Reconstruction of particle energy spectrum for angular dependent distribution at the entrance of electrostatic spectrometer

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Abstract. The algorithm of reconstruction of particle energy spectrum from electrostatic spectrometer data under condition of angular dependence of the energy distribution of the charged particles flow at the spectrometer entrance. It is shown that, assuming a linear relationship between the potentials, a standard method of recovering the spectrum by means of dividing the recorded signal by the scanning voltage gives the correct result in the first approximation.

If the energy distribution at the electrostatic spectrometer entrance does not depend on the angular distribution, the reconstruction of spectrum using the standard procedure of dividing the recorded signal by the scanning voltage gives the correct result in the first approximation [1, 2]. At the entrance of electrostatic dispersion spectrometers, particles have different angular distribution at different energies. These spectrometers therefore have different instrument functions, and the procedure of spectrum reconstruction using these spectrometers has not been justified yet. Meanwhile, for a large number of such spectrometers used, for example, in the mass spectrometry, the condition of the energy distribution independence from angular distribution fails.

To justify the recovery procedure of the spectrum we will use the results from Ref. [1, 2]. The signal at the spectrometer outlet is related to the particles energy and angular distribution function by the equation

\[ I = I_0 \int_0^\infty \int_0^{\xi_0} \delta(E) f(\eta, \xi, \alpha, \beta, E) J(\alpha, \beta, \eta, \xi) \sin(\alpha) d\xi d\eta dE, \]

where \( \alpha \) and \( \beta \) are the incidence angles of particles at the inlet diaphragm:

\[ \alpha = \alpha \left( \eta, \xi, \eta_1, \xi_1, \frac{qU_1}{E}, \ldots, \frac{qU_n}{E} \right), \beta = \beta \left( \eta, \xi, \eta_1, \xi_1, \frac{qU_1}{E}, \ldots, \frac{qU_n}{E} \right), \]

\[ J(\alpha, \beta, \eta, \xi) = \frac{\partial^2(\alpha, \beta)}{\partial(\eta, \xi)}, \]

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where \( J \) is the Jacobian of transformation; \( f(\eta, \zeta, \alpha, \beta, E) \), the particle coordinates, angles and energy distribution function, normalized to unity, at the inlet aperture diaphragm; \( E \), the particle energy; \( \delta(E) \), the efficiency of particle registration by the detector at the outlet; \( U_i \) are the electrode potentials relative to the zero potential of the inlet aperture; \( (\eta_1, \zeta_1) \), the coordinates in the outlet diaphragm plane. The integral is taken over the areas of inlet and outlet diaphragm slits.

The distribution function can be expressed as

\[
f(\eta, \zeta, \alpha, \beta, E) = f_1(\eta, \zeta, \alpha, \beta, E)f_2(E),
\]

(4)

where \( f_2(E) \) is the particle energy distribution function, \( f_1(\eta, \zeta, \alpha, \beta, E) \) is the particle angular and cross-section distribution function in the inlet diaphragm plane.

Note that the angular and cross-section distribution function depends on the energy, and therefore the instrument functions for different energies will be different. Thus, if the instrument function is unknown beforehand, seeking of an exact solution is senseless. We can find an approximate solution under condition that the relative width of the instrument function is much less than unity and assuming a linear relationship between the potentials:

\[
\frac{U_2}{U_1} = \lambda_2, ..., \frac{U_n}{U_1} = \lambda_n,
\]

(5)

where \( \lambda_2, ..., \lambda_n \) are the constants.

From (1) it follows:

\[
I \approx I_0 \delta(W) f(W) \int \int f_1(\eta, \zeta, \alpha, \beta, W) J(\alpha, \beta, \eta_1, \zeta_1) \sin \alpha dS_1 dS_0 dE,
\]

(6)

where \( W \) is the tuning energy of spectrometer,

\[
W = qkU_1,
\]

(7)

\[
\alpha = \alpha(\eta, \zeta, \eta_1, \zeta_1, \frac{qU_1}{E}, \lambda_2, ..., \lambda_n), \quad \beta = \beta(\eta, \zeta, \eta_1, \zeta_1, \frac{qU_1}{E}, \lambda_2, ..., \lambda_n).
\]

(8)

We will show that the integral in the right-hand side of (6) in the first approximation can be represented in the form

\[
\int_0^\eta \int_0^\zeta f_1(\eta, \zeta, \alpha, \beta, W) J(\alpha, \beta, \eta_1, \zeta_1) \sin \alpha dS_1 dS_0 dE = CU_1,
\]

(9)

where \( C \) is a constant, independent from the input angular distribution.

Let us introduce the distribution function of the beam with energy \( E \) in the plane of the outlet aperture \( \psi(\eta_1, \zeta_1, qU_1/E, W) \) (see figure 1).

**Figure 1.** The distribution of particle flux in the plane of the outlet aperture: the distribution function of the particle flux (1), the slit in the outlet aperture (2).
\[ \psi \left( \eta, \xi, \frac{qU_1}{E}, W \right) = \int_{\xi_0}^\infty f_i \left( \eta, \xi, \alpha, \beta, W \right) J \left( \alpha, \beta, \eta, \xi \right) \sin \alpha d\xi_0 . \]  

(10)

Function \( \psi \left( \eta, \xi, \frac{qU_1}{E}, W \right) \) satisfies the condition of normalization:

\[ \int \psi \left( \eta, \xi, \frac{qU_1}{E}, W \right) d\xi_1 = 1 , \]

(11)

where the integral is taken over the entire area of the outlet aperture.

The integral of this function over the output diaphragm slit surface gives an instrument function:

\[ \int_{\xi_1} \psi \left( \eta, \xi, \frac{qU_1}{E}, W \right) d\xi_1 = A \left( \frac{qU_1}{E}, W \right) . \]

(12)

We will assume that for small change of the parameter \( z = E / qU_1 \) the form of the function \( \psi \left( \eta, \xi, \frac{qU_1}{E}, W \right) \) is not changed in the first approximation, and the shift of the function takes place along the \( \xi_1 \) coordinate:

\[ \psi \left( \eta, \xi, \frac{qU_1}{E}, W \right) = \psi \left( \eta, \xi_1 + \frac{1}{z + \xi_1}, W \right) \].

(13)

In fact, this condition is similar to the one formulated in the monograph [3] with, however, one significant difference: in [3] this parameter is the tuning energy \( W \), whereas in our case this is the ratio of the scanning voltage to the energy of the particles or, with account of (7), the ratio of the tuning energy to the particle energy.

The integral (9) becomes

\[ \int_{\xi_1}^{\infty} \int_{\xi_0}^{\infty} \int_{\xi}^{\eta} \psi \left( \eta, \xi, \frac{qU_1}{E}, W \right) d\eta d\xi dE = qU_1 \int_{\xi_1}^{\infty} \int_{\xi_0}^{\infty} \int_{0}^{\infty} \psi \left( \eta, \xi_1, \frac{1}{z}, W \right) \frac{dz}{d\xi_{11}} d\xi_{11} d\eta d\xi . \]

(14)

If the relative width of the instrument function is much less than unity, the parameter \( z_i \) and the shift \( \xi_{11} \) in the linear approximation are related by the equation

\[ \frac{dz_i}{d\xi_{11}} \approx \text{const} = C_i . \]

(15)

The integral of the function \( \psi \) taken over \( \xi_{11} \) and \( \eta_1 \) equals unity. The remaining integral represents the average width of the outlet slit \( D \). Consequently, the integral in the expression (9) in the first approximation is given by the equation

\[ \int_{\xi_1}^{\infty} \int_{\xi_0}^{\infty} \int_{0}^{\infty} f_i \left( \eta, \xi, \alpha, \beta, W \right) J \left( \alpha, \beta, \eta, \xi \right) \sin \alpha d\xi_0 d\xi_1 dE = qU_1 C_i D . \]

(16)

Thus, in the first approximation the integral does not depend on the angular distribution of particles at the spectrometer entrance. Our analysis given by (9) shows that for electrostatic dispersion spectrometers with linearly related potentials, dividing the recorded signal by a scanning voltage while reconstructing the energy spectrum gives in the first approximation the correct result. It is valid even in the case when particles with different energies have different angular distribution at the analyzer inlet. We should note that the obtained results are also important for spectrometers with preretardation. The formula for the spectrum reconstruction for such spectrometers was obtained in [4, 5], where an expression similar to (9) was assumed. Namely, it was assumed that at a fixed potential bias in the dispersion part of the spectrometer, the integral over the instrument function of the
dispersion part of the spectrometer will be the same, if after passing the retardation system the angular
distributions of particles are different at different initial energies.

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