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The graphical analysis of a Lorentzian function and a differentiated Lorentzian function

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Abstract. A simple graphical method is proposed for measuring the width of a Lorentzian curve when the base line is uncertain, and is compared with other possible methods. A similar method for measuring the width of a differentiated Lorentzian curve is also given.

1. Introduction

It is a common problem in experimental physics to fit data involving two variables to a theoretical curve containing two unknown parameters, and thence to determine these parameters for the curve of 'best fit'.

In general it is most desirable to solve problems of this type using a computer. However, it is useful to have recourse to a simpler alternative method which could be used if a computer is not available, or if the time required to write a programme is not justified by the extra accuracy obtained.

The possibility of devising an alternative method will depend on the equation of the theoretical curve. If it is of simple mathematical form it is often possible to manipulate its equation so as to allow a 'linear plot' of the data points.

Methods of doing this for a Lorentzian curve, and a differentiated Lorentzian curve, will be discussed.

2. Analysis of a Lorentzian function

2.1. *Thomsen's method*

Thomsen (1966) gives a method of determining the centre of a Lorentzian function (see figure 1) given by

$$y = \frac{A{x_{1/2}}^2}{{x_{1/2}}^2+(x-a)^2}. \qquad (1)$$

The nomenclature is slightly different from Thomsen's. (a, A) are the coordinates of the peak, and $2x_{1/2}$ is the width at half the maximum.

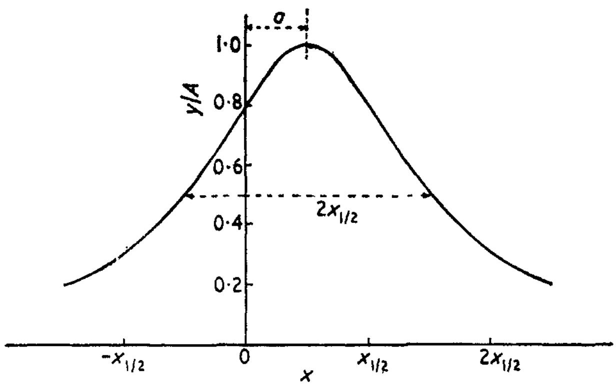

Figure 1. Lorentzian function.

In Thomsen's method, the quantity

$$u = \frac{1}{x}\left(\frac{y_0}{y} - 1\right)$$

is calculated, where y_0 is the value of y at the arbitrarily chosen origin of x. (It is convenient, but not essential, that this origin should be near the centre of the curve.) There is a linear relationship between u and x given by

$$u = \frac{x-2a}{x_{1/2}{}^2 + a^2}.$$

A plot of u against x will therefore give a straight line from which can be determined the value of a and hence the exact x coordinate of the peak.

Although Thomsen's method was devised primarily to determine the x coordinate of the peak, it has two by-products: (i) the value of $x_{1/2}$ from the slope and a, and (ii) the accuracy with which the experimental points can be represented by a Lorentzian function.

2.2. *Effect of uncertainty in the base line*

It often happens that the data are known to fit a Lorentzian function but the base line (i.e. the position of the x axis) is unknown. Unless the data cover a range of several line-widths on either side of the peak, there may be an appreciable error in estimating the base line, which will cause non-linearity in the relationship between u and x.

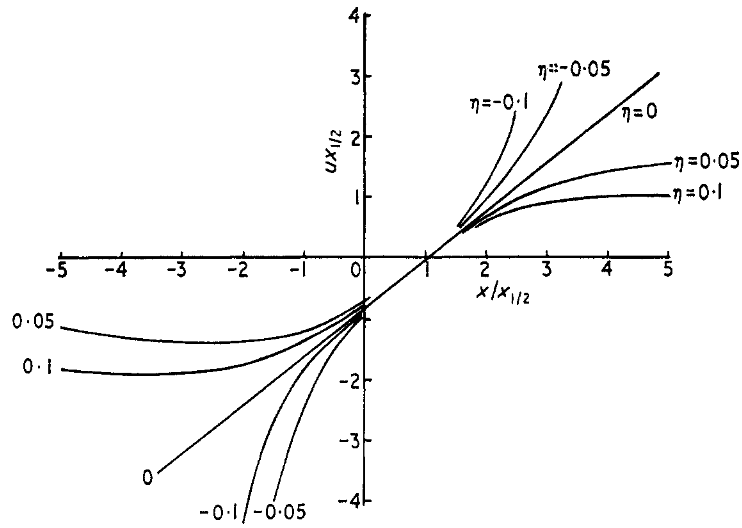

Figure 2. Plot of u against x with uncertain base line, $\alpha = \frac{1}{2}$.

If we rewrite (1) as

$$y = \frac{Ax_{1/2}{}^2}{x_{1/2}{}^2 + (x-a)^2} + \eta A$$

where η is the error in the position of the base line, expressed as a fraction of A, we find that

$$u = \frac{x-2a}{x_{1/2}{}^2 + a^2 + \eta x_{1/2}{}^{-2}(x_{1/2}{}^2 + a^2)\{x_{1/2}{}^2 + (x-a)^2\}}. \tag{2}$$

The effect of a non-zero η is shown in figure 2, in which $ux_{1/2}$ is plotted against $x/x_{1/2}$ for a typical value of a, $\frac{1}{2}x_{1/2}$. It can be shown that a very similar result is found for other values of a in the range $-\frac{1}{2}x_{1/2} \leqslant a \leqslant \frac{1}{2}x_{1/2}$.

Although the line is curved, the intercept at $u = 0$ and hence the x coordinate of the peak can still be determined with a reasonably good accuracy if $|\eta| < \sim 0{\cdot}1$. However, it is now impossible to measure $x_{1/2}$ accurately from the slope, and to determine how well the data fit a Lorentzian function. These are best determined by a different method.

2.3. *Measurement of $x_{1/2}$ with an uncertain base line*

It is convenient to measure y downwards from the peak, since its y coordinate can usually be found with considerable accuracy. Hence we are led to define a quantity

$$Y = y_{\text{peak}} - y = \frac{A(x-a)^2}{x_{1/2}{}^2 + (x-a)^2}. \tag{3}$$

(We note that y_{peak} is the true height of the peak $A + \eta A$, not the value of y at $x = 0$.)

If $a = 0$, $A/Y = 1 + x_{1/2}{}^2/x^2$. Two methods suggest themselves: (i) to plot $1/Y$ against $1/x^2$ or (ii) to plot x^2/Y against x^2. Either of these will give a straight line from which $x_{1/2}$ can be determined, but a little thought will show that method (ii) is preferable. The reason is that if the probable experimental error ΔY is approximately the same for all points, the quantity $\Delta(x^2/Y)$ varies much less than $\Delta(1/Y)$, so that when the graph is drawn a much smaller error is introduced if equal weights are given to each point. Even so, there is still such a variation in $\Delta(x^2/y)$ that it is advisable to weight each point appropriately.

The intercept on the x^2 axis is $-x_{1/2}{}^2$.

2.4. *Effect of uncertainty in the origin of x in this method*

It is not possible in practice to judge the centre of the Lorentzian function with perfect accuracy, so that in equation (3) $a \neq 0$. One way of proceeding is to find the centre as outlined in § 2.1, and then to plot x^2/Y against x^2. There is a simpler method, however, based on the fact that the centre can be judged by eye to within about $\frac{1}{10}$ of $x_{1/2}$, so long as there are enough experimental points, and their accuracy is reasonably good.

One consequence of having $a \neq 0$ is that $Y(x)$ is not quite equal to $Y(-x)$. A method which suggests itself is to plot x^2/Y_{m} against x^2, where $Y_{\text{m}} = \frac{1}{2}\{Y(x) + Y(-x)\}$. $x_{1/2}{}^2$ would be inferred from the intercept on the x^2 axis as before. The error would be small, as we shall show.

It can be shown that

$$\frac{Ax^2}{Y_{\text{m}}} = x^2 + x_{1/2}{}^2 + \frac{a^2 x_{1/2}{}^2(3x^2 - a^2 - x_{1/2}{}^2)}{(x^2-a^2)^2 + x_{1/2}{}^2(x^2+a^2)}.$$

It is convenient to define dimensionless parameters

$$\xi = \frac{x}{x_{1/2}}, \qquad \alpha = \frac{a}{x_{1/2}}$$

and we find

$$\frac{A}{Y_{\text{m}}}\xi^2 = 1 + \xi^2 + \frac{\alpha^2(3\xi^2 - \alpha^2 - 1)}{(\xi^2-\alpha^2)^2 + \xi^2 + \alpha^2}. \tag{4}$$

The error term (the last term on the right-hand side) is tabulated below, for $\alpha = 0{\cdot}1$ and $0{\cdot}3$.

Table 1. Error term as a function of ξ

ξ	0·1	0·2	0·3	0·5	1	1·5	2	3	5
$\alpha = 0{\cdot}1$	−0·490	−0·175	−0·070	−0·008	0·010	0·008	0·006	0·003	0·001
$\alpha = 0{\cdot}3$	−0·897	−0·659	−0·410	−0·084	0·090	0·073	0·051	0·026	0·010

The error introduced in the intercept due to this error term will be very small so long as: (i) the centre of the line is judged to within $\frac{1}{10}$ of $x_{1/2}$ and (ii) points within about $\frac{1}{2}$ of $x_{1/2}$ of the peak ($\xi < 0{\cdot}5$) are given less weight.

It can be shown that the above method gives a smaller error term than would be obtained by plotting either

$$\frac{x^2}{2}\left\{\frac{1}{Y(x)}+\frac{1}{Y(-x)}\right\} \quad \text{or} \quad \frac{x^2}{\{Y(x)\,Y(-x)\}^{1/2}}.$$

2.5. *Effect of a sloping background*

It may happen that the background has a small slope which can be taken as being approximately constant, so that the curve is represented by

$$\frac{y}{A} = \frac{{x_{1/2}}^2}{{x_{1/2}}^2+(x-a)^2}+\eta+\frac{\beta x}{x_{1/2}}.$$

β is a dimensionless constant, being the increase in the background level expressed as a fraction of A, owing to an increase of $x_{1/2}$ in the value of x.

It may appear at first sight that the method of plotting x^2/Y_{m} against x^2 would entirely eliminate the error due to a constant slope. This is not quite true, the reason being that there will now be an error in estimating the y coordinate of the peak because of the displacement of the position of the true peak by the sloping background.

If the experimental curve extends over a sufficient range of x, it would be possible to estimate the slope of the background, and hence to determine the true position of the peak and its y coordinate. The error would then be eliminated. If this cannot be done, a small error will arise, so that

$$\frac{A}{Y_{\mathrm{m}}}\xi^2 = 1+\xi^2+E.$$

The error term E is tabulated below for $\alpha = 0{\cdot}1$ and $\beta = \pm 0{\cdot}05$ (cf. table 1, for which $\beta = 0$).

Table 2. Error term E as a function of ξ, $\alpha = 0{\cdot}1$

ξ	0·1	0·2	0·5	0·6	1	2	3
$\beta =$ 0·05	−0·608	−0·269	−0·042	−0·027	−0·012	−0·029	−0·059
$\beta =$ −0·05	−0·337	−0·084	0·019	0·024	0·028	0·033	0·052

It is seen that for these values of α and β the errors are small so long as the points within the range $|\xi| < 0{\cdot}6$ are given less weight.

2.6. *Effect of a small number of data points*

The method of § 2.4 presupposes that there are enough data near the peak to be able to estimate its height with accuracy. If this is not so,

$$Y = \frac{A(x-a)^2}{{x_{1/2}}^2+(x-a)^2}+\zeta A$$

where ζ is the error in estimating the height of the peak, expressed as a fraction of A. In this case,

$$\frac{A}{Y}\xi^2 = 1+\xi^2+\frac{\alpha(2\xi-\alpha)-\zeta(1+\xi^2)\{1+(\xi-\alpha)^2\}}{(\xi-\alpha)^2+\zeta\{1+(\xi-\alpha)^2\}}.$$

If the peak can be determined to within 1% of A ($\zeta \leqslant 0{\cdot}01$) the error in measuring $x_{1/2}$ is only a few per cent, so long as $|\alpha| < 0{\cdot}1$, and the points near the peak ($\xi^2 < 1$) are given little or no weight. One plot is made of (x^2/Y) against x^2 for each wing, and the average of the two intercepts used to determine $x_{1/2}$. If the peak cannot be determined to within 1% of A, it is advisable to use a least-squares method to evaluate $x_{1/2}$ accurately.

3. Analysis of a differentiated Lorentzian function

It is sometimes necessary to analyse a curve which is a differentiated Lorentzian function (see figure 3) given by

$$y = \frac{2xAx_{1/2}^2}{(x_{1/2}^2 + x^2)^2}. \qquad (5)$$

For example, such a curve might be the result of a 'level crossing' experiment (Franken 1961) in which the external magnetic field is modulated and the resulting modulated signal detected by a phase sensitive detector (for example, Gough and Series 1965).

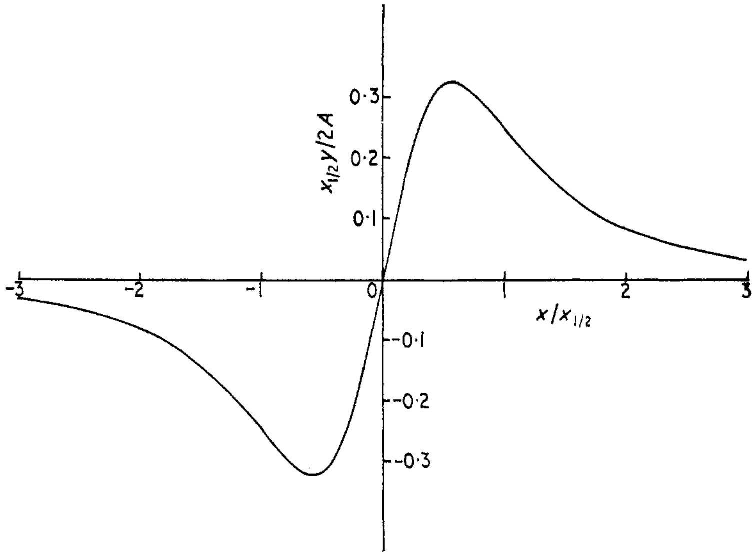

Figure 3. Differentiated Lorentzian function.

3.1. *The exact position of the origin*

Sometimes the main object of the analysis is to determine the position of the origin as accurately as possible using all the available information. In this case, we usually have no knowledge of the origin of x or y. Because of the complex form of equation (5) no simple graphical method readily suggests itself.

One simple way of solving the problem, however, is to plot the two halves of the curve on separate pieces of translucent graph paper, place one over the other, and match them as well as possible. It is a simple matter to deduce the origin from the position of best fit.

In passing it could be mentioned that this method is possible for any symmetrical or antisymmetrical curve, although no use is made of any knowledge of the equation of the curve.

3.2. *The width of the curve*

It is sometimes necessary to measure $x_{1/2}$ of a differentiated Lorentzian curve.

One method, suggested by Series, was used in an experiment to determine the mean lifetime of the 6 $^2D_{3/2}$ state of thallium I by Gough and Series (1965). The method, which is very similar to that described in § 2.3, is to plot $(x/y)^{1/2}$ against x^2, giving a straight line with an intercept of $-x_{1/2}^2$ on the x^2 axis.

It can be shown that this method is better than plotting $(x^3y)^{-1/2}$ against x^{-2}. As in § 2.3, it is advisable to weight each point appropriately.

Since y is antisymmetric and has a large gradient at the origin, there is no difficulty in locating the origin of x to within about $0{\cdot}05x_{1/2}$.

It is possible to correct for a small error which might arise in estimating the origin of x by a device similar to that of § 2.4, based on the fact that $y(x)$ is slightly different from $-y(-x)$.

$(x/y_{\mathrm{m}})^{1/2}$ is plotted against x^2, where $y_{\mathrm{m}} = \frac{1}{2}\{y(x)-y(-x)\}$.

Thus, if the origin of the curve has coordinates (a, b), the measured values of x and y obey the equation

$$y-b = \frac{2(x-a)Ax_{1/2}^2}{\{x_{1/2}^2+(x-a)^2\}^2}$$

whence we find that

$$(2A)^{1/2}x_{1/2}\left(\frac{x}{y_{\mathrm{m}}}\right)^{1/2} = \frac{\{x_{1/2}^2+(x+a)^2\}\{x_{1/2}^2+(x-a)^2\}}{(x_{1/2}^4+2x_{1/2}^2x^2-2x_{1/2}^2a^2+x^4+2a^2x^2-3a^4)^{1/2}}.$$

Putting this equation equal to $x^2+x_{1/2}^2+\Delta$, where Δ is a small correction term, we find that

$$\frac{\Delta}{x_{1/2}^2} = -1-\xi^2+\frac{\{1+(\xi+\alpha)^2\}\{1+(\xi-\alpha)^2\}}{(1+2\xi^2-2\alpha^2+\xi^4+2\alpha^2\xi^2-3\alpha^4)^{1/2}} \tag{6}$$

where $\alpha = a/x_{1/2}$ and $\xi = x/x_{1/2}$ as before.

Any error in estimating the y coordinate of the origin is eliminated by this method. It should be possible to determine its x coordinate visually to within $0{\cdot}05x_{1/2}$. If $\alpha = 0{\cdot}05$ in equation (6), this gives $|\Delta/x_{1/2}^2|$ to be less than $0{\cdot}0076$.

In contrast to the Lorentzian function, it is not a simple matter to correct for a sloping background because the curve is antisymmetrical.

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