# The method of finding all numerical descriptions of a given Mössbauer spectrum tested on $Re_2Fe_{14}B$ - type of spectra

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The numerical method of looking for all possible different Lorentzian descriptions of Mossbauer spectra, based on one given initial description is proposed. The method enables finding all descriptions which fulfill a given precision condition, ΣΔw, on vertical scale (the difference in each point between the investigated spectrum and the description is smaller than ΣΔw) and differing in the line position between each other by at least Δr (at least one line position is different by at least the given Δr value). The amplitudes and widths of all lines remain the same as in the starting description.

The proposed method can, by using a fast computer, give a set of all mathematical descriptions of a given Mössbauer spectrum. From this set one can choose solutions which are interesting from the physical point of view, what can make easier the interpretation of the experimental results [1,2].

The method is based on the relation between the error of the Lorentzian line position Δs and the maximal error in description of the vertical scale Δw (Fig. 1, formula 1).

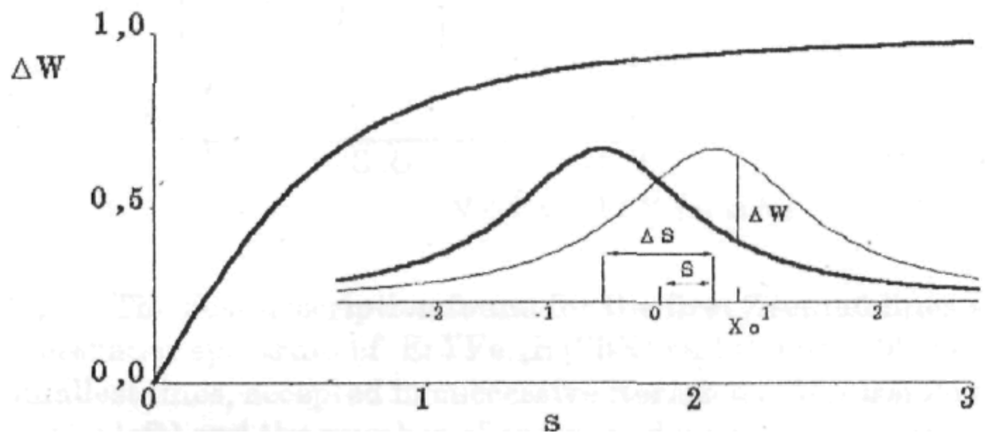


Fig. 1. The maximal difference between the two Lorentzian lines Δw (expressed as the fraction of the line amplitude) as a function of difference in the position of lines (expressed in Γ/2). $x_o$ (given by formula 1) is the position of the maximal difference Δw between the two Lorentzian lines separated by Δs.

$$\Delta w = \frac{1}{(x_o - s)^2 + 1} - \frac{1}{(x_o + s)^2 + 1}, \text{ where } x_o = \sqrt{\frac{s^2 - 1 + 2\sqrt{s^4 + s^2 + 1}}{3}} \qquad (1)$$

and s=Δs/2, s being the half of the position error.

For s < 1 (when the position error is smaller than the line half width Γ)

$$\Delta w \approx 1.299 * s * (1 - 0.75 * s^2) \qquad (2)$$

By using the above relations one can organize the procedure of looking for line positions in such a way that none of the possible solutions will be omitted.

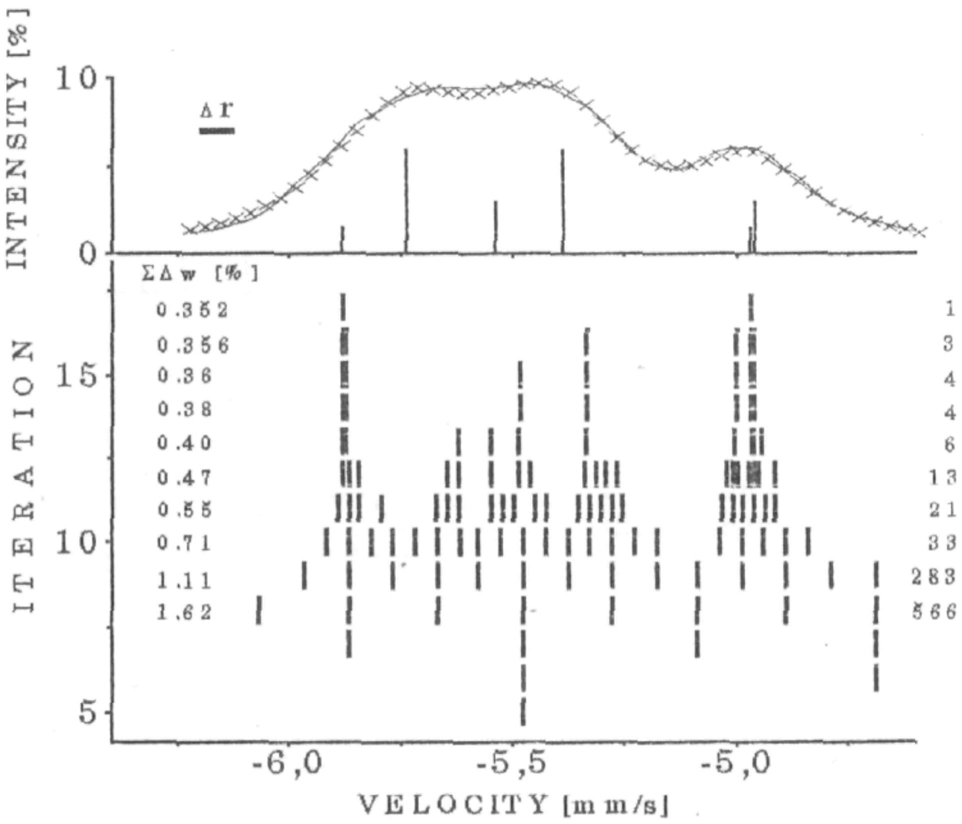


Fig. 2. The best description found for the first Zeenian lines extracted from the Mossbauer spectrum of $ErYFe_{14}B$ (78K) and the possible positions of the two smallest lines, accepted in successive iterations. Admissible error ΣΔw (numbers on the left) and the number of accepted descriptions (on the right) have been written in the picture for the last ten iterations. (In the applied procedure, the search for the positions of the smallest lines started in the sixth iteration. The position indicated in the fifth iteration is the arbitrarily chosen starting position.)

Assuming a search step $2\Delta s$ on the velocity scale its sure to meet with the position for which the error in the horizontal scale is not bigger than $\Delta s$. Then the contribution to the vertical scale error, coming from this line, will be not bigger than $\Delta w$ given by formula 1. The descriptions which yield the error greater then $\Sigma\Delta w$, which take into account the possibility of the summation of errors from all lines and the error of the initial description, can be neglected. (Error of initial description can play the role of the smallest possible error. This error can't be equal to zero at the least due to the statistical distribution of points.)

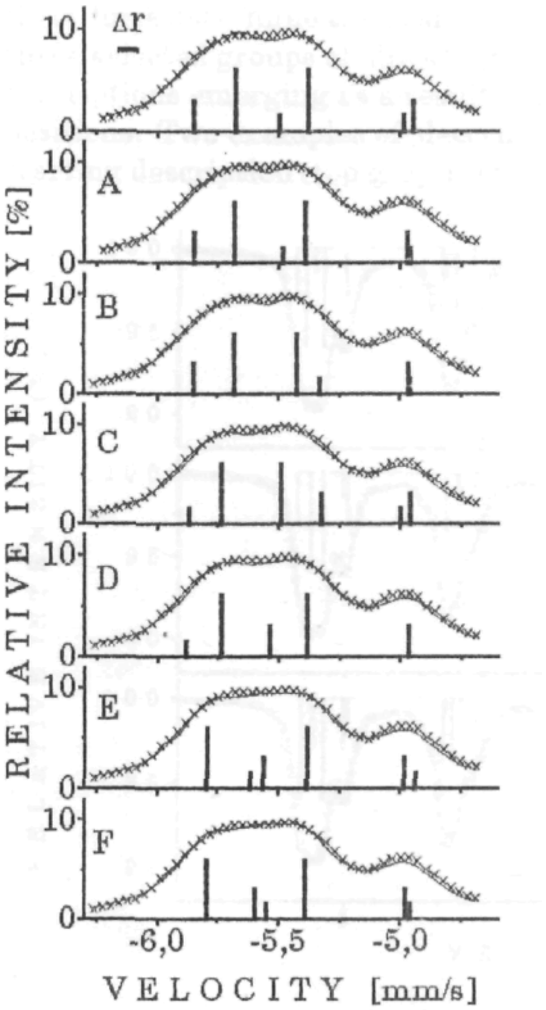


Fig. 3. The set of first Zeeman lines extracted from the Mössbauer spectrum of the compound $ErYFe_{14}B$ (78K) together with the initial description (top graph) and six different descriptions found for $\Sigma\Delta w = 0,4\%$ and $\Delta r = 0.068$ mm/s. Stick diagrams show the line positions and their amplitudes. The description A is equivalent with the starting description (top graph).

Taking into account the time of computation, an iterative method of looking for the line positions was developed. The value of $\Delta s$ was divided by 2 in each next step. Each position $s_i$ accepted in a previous description step was replaced by three positions $s_i - \Delta s_i$, $s_i$, $s_i + \Delta s_i$ in the next iteration. The descriptions which do not fulfill $\Sigma\Delta w_i$ requirement were neglected. The method is presented on the example of the first Zeeman lines extracted from the Mössbauer spectrum of $ErYFe_{14}B$ measured at 78 K. Possible positions, accepted in successive iterations, for the two smallest lines are shown in Fig. 2. The top spectrum presents the best possible description, (different from the starting description and better from it). Six descriptions found for $\Sigma\Delta w = 0.4\%$ and $\Delta r = 0.068$ mm/s (13th iteration in Fig, 2), are shown in Fig. 3 with the starting description shown in top graph. The achieved precision of line positions $\Delta s$ was smaller than 0.003 mm/s. The graph A is equivalent to the initial description and graph D is the precursor of the best description presented in Fig. 2.

When analyzing Mössbauer magnetic spectra, in which the positions of three lines determine the positions of the remaining lines, it is enough to analyze three selected groups of lines (e.g. lines 1st, 2nd and 6th) and later to analyze the descriptions emerging as a result of all possible correlations of the obtained positions. Two examples of descriptions found by using this method, with the starting description (top graph) are presented in Fig. 4.

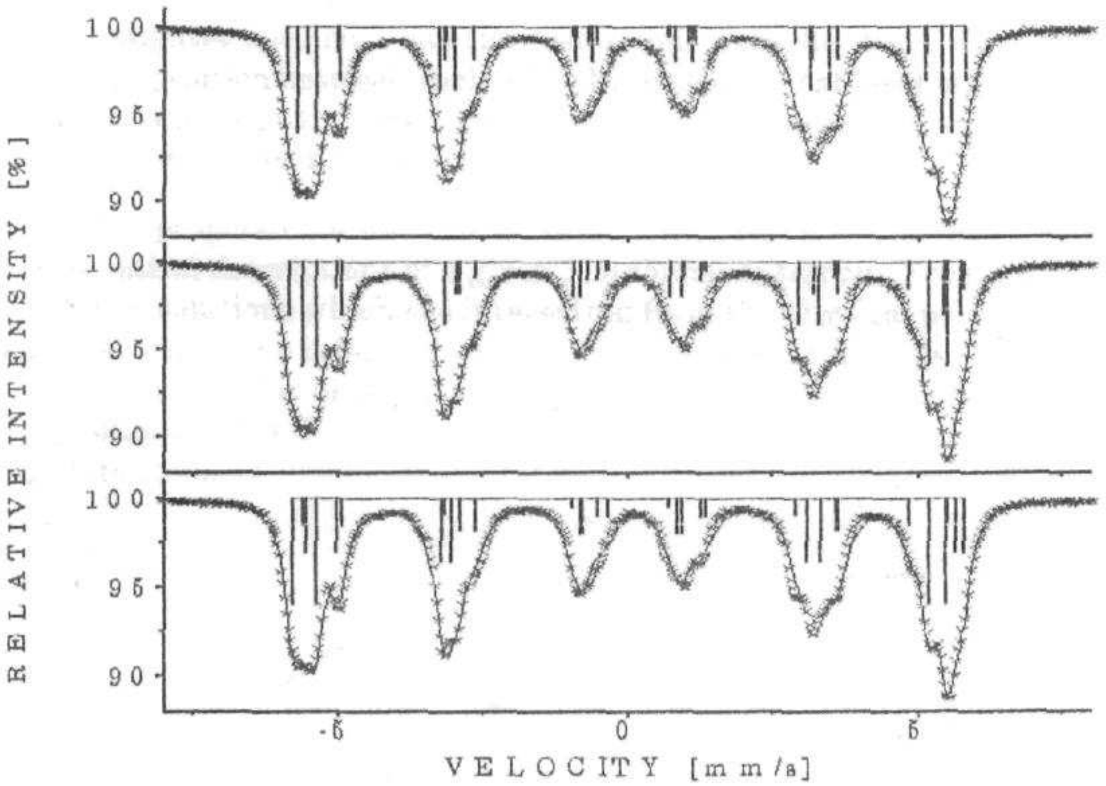


Fig. 4. The Mössbauer spectrum of the $ErYFe_{14}B$ compound (measured at 78K), with the starting description (top graph) and two examples of other descriptions.


References:

1. H. Onodera, A.Fujita, H.Yamamoto, M. Sagawa and S. Hirosawa, J. Maf. Mag. Mat. 68 (1987) 6-14.
2. J.J. Bara, B.F. Bogacz and A. Szytuła, J. Mag. Mag. Mat. 75 (1988) 293-297.