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A modified formula for the Voigt spectral line profile

G D Roston, M F Ahmed, M S Helmi and O S Mahran
Department of physics – Faculty of science - Alexandria University-Egypt

Abstract. A modified formula for the Voigt spectral line profile has been obtained. The Voigt formula has been transferred from the integral formula to a second order differential equation. It was found that the results of the obtained formula are in a perfect agreement with the corresponding published results which are obtained by different numerical calculation methods for a wide range of the line damping parameter (a) for $(0 \leq a \leq 200)$. Also, four special formulas are obtained at different ranges of the line profile, Gaussian profile at (a → 0), Lorentzian profile at (a → ∞), line center at (x → 0) and line wings at (x→ ∞).

1. Introduction

The spectral line pressure broadening can be described using the Voigt profile which is a convolution of both Doppler and Lorentzian profiles which is given by:

$$V\,(a,\,x) = \frac{\boldsymbol{a}}{\boldsymbol{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\,(y)^{2}}}{\boldsymbol{a}^{2} + (\boldsymbol{x}-\boldsymbol{y})^{2}}\, dy \tag{1}$$

Where (a) is the spectral line damping parameter which is given by

$$a = \sqrt{ln2} \cdot \frac{\Delta\nu_L}{\Delta\nu_D} \qquad \text{and} \qquad x = 2\sqrt{ln2}\,\frac{(\nu_0-\nu-\Delta\,)}{\Delta\nu_D}$$

Here, $\Delta\nu_L$ and $\Delta\nu_D$ are the Lorentzian and Doppler widths and Δ is the pressure shift of the spectral line with respect to the unperturbed frequency ν_0. Many accurate tables of the Voigt profile [1-4] have been developed for some values of the parameter (***a***). G. D. Roston and F. S. Obeid [4] obtained an analytical formula for this profile as a solution of the second-order differential equation using homogeneous and non-homogeneous solutions for some values of (**a**) $(0 \leq a \leq 1)$, but the obtained formula obtained by [4] contain two terms which should be solved numerically. The aim of this work is to convert those two numerical terms to analytical terms to obtain a total analytical formula for the Voigt spectral line profile.

2. Theoretical

According to Roston and Obaid [4] and Andersen [5], the Voigt profile has been converted from the integral formula to the second- order differential equation as:

$$\frac{\partial^2 V(a,x)}{\partial x^2} + 4\,x\,\frac{\partial V(a,x)}{\partial x} + (4\,a^2 + \,4x^2 + \,2)V = \frac{4a}{\sqrt{\pi}} \tag{2}$$

The solution of Eq. (2) is obtained by [6] as

$$V(x) = e^{a^2-x^2} cos(2ax)erfc(a) - \frac{2}{\sqrt{\pi}}e^{-x^2}$$

$$[\cos(ax)\int_0^x sin\,(2ax)\;e^{x^2} - sin(2ax)\int_0^x \cos(2ax)\,e^{x^2}dx] \tag{3}$$

Where **erfc** is the complementary error function. Eq. (3) was not totally analytical, the second and the third terms should be solved numerically. For that, the two integrals must be converted to analytical formulas as follows:

(1). $\int_0^x sin(2ax)\ e^{x^2} dx = \frac{1}{2i} \int_0^x e^{x^2} \left(e^{2iax} - e^{-2iax}\right) dx$

$$= [\tfrac{1}{2i} \cdot \tfrac{1}{2} \sqrt{\pi} e^{a^2} erfi(x + ia) - \tfrac{1}{2i} \cdot \tfrac{1}{2} \sqrt{\pi} e^{a^2} erfi(x - ia)]_0^x$$

$$= \frac{1}{4} \sqrt{\pi}\ e^{a^2} \left[erf(a - ix) + erf(a + ix) - 2erf(a)\right] \tag{4}$$

(2). $\int_0^x cos(2ax)\ e^{x^2} dx = \frac{1}{2} \int_0^x e^{x^2} \left(e^{2iax} + e^{-2iax}\right) dx$

$$= [\tfrac{1}{2} \cdot \tfrac{1}{2} \sqrt{\pi} e^{a^2} erfi(x + ia) + \tfrac{1}{2} \cdot \tfrac{1}{2} \sqrt{\pi} e^{a^2} erfi(x - ia)]_0^x$$

$$= \frac{i}{4} \sqrt{\pi}\ e^{a^2} \left[erf(a - ix) - erf(a + ix)\right] \tag{5}$$

By inserting Eq. (4) and Eq. (5) in Eq. (3) we get:

$$V\ (a,x) = erfc(a)\ e^{a^2 - x^2} cos(2ax) - \frac{2}{\sqrt{\pi}} e^{-x^2} \{\tfrac{1}{4} \sqrt{\pi}\ e^{a^2} cos(2ax)\ [erf\,(a\text{-}ix)$$

$$+ erf\,(a+ix) - 2erf\,(a)] - \tfrac{i}{4} \sqrt{\pi}\ e^{a^2}\ sin\,(2ax)\ \ [erf\,(a\text{-}ix) - erf\,(a+ix)]\}$$

$$= e^{a^2 - x^2} \{erfc\ (a)\ cos(2ax) - \tfrac{1}{2} [\ cos(2ax)\ [erf\,(a\text{-}ix) + erf\,(a+ix)$$

$$- 2erf\,(a)] - isin(2ax)\ [erf\,(a\text{-}ix) - erf\,(a+ix)]]\} \tag{6}$$

The two functions *erf* (*a-ix*) and *erf* (*a*+*ix*) given by Abramowitz and Stegun [6] as:

1. $erf\,(a\text{-}ix) = erf\,(a) + \frac{e^{-a^2}}{2\pi a}[(1 - \cos(2ax)) - i\sin(2ax)]$

$$+ \frac{2}{\pi} e^{-a^2} \sum_{n=1}^{\infty} \frac{e^{-n^2/4}}{n^2 + 4a^2} [\ f_n(a,x) - iR_n(a,x)] + \varepsilon(a,x)$$

2. $erf\,(a+ix) = erf\,(a) + \frac{e^{-a^2}}{2\pi a}[(1 - \cos(2ax)) + i\sin(2ax)]$

$$+ \frac{2}{\pi} e^{-a^2} \sum_{n=1}^{\infty} \frac{e^{-n^2/4}}{n^2 + 4a^2} [\ f_n(a,x) + iR_n(a,x)] + \varepsilon(a,x)$$

The functions $f_n(a,x)$, $R_n(a,x)$ and $\varepsilon(a,x)$ are given by Abramovitz and Stegun [6] as:

$f_n(a,x) = 2a - 2a\ cosh\ (nx)\ cos\ (2ax) + nsinh\ (nx)\ sin\ (2ax)$

$R_n(a,x) = 2a\ cosh\ (nx)\ sin\ (2ax) + n\ sinh\ (nx)\ cos\ (2ax)$, $\quad \varepsilon(a,x) \approx 10^{-16}\ |erf(a + ix)|$.

Introducing the expansions of erf (*a-ix*) and erf (*a*+*ix*) in Eq. (6) we get:

$$V(a,x) = e^{-x^2} \{erfc\ (a) \cos(2ax) e^{a^2} + \frac{1}{2\pi a} (\cos^2(2ax) + \sin^2(2ax)) - \frac{1}{2\pi a} (cos(2ax)$$

$$+ \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{e^{-n^2/4}}{n^2 + 4a^2} [sin(2ax)\ R_n(a,x) - cos(2ax) f_n(a,x)]\} \tag{7}$$

The obtained formula is in agreement with the formula obtained by Limandri et al [7]. Substituting the values of $f_n(a,x)$ and $R_n(a,x)$ in Eq. (7), we get

$$V(a,x) = e^{-x^2}\{erfc(a)\, e^{a^2}\cos(2ax) + \frac{1}{2\pi a}(1-\cos(2ax)) + \frac{4a}{\pi}\sum_{n=1}^{\infty}\frac{e^{-n^2/4}}{n^2+4a^2}[\cosh(nx)-\cos(2ax)] \quad (8)$$

This is the final formula for the Voigt profile, which is valid in the wide range of spectra [$0 \leq a \leq 5$ and $-10 \leq x \leq 10$], but for $a > 5$, erfc (a) in the first term of Eq. (8) is very small and approaches to zero. For that, the expansion of [$erfc(a)\, e^{a^2}$] given by [1] can be used as:

$$erfc(a)\, e^{a^2} = \frac{1}{\sqrt{\pi}}\frac{1}{a}\sum_{n=0}^{\infty}\frac{(-1)^n(2n)!}{n!(2a)^{2n}} \quad (9)$$

By substituting Eq. (9) in Eq. (8), we have

$$V(a,x) = e^{-x^2}\{\frac{1}{\sqrt{\pi}}\frac{1}{a}\sum_{n=0}^{\infty}\frac{(-1)^n(2n)!}{n!(2a)^{2n}}\cos(2ax) + \frac{1}{2\pi a}(1-\cos(2ax)) + \frac{4a}{\pi}\sum_{n=1}^{\infty}\frac{e^{-n^2/4}}{n^2+4a^2}[\cosh(nx)-\cos(2ax)]\} \quad (10)$$

This formula is valid for larger values of (a) [$5 < a \leq 15$ and $-10 \leq x \leq 10$].

Special cases at different ranges of the line profile

1-At ($a \simeq 0$) , $V(0, x) = e^{-x^2}$ (Doppler profile) .

2-At ($a \simeq \infty$), $V(a \to \infty, x) = \frac{1}{\sqrt{\pi}}\frac{a}{a^2+x^2}$ (Lorentzian profile)

This formula is valid for [$15 < a \leq 200$ and $-200 \leq x \leq 200$].

3-At the line center where ($\nu = \nu_0$) and $x = 0$, $V(a, 0) =$ erfc $(a)\, e^{a^2}$

4-At the line wing where ($x = \infty$), $V(a, x \to \infty) = \frac{1}{\sqrt{\pi}}\frac{a}{x^2}$

3. Results and discussions

3.1.The effect of (n) parameter

As the Voigt profile (Eqs.8,10) is dependent on the number of summation (n) which effects on the shape and the accuracy of the spectral line, It was found that the best fitting between the calculated profiles and the corresponding numerical profiles takes place at (n =25), and for n > 25 does not make any variations. For small values of (a) [0.01 - 4] we get a good fitting at of (n) [7 - 20] as shown in Fig.(1) with the fitting polynomial equation given by:

$$n = 6.02 + 8.214a - 1.179a^2.$$

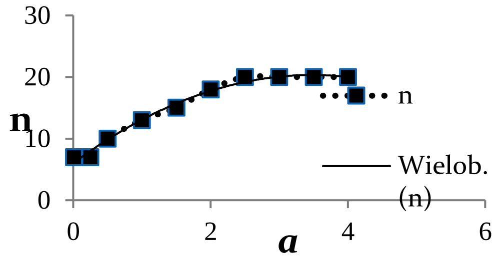

Figure (1): The relation between the values of (n) and the damping parameter (a) [0.01 – 4] and the fitting polynomial equation

3.2 Comparison between the obtained and the corresponding published results

The comparison between the results of the obtained formulas and the corresponding published data of [1-3] are illustrated in the table.

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Table: The comparison between the obtained results and Mofreh R.Zaghloul [1], Mamedov [2] and Z.Shippony and W.G.Read[3].

x	This work	Zaghloul [1]
At damping parameter (*a* = 0.01)		
1	0.368702417397766	0.368702416670236
2	0.0206200654455691	0.0206200653731694
3	0.000908830706741581	0.000908830706010574
4	0.000392604421617868	0.00039260442161698
5	0.00030237707114623	0.000240803391951175
At damping parameter (a = 0.5)		
1	0.354900332867578	0.354900332432228
2	0.103358823741367	0.103358823749883
3	0.037126366054692	0.037126366055133
4	0.019224945518739	0.019224945518740
5	0.011900325522594	0.011900325522594
At damping parameter (a = 5)		
1	0.106797738398065	0.106797738687967
2	0.0964981126066414	0.0964981125848205
3	0.0829877379769018	0.082987737977024
4	0.0692362095804915	0.0692362095804913
5	0.056965439888177	0.0569654398881766
At damping parameter (a = 15)		
1	0.0373653474578327	0.0373653478628073
2	0.0368810149294909	0.0368810149383951
3	0.0361008874912074	0.0361008874910956
4	0.035062152853902	0.0350621528539018
5	0.0338107397543061	0.033810739754306

x	This work	Mamedov [2]
At damping parameter (a = 0.01)		
1.00E-09	9.88815461046343E-01	9.88815461046342E-01
5.00E-05	9.88815458602020E-01	9.88815458602018E-01
1.00E-04	9.88815451269048E-01	9.88815451269048E-01
5.00E-02	9.86374167467079E-01	9.86374167467078E-01
2	2.06200654455691E-02	2.06200654455695E-02
9	7.09844469661236E-05	7.09844886591770E-05
At damping parameter (a = 0.5)		
1.00E-09	6.15690344192926E-01	6.15690344192925E-01
5.00E-05	6.15690362791042E-01	6.15690343294561E-01
1.00E-04	6.15690418585387E-01	6.15690340599466E-01
5.00E-02	6.14792754945695E-01	6.14792754945695E-01
2	1.03358823741367E-01	1.03358823741366E-01
9	3.53780588850978E-03	3.53780778549224E-03
At damping parameter (a = 5)		
1.00E-09	1.10704637733069E-01	1.10704637793912E-01
5.00E-05	1.10704637722967E-01	1.10704637715343E-01
1.00E-04	1.10704637692662E-01	1.10704637694591E-01
5.00E-02	1.10694536873867E-01	1.10694536864910E-01
2	9.64981126066414E-02	9.64948274000898E-02
9	2.68729312688368E-02	2.68729317409139E-02

x	(This work)	Z.Shippony and W.G.Read [3]
At damping parameter (*a* = 1)		
1	0.304744205256913	0.3047442052569126
2	0.140239581366278	0.1402395813662779
3	0.065317777289047	0.0653177772890470
4	0.0362814564899886	0.0362814564899886
5	0.023003132594060	0.0230031325940600
At damping parameter (a = 2)		
1	0.218492615274891	0.2184926152748907
2	0.147952759512016	0.1479527595120158
3	0.0927107664264434	0.0927107664264433
4	0.0596869296104459	0.0596869296104459
5	0.0406436763334944	0.0406436763334944
At damping parameter (a = 3)		
1	0.129888159930841	0.1298881599308405
2	0.112139477902116	0.1121394779021160
3	0.0909339041947653	0.0909339041947653
4	0.0715704334263653	0.0715704334263653
5	0.0559973771425239	0.0559973771425239
At damping parameter (a = 4)		
1	0.164261136392986	0.1642611363929863
2	0.130757469669849	0.1307574696698486
3	0.0964025055830446	0.0964025055830445
4	0.0697909616496483	0.0697909616496483
5	0.0512259965673866	0.0512259965673866
At damping parameter (*a* = 5)		
1	0.106797738398065	0.1067977383980653
2	0.0964981126066414	0.0964981126066414
3	0.0829877379769018	0.0829877379769018
4	0.0692362095804915	0.0692362095804914
5	0.056965439888177	0.0569654398881770

It is seen from the last tables that the results of the obtained formulas are in good agreement with the corresponding theoretical and numerical values.

4. Conclusions

1-A modified formulas for the Voigt profile Eq. (8, 10) makes the calculation of the Voigt profile easier in a wide range of the spectral line profile.

2-Using the obtained formulas, four special formulas were also obtained for [($a \to 0$) Gaussian profile, ($a \to \infty$) Lorentzian profile , for ($x \to 0$) at line center and ($x \to \infty$) at line wing].

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