



Mathematical Analysis of Asymmetrical Spectral Lines. Case study: Exponentially Modified Functions

J. Dubrovkin

Computer Department, Western Galilee College
2421 Acre, Israel

Abstract: Asymmetrical spectral lines were modeled as a set of exponentially modified asymmetrical functions which were decomposed into a weighted sum of symmetrical and asymmetrical parts. In each model the asymmetrical part was equal to the first-order derivative of the symmetrical part. Invariant expressions of the first three central statistical moments of these lines have been found. Maximum peak positions and widths of the lines and of their symmetrical parts were evaluated numerically. Asymmetrical lines were also studied using their decomposition to the product of symmetrical and asymmetrical parts.

Keywords: asymmetrical line modeling; exponentially modified functions; statistical moments.

I. Introduction

Spectrometry is one of the most widespread theoretical and experimental physical methods, which has been employed in various fields of science and technology for more than a century [1]. Measured spectra are usually a set of overlapping spectral lines and bands (elementary spectral components- ESCs) which parameters are the main information source of the qualitative and quantitative properties of the samples under study. Precise determination of these parameters often requires spectral curve fitting to some modeling functions especially in the case of strongly overlapped ESCs [2]. If lines and bands are symmetrical then they are usually approximated by Gaussian, Lorentzian and Voigt functions. However, in real life, symmetrical ESCs are disturbed by the inter- and intra-atomic and molecular interactions [1, 3] and by spectral instruments (e.g., due to the non-zero time constant of the fast-scan instruments [4]). This is why, symmetrical functions have been modified by introducing asymmetry which was controlled by the asymmetry parameters [5, 6]. Symmetry means that the asymmetry parameters are zero.

The line shape theory in spectroscopy and chromatography has been discussed in numerous studies; many analytical expressions for line shapes were theoretically obtained (see references in [1-6]). However, these expressions are not often useful for practical applications. Therefore, it is common to describe ESCs by mathematical functions which are approximations to theoretical models or experimentally obtained data. This method includes phenomenological approach which is based on the choosing the model parameters for the best model fitting to the measured analytical signal without rigorous physical foundation. It is very important to underline that there is no "universal" modeling function that can describe all asymmetry ESCs. However, choosing physically-based line models is the preferred method in this case. In this connection the exponentially modified Gaussian model [7] is interesting since it reflects the impact of the first-order decay in the measuring tool on the obtained signal dependence on time (e.g., on chromatographic peak [7]).

Earlier we performed mathematical analysis of the non-integral asymmetry ESCs by decomposing these components into a product of symmetrical and asymmetrical parts [6]. The dependences of the maximum peak positions and the widths of ESCs on the asymmetry parameters have been estimated. In the present study we describe a set of the exponentially modified symmetrical functions which will be used for approximating asymmetrical ESCs. Our goal is to develop flexible mathematical models of asymmetrical spectral components. For simplicity, we use the short term "line" instead of the long term "line and band". The standard algebraic notations are used throughout the article. All calculations were performed and the plots were built using the MATLAB program.

II. Theory

Consider symmetrical Gaussian, Lorentzian and Voigt lines which maxima are located at zero on the x axis, and their intensities are equal to one [1]:

$$F_G(x) = \exp(-x^2), \quad (1)$$

$$F_L(x) = 1/(1+x^2), \quad (2)$$

$$F_V(x) = \int_{-\infty}^{\infty} F_G(x's_G) F_L((x-x')s_L) dx', \quad (3)$$

where $x = \beta i/w$; $\beta_G = 2\sqrt{\ln 2}$ and $\beta_L = 2$ are the line shape parameters for (1) and (2), respectively; $i = -m, -m+1, \dots, 0, \dots, m-1, m$; w is the full line width at half maximum, $s_G = w/w_G$, and $s_L = w/w_L$.

The full line width of the Voigt line [8]:

$$w_V = 0.5346w_L + \sqrt{0.2166w_L^2 + w_G^2} \quad (4)$$

It is follow from Eq.4 that if $w_V = 1$, then

$$w_G = \sqrt{(1 - w_L)(1 - 0.0692w_L)} \cong \sqrt{1 - w_L}, \quad (5)$$

where $w_L \in [0, 1]$.

Suppose that in the first approximation a measured line is obtained by convolution of the ideal line with an exponential decay kernel function (K):

$$F_{ms}(x) = \int_{-\infty}^{\infty} K(x - x') F(x') dx', \quad (6)$$

where

$$K(t) = (1/\tau) \exp(-t/\tau), \quad (7)$$

$t = x - x' \geq 0$, τ is the asymmetry parameter (e. g., it is the instrument time constant).

Substituting Eq.7 into Eq.6 and setting $x' = x - t$, we have [9]:

$$F_{ms}^G(x) \sim \exp(-x/\tau) \operatorname{erfc}(1/2\tau - x), \quad (8)$$

where erfc is the complementary error function.

If for $\tau > 0$ $1/2\tau - x \gg -1$ then $\operatorname{erfc}(1/2\tau - x) \rightarrow 2$, therefore the right wing of $F_{ms}^G(x)$ decays exponentially.

Since derivation of the precise analytical expression for convoluted Lorentzian (2) using elementary functions is very cumbersome [9], the numerical calculation has been performed using Fourier transform (FT) method.

It was found that the MATLAB function $\operatorname{erfc}(1/2\tau - x)$ failed when $\tau \rightarrow 0$. Therefore, the frequency domain (ω) convolution was performed instead of Eq.6:

$$\tilde{F}_{ms}(\omega) = \tilde{K}(\omega) \tilde{F}(\omega), \quad (9)$$

where tilde is the sign of Fourier transform,

$$\tilde{K}(\omega) = 1/(1 + j\omega\tau), \quad (10)$$

$$\tilde{F}_G(p) = w \sqrt{\pi}/\beta_G \exp(-p^2/4\beta_G^2), \quad (11)$$

$$\tilde{F}_L(p) = w\pi/\beta_L \exp(-|p|/\beta_L), \quad (12)$$

$$\tilde{F}_V(p) = \tilde{F}_G(p_G) \tilde{F}_L(p_L), \quad (13)$$

$j = \sqrt{-1}$, $p = w\omega$.

Spectra in the spatial domain are obtained by the inverse FT (IFT) of Eq. 9. Since Eqs. 11 and 12 are even functions, a measured line can be represented as the sum of symmetrical and asymmetrical parts:

$$F_{ms}(x) = (F_{ms}^{sym}(x))^+ + (F_{ms}^{asym}(x))^+, \quad (14)$$

where

$$(F_{ms}^{sym}(x))^+ = 2 \int_0^{\infty} \frac{\tilde{F}(\omega) \cos(\omega x)}{1 + \tau^2 \omega^2} d\omega, \quad (15)$$

$$(F_{ms}^{asym}(x))^+ = 2\tau \int_0^{\infty} \frac{\tilde{F}(\omega) \sin(\omega x)}{1 + \tau^2 \omega^2} \omega d\omega \quad (16)$$

According to Eqs. 15 and 16, Eq. 14 is the weighted sum of symmetrical part and its derivative:

$$F_{ms}(x) = (F_{ms}^{sym}(x))^+ - \tau d(F_{ms}^{sym}(x))^+/dx \quad (17)$$

The common calculation method of the statistical moments of Gaussian line was described by [7]. We used other method based on the decomposition (17) (see Appendix A). It was shown that the first and the third central statistical moments (μ) do not depend on the symmetrical part $(F_{ms}^{sym}(x))^+$, if the derivatives of the Fourier transform of any line at the origin are continuous:

$$\mu_1 = \tau, \quad \mu_3 = 2\tau^3 \quad (18)$$

Since the 1st-order derivative of the FT of Lorentzian line has discontinuity in zero point, the moments have been obtained numerically:

$$\mu_1 \cong 0.9777\tau, \quad \mu_3 \cong 1.826\tau^3 + 0.045\tau^2 - 4.593\tau \quad (19)$$

Eqs. 18 are easily obtained for Losev model [10] by decomposing the model into a product of symmetrical and asymmetrical parts [6]. The symmetrical part is equal to

$$(F_{ms}^{sym}(x))^* = \operatorname{sech}(x), \quad (20)$$

where $\operatorname{sech}(x)$ stands for the hyperbolic secant.

Substituting Eq. 10 and Fourier transform of Eq. 20 [11] into Eq. 9, we have

$$\tilde{F}_{ms}(\omega) = \sqrt{\pi/2} \operatorname{sech}(\pi\omega/2)/(1 + j\omega\tau) \quad (21)$$

The next step in the calculation of moments (18) is differentiation of Eq. 21 (Eq. A1).

Eq. 17 can be slightly modified:

$$F_{ms}(x) = (F_{ms}^{sym}(x))^+ - q\tau d(F_{ms}^{sym}(x))^+/dx, \quad (22)$$

where $q \in [0, 1]$ is the weight of the derivative of the symmetrical part. Coefficient q controls the line asymmetry for a given constant symmetrical part. The odd-order moments (Eq. 18) are:

$$\mu_1 = q\tau, \quad \mu_3 = 2(q\tau)^3 \quad (23)$$

The family of simple functions F_{ms}^{sym} is easily obtained in the frequency domain using symmetrical part of Fourier transformed Gaussian line (Eq.11, $w = 1$) :

$$\tilde{F}_{ms}^{sym}(\omega) \sim \exp(-\omega^2/16\ln 2)/(1 + \tau^2 \omega^2)^n, \quad (24)$$

where $n \geq 1$ may be a fraction. Equation similar to (24) is constructed for Losev model (Eq. 20):

$$\tilde{F}_{ms}^{sym}(\omega) \sim \text{sech}(\pi\omega/2)/(1 + \tau^2 \omega^2)^n, \quad (25)$$

where $n \geq 0$. The odd-order moments of the modified functions (Eqs. 24 and 25) are represented by Eqs. 23.

The second-order central moment of the F_{ms} (Eq. 24) depends only on the symmetrical part (see Appendix A):

$$\mu_2 = C + 2n\tau^2, \quad (26)$$

where $C = 1/8\ln 2$ and $\pi^2/4$ for Gaussian (Eq. 24) and Losev line (Eq. 25), respectively. It is common to use *skewness* as a measure of the asymmetry of spectral lines:

$$\gamma_{as} = \mu_3/\mu_2^{3/2} \quad (27)$$

Substituting Eqs. 23 and 26 into Eq. 27, we have

$$\gamma_{as} = 2q^3/(2n + C/\tau^2)^{3/2} \quad (28)$$

It is known that the value of γ_{as} strongly depends on the range of integration while calculating the central moments. This is an essential drawback because, in practice, the range of integration is limited by the finite wings of the observed line profiles. Therefore, instead of the skewness, we introduced [6] the ratios of: the first-order derivative extremes:

$$\gamma_{d1} = F'_{max}/|F'_{min}| \quad (29)$$

and of the amplitudes of the left and the right satellites in the second-order derivative:

$$\gamma_{d2} = F''_{sL}/F''_{sR} \quad (30)$$

Coefficient γ_{d2} is indicative of the line asymmetry at larger distances from the line centre than γ_{d1} .

Asymmetrical line may be represented as a sum the even and the odd parts in the spatial domain without applying IFT. (see Appendix B). Particularly, for Dobosh model [12]:

$$(F_{ms}^{even}(x))^+ = (\exp(\tau)/(1 + x^2)) \cosh(\tau \operatorname{atan}(x)), \quad (31)$$

where *cosh* stands for the hyperbolic cosine. In this case the term $(\tilde{F}_{ms}^{sym}(x))^+$ in Eq. 22 and in the following equations is replaced by $(F_{ms}^{even}(x))^+$. However, generally speaking, $(F_{ms}^{even}(x))^+ \neq (\tilde{F}_{ms}^{sym}(x))^+$.

Line asymmetry can be also studied by decomposition of $F_{ms}(x)$ to the product of symmetrical and asymmetrical parts [6]. However, here we used more general mathematical equations:

$$F_{ms}(x) = (F_{ms}^{sym}(x))^+ + (F_{ms}^{asym}(x))^+ = (F_{ms}^{sym}(x))^+ (F_{ms}^{asym}(x))^*, \quad (32)$$

where

$$(F_{ms}^{asym}(x))^* = 1 + (F_{ms}^{asym}(x))^+/(F_{ms}^{sym}(x))^+, \quad (33)$$

$$(F_{ms}^{asym}(x))^+ = -q\tau d(F_{ms}^{sym}(x))^+/dx. \quad (34)$$

Eq. 34 and the second term of Eq. 22 are similar.

For the modified Losev model (Eqs. 20 and 22) Eq. 33 has simple analytical form:

$$(F_{ms}^{asym}(x))^* = 1 + \tau q * \tanh(x), \quad (35)$$

where *tanh*(*x*) stands for the hyperbolic tangent.

The asymptotic properties of Eq. 35 are

$$(F_{ms}^{asym}(x))^* \rightarrow \begin{cases} 1 + \tau q, x \rightarrow +\infty \\ 1 - \tau q, x \rightarrow -\infty \end{cases} \quad (36)$$

For the modified Dobosh model (Eqs. B4 (Appendix) and 33)

$$(F_{ms}^{asym}(x))^* = 1 - \tau q (\tau \tanh(\operatorname{atan}(x)) - 2x)/(1 + x^2) \quad (37)$$

For $|x| \rightarrow \infty$ $(F_{ms}^{asym}(x))^* \rightarrow 1$.

III. Computer modelling

The dependences of the maximum peak position on the asymmetry parameter for the exponentially modified Gaussian, Lorentzian, Voigt, and Losev lines are given in Fig. 1. The quantitative relationships between line asymmetry and parameters x_m and μ is established in chromatography by asymmetry factor [7]:

$$\chi = (x_m - t_0)/(\mu_1 - t_0), \quad (38)$$

where t_0 is the hold-up time. In spectroscopy t_0 can be approximately defined as a *x*-value for which the line intensity is equal to the baseline level. From Fig. 1 it is seen that for $\tau \ll 1$ $x_m \cong \tau = \mu_1$ (Eq. 18), and $\chi \cong 1$. If the asymmetry parameter increases then $x_m < \mu_1$ and $\chi > 1$, since $|t_0| \gg x_m$.

For given τ

$$x_m^{Gauss} \leq x_m^{Voigt} \leq x_m^{Lorentz} \quad (39)$$

Maximum peak position of high asymmetrical lines is significantly shifted from zero point (Fig 1) and the lines are broadened (Fig.2). The symmetrical parts become wider than the lines (Fig. 2).

For given τ :

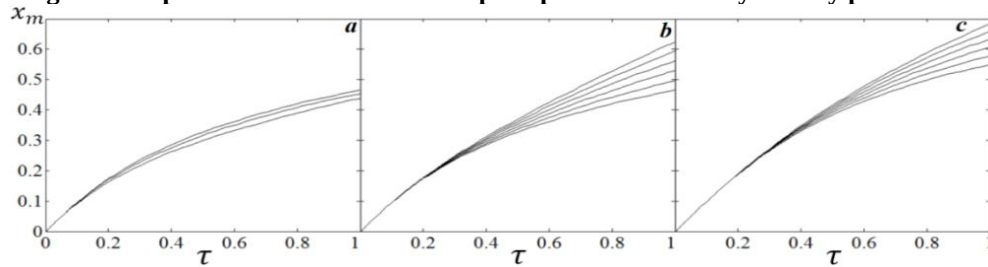
$$w^{Gauss} \leq w^{Voigt} \leq w^{Lorentz} \quad (40)$$

The same results have been obtained for Gaussian line which FT was modified according to Eq. 24 (Fig. 3). However, similar modification of Losev line (Eq. 25) produces dissimilar dependences $w(\tau)$ (Fig.4). It is very interesting that for $n = 0.4$ $w(\tau) \cong w_{LV}^{sym} = 2 \operatorname{arccosh}(2) = 2.6339$ [6].

The dependences of the skewness of Gaussian and Lorentzian lines on the asymmetry parameter differ by sign and magnitude (Fig. 5a). According to Eq. 28 increasing of the weight (q) of the derivative of the line symmetrical part (Eq. 22) significantly increases the skewness. Increasing of parameter n of the modified symmetrical parts (Eq. 24) causes inverse effect. Similar results were obtained numerically for the line asymmetry coefficients γ_{d1} and γ_{d2} (Eqs. 29 and 30). So for a given symmetrical part increasing of the q -value increases γ_{d1} and γ_{d2} (Fig. 5b and c). If n values increase, the symmetrical part and its derivative are changed and lines become more asymmetrical. Changing of the q -values has strong effect on the line form, width and maximum peak position (Figs. 6-8). Shifts of maximum peak positions and line widths increase with increasing asymmetry. So, it can be concluded that required asymmetry may be obtained by varying of the q and n parameters.

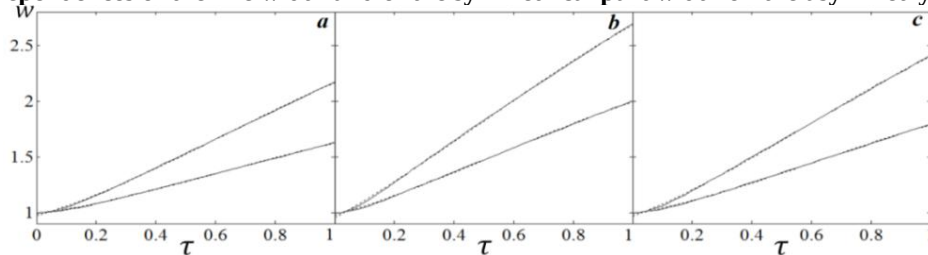
Decomposition of asymmetrical lines to the product of symmetry and asymmetry parts (Eqs. 32 – 34) is illustrated in Figs.9-11. Wings of the asymmetrical parts of Gaussian and Lorentzian lines are significantly

Figure 1. Dependences of the maximum peak position on the asymmetry parameter



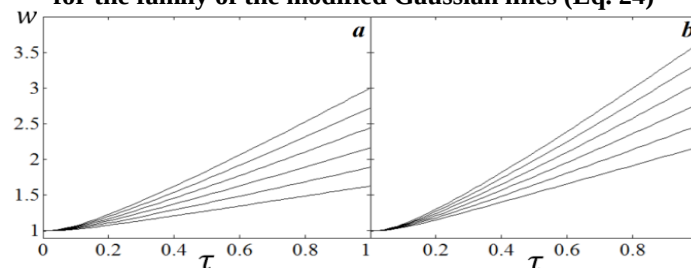
(a) Exponentially modified Gaussian, Voigt ($w_L = 0.5$) and Lorentz lines (from top to bottom plots, respectively). The families of modified Gaussian (Eq. 24) (b) and Losev (Eq. 25) (c) lines. $n = 1, 1.2, \dots, 2$; and $0, 0.2, \dots, 1$, respectively, from bottom to top plots.

Figure 2. Dependences of the line width and of the symmetrical part width on the asymmetry parameter



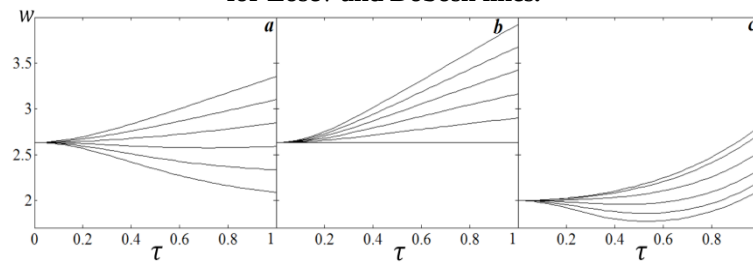
Exponentially modified Gaussian (a), Lorentz (b) and Voigt (c) ($w_L = 0.5$) lines. Bottom and top plots are widths of the lines and of their symmetrical parts, respectively.

Figure 3. Dependences of the line width and of the symmetrical part width on the asymmetry parameter for the family of the modified Gaussian lines (Eq. 24)



Lines (a) and their symmetrical parts (b). $n = 1, 1.2, \dots, 2$ from the bottom to the top plots, respectively.

Figure 4. Dependences of the line width and of the symmetrical part width on the asymmetry parameter for Losev and Dobosh lines.

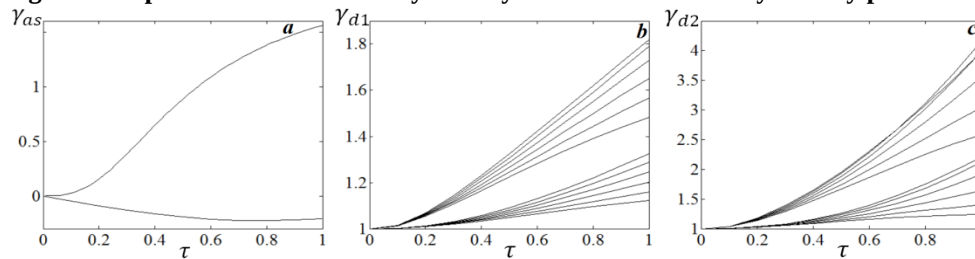


Losev lines (Eq. 25) (a) and their symmetrical parts (b). $n = 0, 0.2, \dots, 1$ from the bottom to the top plots, respectively.

Dobosh lines (c) (Eqs. 22 and 31). $q = 0, 0.2, \dots, 1$ from the top to the bottom plots, respectively.

different (Fig. 9). In contrary, asymmetrical parts of Voigt and Lorentz lines have similar form since the dominant component of the Voigt wings is Lorentzian line. If parameter n (Eq. 24) increases, then symmetrical part is broadened, therefore the slope of the plots $(F_{ms}^{asym}(x))^*$ (Eq. 33) decreases (Fig. 10c).

Figure 5. Dependences of the line asymmetry coefficients on the asymmetry parameter

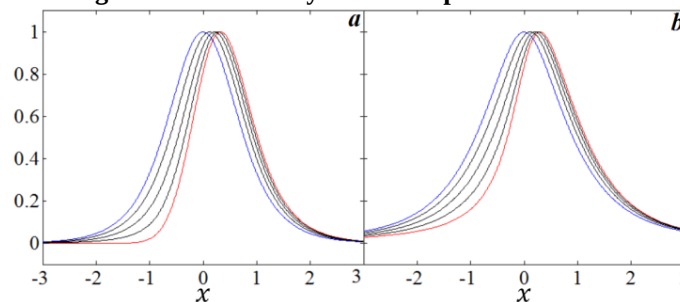


(a) Skewness of Gaussian ($q = 1, n = 1$) and Lorentzian lines (top and bottom plot, respectively).

(b, c) Family of modified Gaussian lines (Eqs. 22 and 24), $q = 0.5$ and 1 for bottom and top groups of the plots, respectively.

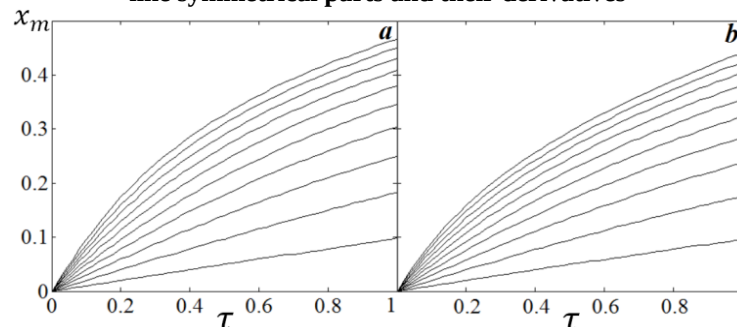
In each group $n = 1, 1.2, \dots, 2$ from the bottom to the top plots, respectively.

Figure 6. Weighted sum of line symmetrical parts and their derivatives



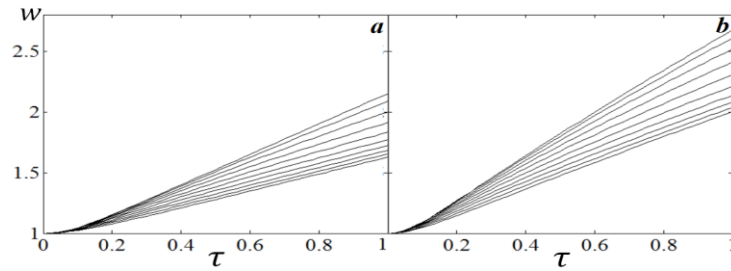
Gaussian (a) and Lorentzian (b) lines. $\tau = 0.5, q = 0, 0.25, \dots, 1$ from the bottom to the top plots, respectively.

Figure 7. Dependences of the maximum peak position on the asymmetry parameter for weighted sum of line symmetrical parts and their derivatives



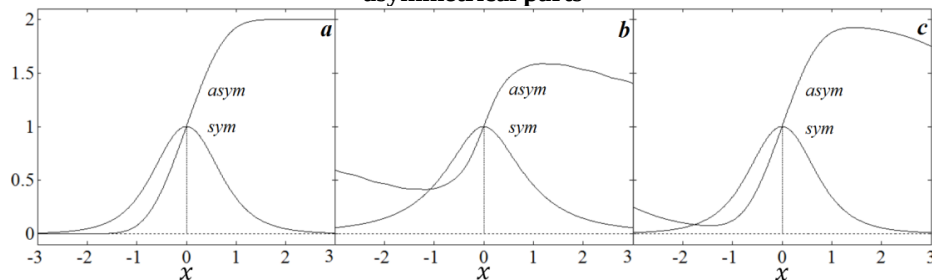
Gaussian (a) and Lorentzian (b) lines. $q = 0, 0.1, \dots, 1$ from the bottom to the top plots, respectively.

Figure 8. Dependences of the line width on the asymmetry parameter for weighted sum of line symmetrical parts and their derivatives



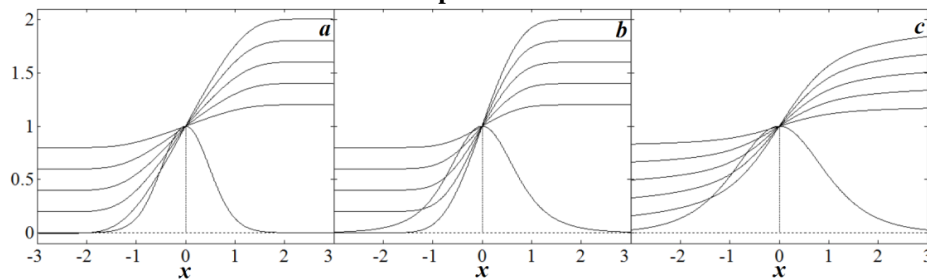
Gaussian (a) and Lorentzian (b) lines. $q = 0, 0.1, \dots, 1$ from the bottom to the top plots, respectively.

Figure 9. Decomposition of Gaussian, Lorentzian and Voigt lines to the product of symmetrical and asymmetrical parts



Exponentially modified Gaussian (a), Lorentz (b), and Voigt (c) ($w_L = 0.5$) lines. $\tau = 0.5$.

Figure 10. Decomposition of the modified Gauss line to the product of symmetrical and asymmetrical parts



(a) $\tau = 0.2, n = 1$, (b) $\tau = 0.5, n = 1$, (c) $\tau = 0.5, n = 2$. $q = 0.2, 0.4, \dots, 1$ from the bottom to the top plots, respectively.

Since the asymmetrical parts of Losev and Gaussian lines have similar form, the asymmetrical parts of Gaussians can be roughly approximated by modified Eq. 36 (Fig. 12):

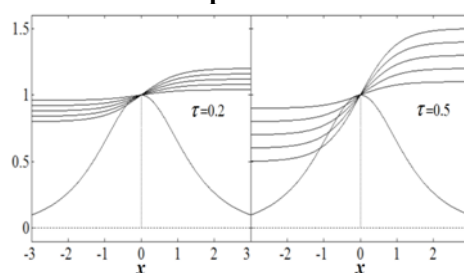
$$(F_{ms}^{asym}(x))^* = 1 + \rho\tau q * \tanh(\theta x), \quad (41)$$

where $\rho = 2, \theta = 1.6$ for $\tau = 0.5$.

The asymmetrical parts of Lorentzian (Fig. 9b) and Dobosh lines (Fig. 13) are similar, since the Dobosh model includes Lorentzian component (Eq. B4 (Appendix B)). The plots $(F_{ms}^{asym}(x))^*$ have extremes which intensities increase with increasing the asymmetry coefficient.

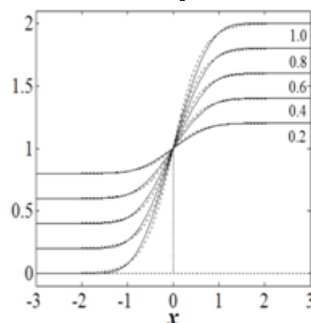
Obtained results clearly demonstrate that decomposition of the asymmetrical lines to the sum and to the product of their symmetrical and asymmetrical parts is useful method for studying the properties of asymmetrical line shapes.

Figure 11. Decomposition of the modified Losev line to the product of symmetrical and asymmetrical parts



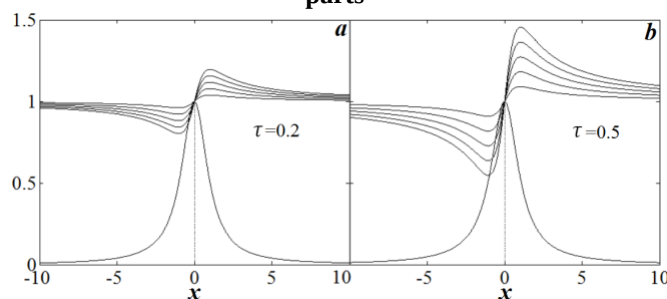
$q = 0.2, 0.4, \dots, 1$ from the bottom to the top plots, respectively.

Figure 12. Approximation of the asymmetrical part of Gaussian line



q -values are given next to the plots. $\tau = 0.5$

Figure 13. Decomposition of the modified Dobosh line to the product of symmetrical and asymmetrical parts



$q=0.2, 0.4, \dots, 1$ from the bottom to the top plots, respectively.

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Appendix

A. Statistical moments of the exponentially modified lines

The n^{th} -order moment of $F(x)$ [7]:

$$M_n = \int_{-\infty}^{\infty} x^n F(x) dx = \tilde{F}^{(n)}(\omega) / (-j)^n, \quad (A1)$$

where tilde stands for the Fourier transform symbol, $\tilde{F}^{(n)}(\omega)$ is the n^{th} -order derivative, ω is the angular frequency, and $j = \sqrt{-1}$. If $F(x)$ can be represented as a sum of symmetrical (F_s) and asymmetrical (F_{as}) parts, then

$$M_n = \int_{-\infty}^{\infty} x^n F_s dx + \int_{-\infty}^{\infty} x^n F_{as} dx = M_n^s + M_n^{as}, \quad (A2)$$

It is easy to show that

$$M_{2t+1}^s = M_{2t}^{as} = 0 \quad (A3)$$

Impact of the line intensity and of the line width on M_n values is eliminated if Eq. A2 is divided by M_0^s .

Using Eq. 17 we obtain:

$$M_{1N} = M_1 / M_0^s = M_1^{as} / M_0^s = (1 / M_0^s) \int_{-\infty}^{\infty} x F_{as} dx = (\tau / M_0^s) \int_{-\infty}^{\infty} x dF_s = (\tau / M_0^s) \int_{-\infty}^{\infty} F_s dx = \tau \quad (A4)$$

Since the derivative of the Fourier transform of Lorentzian line has a discontinuity in the zero point, Eq. A4 is not applicable for this line. However, dependence $M_{1N}(\tau) \cong 0.9777\tau$, numerically obtained in the interval $\tau = [0, 1]$ is very close to Eq. A4.

The central n^{th} -order moment of $F(x)$ [7]:

$$\mu_n = (1/M_0^s) \int_{-\infty}^{\infty} (x - M_{1N})^n F(x) dx \quad (A5)$$

Substituting Eq. A2 into Eq. A5 for $n = 3$ and taking into account that for Gaussian line $\mu_1 = M_{1N}$ and $M_3^{as} = \int_{-\infty}^{\infty} x^3 dF_s = 3\tau M_2^s$, we have:

$$\mu_3 = (-3\tau M_2^s - \tau^3 M_0^s + M_3^{as})/M_0^s + 3\tau^3 = 2\tau^3 \quad (A6)$$

For Lorentzian line dependence $\mu_n(\tau)$, numerically obtained in the interval $\tau = [0, 1]$, is described as

$$\mu_3 \cong 1.826\tau^3 + 0.045\tau^2 - 4.593\tau \quad (A7)$$

Substituting Eq. A2 into Eq. A5 for $n = 2$ and taking into account that $\mu_1 = M_{1N}$, we have:

$$\mu_2 = (M_2^s + \tau^2 M_0^s - 2\tau M_1)/M_0^s = M_2^s - \tau^2 \quad (A8)$$

According to Eqs. A1 and A2 the second-order moment M_2^s is equal to the second-order derivative of the Fourier transform of the line symmetrical part. For modified Gaussian line (Eq. 24):

$$M_2^s = 1/8 \ln 2 + 2n\tau^2 \quad (A9)$$

B. Decomposition of asymmetrical line to the sum of the even and the odd parts

From the following equations

$$F_{ms}(x) = (F_{ms}^{even}(x))^+ + (F_{ms}^{odd}(x))^+, \quad (B1)$$

$$F_{ms}(-x) = (F_{ms}^{even}(x))^+ - (F_{ms}^{odd}(x))^+, \quad (B2)$$

we have

$$(F_{ms}^{even}(x))^+ = (F_{ms}(x) + F_{ms}(-x))/2, \quad (B3)$$

In general case $(F_{ms}^{odd}(x))^+$ is different from the derivative of the symmetrical part (Eq. 34). Particularly for Dobosh model [12]:

$$F_{ms}(x) = \exp(\tau)/(1+x^2) \exp(-\tau \operatorname{atan}(x)), \quad (B4)$$

$$(F_{ms}^{even}(x))^+ = \exp(\tau)/(1+x^2) \cosh(\tau \operatorname{atan}(x)) \quad (B5)$$