A novel analytical method of Mössbauer spectra resolution improvement has been developed. This method gives an opportunity to narrow the effective line of a source and an absorber by simple integral transformations of an experimental spectrum, that is, to transform the Lorentzian linewidth to the Lorentzian power one. The resulting spectrum may be considered as a new experimental one since the statistical error in each point of the spectrum is evaluated exactly. The procedure of sharpening gives many advantages for Mössbauer spectra analysis. To illustrate this, a number of applications of the proposed method is demonstrated.

1. Introduction

The reconstruction of the spectral density of states and the determination of the hyperfine structure parameter distribution from an experimental Mössbauer spectrum makes it possible to obtain more detailed information about the hyperfine interaction character. From a mathematical point of view, both problems are similar and come to the solution of the integral equation

$$I(v) = \int_{-\infty}^{\infty} \rho(x)L(v-x)dx.$$  \hspace{1cm} (1)

where $I(v)$ is the experimental Mössbauer spectrum and $\rho(x)$ is an unknown function. In the first case, $\rho(x)$ is the spectral density of states and $L(v)$ is the Lorentzian having the double natural linewidth (the presence of a single line source and a thin absorber are presupposed). In the second case, $\rho(x)$ is the distribution of magnetic hyperfine fields, electric field gradients or isomer shifts, and $L(v)$ is the Lorentzian sextet, doublet or singlet, respectively ($^{57}$Fe is assumed to be the Mössbauer probe for the definiteness). There exist four approaches to determine $\rho(x)$.

In the first approach, $\rho(x)$ is approximated by an analytical multiparameter function (see, for example, [1, 2], where a binomial hyperfine field distribution is given). Then the parameters of this function are calculated by fitting the experimental spectrum to the simulated one (according to the $\chi^2$ criterion). However, this approach
can be applied only for those particular cases where the choice of \( \rho(x) \) as a definite function is physically substantiated.

In the second approach, Fourier analysis is used [3–5]. In this technique, the Fourier image of an experimental spectrum is evaluated by appropriate high-frequency cutting. Then \( \rho(x) \) itself is reconstructed by the inverse transformation. However, this method suffers from a serious drawback, which is the appearance of uncontrolled oscillations in the resulting spectrum or distribution.

The third approach [6,7] is based on the assumption that \( \rho(x) \) is not zero on a fixed interval. Then it can be represented as a Fourier series. The coefficients of this expansion are derived using the \( \chi^2 \) criterion.

In the fourth approach [8,10], the regularization technique [11–13] is applied for the solution of the integral equation (1). This technique allows us to exclude the solutions unstable with respect to weak fluctuations in data by imposing restrictions on the magnitudes of the derivatives of \( \rho(x) \).

In the present paper, a novel approach to the problem of increasing Mössbauer spectrum resolution is proposed [14]. Its essence is in the consecutive sharpening of the convolution function \( L(v) \) and, therefore, the spectrum \( l(v) \). By means of simple transformations, the convolution line can be changed from a Lorentzian to any power \( n \) of a Lorentzian. It is is necessary, the sharpening process may be stopped at any step \( n \). Since the statistical error in the sharpened spectra is evaluated exactly, they can be used for determining any Mössbauer parameter by a fitting procedure.

In section 2, mathematical principles of the line sharpening are described and main formulae are derived. The problems of the numerical calculation of the sharpened spectra are discussed in section 3. In section 4, particular examples and applications of the proposed method are given.

2. Mathematical foundation of the method

Let us assume that \( I_1(v) \) is the Mössbauer spectrum corresponding to a thin absorber. Then,

\[
I_1(v) = \frac{\Gamma}{2\pi} \int_{-\infty}^{\infty} \frac{\rho(x)dx}{(v-x)^2 + \Gamma^2/4},
\]

where \( \Gamma \) is the double natural linewidth and \( \rho(x) \) denotes the spectral density of states. We will consider the auxiliary function \( J(v) \) resulting from spectrum \( I_1(v) \) with the help of the dispersion relation

\[
J(v) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{I_1(v-y) - I_1(v+y)}{2y} dy.
\]