A METHOD FOR APPROXIMATE CONSTRUCTION OF THE
BASIC COMPONENT IN THE CLASS OF FUNCTIONS
OF BOUNDED VARIATION

P. N. Zaikin and E. Yu. Shchetinin

The article considers the construction of a stable approximation of the basic component in an experimental spectrum. Conditions of independence and nondegeneracy are introduced for the local resonance nonhomogeneities and the basic component, which is treated as a continuous smooth function whose local variation is substantially less than the variation of the local nonhomogeneities. The problem of approximating the basic component is shown to have a unique solution under these conditions. A stable algorithm is developed for the construction of the basic component. The algorithm is applied to construct the basic component from typical spectrometric data, and the results are compared with other known basic-component fitting methods.

1. MATHEMATICAL MODEL OF THE BASIC COMPONENT

The basic component \( l(x) \) in a region with local nonhomogeneities is approximated by an expression of the form

\[
l(x) = \sum_{i=1}^{k} r_k x^k, \quad \text{если} \quad x \in [x_i^*, x_{i+1}^*], \quad i = 1, n
\]

where the function \( l(x) \) is the basic component near an isolated resonance. Following the common practice [1, 2], we approximate the function \( l(x) \) by a polynomial of 1st or 2nd degree:

\[
l_i(x) = \sum_{k=0}^{K} r_k x^k, \quad \text{если} \quad x \in [x_i^*, x_{i+1}^*], \quad K = 0, 1, 2.
\]

\[
l_i(x) = 0, \quad \text{если} \quad x \not\in [x_i^*, x_{i+1}^*]
\]

\[
l_i(x) \in C.
\]

\( x_i^* \) are the contact points of \( l_i(x) \), where we impose the continuity conditions

\[
l_i(x_i^*) = l_{i+1}(x_i^*)
\]

and conditions of continuity of first derivatives for the second-order polynomial approximation:

\[
l_i'(x) = l_{i+1}'(x)
\]

The points \( x_i \) may be chosen in different ways, for instance,

\[
x_i^* = \frac{(\xi_{i+1} - \xi_i)}{2},
\]

Translated from Chislennye Metody v Matematicheskoi Fizike, Published by Moscow University, Moscow, 1996, pp. 137-146.
where $\xi_i$ is the position of the $i$-th resonance component on the grid $\{x_j\}, j = 1, \ldots, m$, of the argument $x$.

2. THE PROBLEM OF SIMULTANEOUS DETERMINATION OF MODEL PARAMETERS AND LOCAL NONHOMOGENEITY INTENSITIES

We model the experimental function $B(x)$ in the form

$$
B(x) = S(x) + l(x)
$$

where

$$
S(x) = \sum_{i=1}^{N} J_i \Phi(x, \xi_i, \rho)
$$

$x \in [x_1, x_m]$, $\Phi(x, p) \in L_2$, $S(x) \in L_2$, $B(x) \in L_2$, $l(x) \in C$.

The column vector $C$ is the vector of sought parameters:

$$
C = \{ \{ r_k \}, \{ J_i \} \}.
$$

The dimension $n$ of the vector $C$ is given by $n = N(N + 1)$; $J_0$ is the isolated resonance threshold intensity; $\xi_i$ is the position of the $i$-th isolated resonance on the interval $[x_1, x_m]$, and all $\xi_i$ are different, i.e., for two different indices $i \neq j$, we have

$$
\xi_i \neq \xi_j
$$

(4.2)

$\Phi(x)$ is the apparatus function describing the line shape of isolated resonances,

$$
\| \Phi \|_{L_2} = 1, \quad \Phi(x) > 0,
$$

(4.3)

$p$ is the vector of nonlinear parameters of the apparatus function $\Phi$ (half-width, asymmetry, decay decrement).

We impose conditions of nonnegativity and boundedness on the intensities $\{J_i\}$:

$$
0 < J_i \leq B(\xi_i).
$$

(5)

Since the experimental function $B(x)$ is usually defined on a nonuniform grid $\{x_j\}, j = 1, \ldots, m$, of the argument $x$ in the form of a finite-dimensional vector $B$, $B_j = B(x_j)$, we pass to a finite-dimensional approximation of the problem. We consider the function $B(x)$ defined on the grid $\{x_j\}, j = 1 \ldots, m$, in the form

$$
B(1:m) = A(m:n) \cdot C(1:n),
$$

(6)

where $K$ is the dimension of the polynomial (1).

The equations modeling the basic component (1)-(4) and the constraint (5) are written in the form of a system of linear algebraic inequalities.