs ($N_{\text{HI}}, b$) for these systems for $b \in [10, 100]$ km s$^{-1}$ is shown in Figure 7.

Using this list of Ly$\alpha$ line parameters ($z_{\text{abs}}, b, N_{\text{HI}}$), we generate a synthetic spectrum of the QSO J2233-606 in the wavelength range 3340 – 3530 $\AA$ with a higher resolution than that of the observed spectrum of $\Delta \lambda = 0.01$ $\AA$, using eqs. (1), (23), (24), and (25). We synthesise a second spectrum using Monaghan’s algorithm, and compute the logarithmic difference $\delta V$ between these two synthetic spectra in the same fashion as in the previous section. In this way, we test again our method against the highest-precision method available, for a typical range in column densities and Doppler parameters present in a QSO spectrum. The result is shown in Figure 7. The upper panels of each row show the observed spectrum and the spectrum synthesised using our method, whereas the lower panels show the logarithmic difference between both synthetic spectra. We choose to cut off the logarithmic difference at $10^{-16}$, since differences smaller than these are out of the range of the highest available numerical precision. It can be seen again, as in Figure 6, that the smallest discrepancies are given at the line cores, and the largest, of the order of $10^{-4}$, are given at the wings (cf. discussion of Figure 6 Section 5). As can be seen from the column density and Doppler parameter distribution in Figure 7, the largest discrepancies in this wavelength range are consistent with the maximum absolute differences shown in Figure 6. Note that in the spectral regions where no apparent absorption features are found, the logarithmic difference does not fall to $-\infty$, as one would naively expect. These features are present in Figure 6 as well. The reason for this ‘valley-shaped’ features is that, even though having small values away from the line center, the function $H$ does not fall to zero, and thus in these regions the wings of two or more lines overlap. Strictly speaking, in these regions there is always some absorption left, i.e. $\tau < 1$, and different methods to compute $H$ will account for this effect differently. Again, since our method neglects terms of order $n \neq 2$, the absorption in these regimes differs from its fiducial value. The lack of this terms in our approximation to $H$ is also pointed out pictorially by the local maxima symmetrically placed around the deeps corresponding to the logarithmic differences at the line cores.

7 SUMMARY

The absorption lines imprinted in the spectra of background sources yield a wealth of information about the physical and chemical properties of the intervening absorbing material, as is the case of intervening neutral hydrogen (HI) systems embedded in the intergalactic medium (IGM) and associated with galaxies and larger structures. In order to extract the desired information from these absorp-
tion lines, their profiles have to be modeled in a proper way. In the case of absorption features found on QSO spectra, absorption line profiles are best modeled by Voigt profiles, which are mathematically given in terms of the Voigt-Hjerting function.

In this work, we presented a simple analytic approximation to the Voigt-Hjerting function with which Voigt profiles can be modeled for an arbitrary range in wavelength (or frequency), column densities up to $10^{22}$ cm$^{-2}$, and for damping parameters satisfying $a \lesssim 10^{-4}$. Starting with an exact expression for the Voigt-Hjerting function in terms of Harris’ expansion that is valid for $a < 1$, we showed that the zeroth order term of this series, a Gaussian function, is suitable for modeling absorption line profiles emerging in a medium with low column density $N_{\text{HI}} \lesssim 10^{15}$ cm$^{-2}$. However, for higher column densities, terms of higher order have to be taken into account. A key point leading to this conclusion is the fact that it is not the damping parameter alone, but rather the factor $a \cdot N_{\text{HI}}$ that determines to which extent terms of order higher than zeroth in Harris’ expansion may or may not be neglected. We showed that the departure of the actual Voigt-Hjerting function from the first two terms in Harris’ expansion is of the order of $10^{-7}$ or less for an arbitrary wavelength range and $a \lesssim 10^{-4}$. Hence, we concluded that with an approximation to first order in $a$ to the Voigt-Hjerting function Voigt profiles can be modeled with moderate to high accuracy.

On this basis, we obtained a simple analytic expression for the Voigt-Hjerting function and consequently for the absorption coeffi-
cient of intergalactic HI, in terms of an approximation for the second term $H_1$ of Harris’ expansion. The main advantages of the analytic expression we presented here are, first, that it is valid for an arbitrary wavelength range, in the sense that is has no singularities. In addition, it is simple and flexible to implement in a variety of programming languages to numerically compute Voigt profiles with moderate speed and moderate to high accuracy. As a matter of fact, our method to compute the Voigt-Hjerting function is faster with respect to other known standard methods, for instance, Humlíček’s or Monaghan’s algorithm. Furthermore, our approximation reaches an accuracy of $10^{-4}$ or better in a wide wavelength range, and of the order of $10^{-2}$ only a negligible wavelength interval, for values of $a$ and $N_{\text{HI}}$ characteristic to intergalactic HI absorbers. Our method thus offers a great compromise between speed, accuracy, and flexibility in its implementation.

Even though we did not extend our discussion in this work to other transitions typically present in quasar absorption spectra and associated to HI absorbers, such as metal lines, our method to synthesise Voigt profiles can certainly be applied to most of these elements as well, since their column densities are obviously the same, and their ranges in $a$ strongly overlap with the range of $a$ for intergalactic HI, for which our approximation to the Voigt-Hjerting function is valid. As a matter of fact, our approximation is valid to model absorption Voigt profiles found in any type of spectrum (stellar, solar, etc.), which arise in a medium whose damping parameter and column density satisfy $a \lesssim 10^{-4}$ and $N_{\text{HI}} \lesssim 10^{22}$ cm$^{-2}$, respectively.

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