Influence of the instrumental functions of electrostatic and magnetic analyzers on the processing of experimental data

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Equations relating the output signal of a dispersion analyzer and the energy distribution function of the charged particles entering it are obtained and solved on the basis of an analysis of the motion of charged particles in such analyzers. The influence of corrections on the reconstruction of the energy distribution in comparison with the standard procedure is considered. © 1997 American Institute of Physics. [S1063-7842(97)01806-0]

INTRODUCTION

Many modern methods for investigating solids and plasmas are based on analysis of the energy spectra of charged particles. Electrostatic and magnetic analyzers are employed in such investigations. The fact that the output signal of an analyzer conveys the shape of the energy spectrum of the particles with distortions raises the problem of reconstructing the true spectrum of the particles from the output signal of the analyzer.

The problem of reconstructing the true distribution for electrostatic analyzers was reduced in several papers (see, for example, Ref. 1) to solving the convolution integral equation

$$I(W) = C \int_0^{+\infty} A(W-E)f(E)dE,$$
(1)

where I(W) is the output signal of the analyzer, f(E) is the energy distribution function of the particles, A(W-E) is the instrumental function of the analyzer, W is the tuning energy of the analyzer, and C is a constant.

When the energy distribution (or the momentum distribution for a magnetic analyzer) is reconstructed, the output signal of the analyzer I(W) [or I(p)] is divided by W (or p, respectively).² The problem of reconstructing the true energy distribution was reduced in Ref. 3 on the basis of an approximation of the experimental data for a concrete analyzer to the solution of an integral equation of the form

$$I(W) = C \int_0^{+\infty} A(W/E) f(E) dE.$$
 (2)

A general solution of this equation was obtained in integral form, and it was also shown that the approximate solution of Eq. (2) for a broad spectrum is obtained by dividing the output signal I(W) of the analyzer by W. In Ref. 4 an equation similar to Eq. (2) was also used on the basis of an approximation of experimental data, and a solution was obtained in the form of a series. However, the question of when the equations of the former and latter types should be used to treat the experimental data remained open in the general case. The purpose of the present work is to attempt to reconstruct the true distribution from the analyzer output signal in the general case.

EQUATIONS OF TRAJECTORIES

To obtain the equations of the trajectories of the particles in an analyzer we use the approach described in Ref. 5, expressing the particle velocity $\boldsymbol{\nu}$ in terms of the radius vector of the particle **R** and the coordinate *S* coinciding with its trajectory

$$\boldsymbol{\nu} = \frac{d\mathbf{R}}{dt} = \frac{d\mathbf{R}}{dS}\frac{dS}{dt} = \frac{d\mathbf{R}}{dS}\nu,\tag{3}$$

where ν is the absolute velocity of the particle.

Then, taking into account the equation of motion of a nonrelativistic charged particle in an electrostatic field

$$m\frac{d\boldsymbol{\nu}}{dt} = -qe\nabla U,\tag{4}$$

where U is the electric field potential, and expressing the kinetic energy in terms of the total energy E_0 , after some relatively simple transformations we obtain

$$2\frac{d^2\mathbf{R}}{dS^2}\left(1-\frac{qeU}{E_0}\right)-\frac{d\mathbf{R}}{dS}\frac{d(qeU/E_0)}{dS}=-\nabla\left(\frac{qeU}{E_0}\right).$$
 (5)

Similarly, in the case of a relativistic charged particle in a constant magnetic field, if we substitute Eq. (3) into the equation of motion

$$\frac{d}{dt}\left(\frac{m\boldsymbol{\nu}}{\sqrt{1-\boldsymbol{\nu}^2/c^2}}\right) = \frac{qe}{c}(\boldsymbol{\nu} \times \mathbf{H}),\tag{6}$$

take into account that the kinetic energy of the particles does not vary in the magnetic field $(d\nu/dS=0)$, and introduce the vector **h**=**H**/*H*, for the path equation we obtain

$$\frac{d^2 \mathbf{R}}{dS^2} = \frac{q e H}{p c} \left(\frac{d \mathbf{R}}{dS} \times \mathbf{h} \right),\tag{7}$$

where $p = m \nu / \sqrt{1 - \nu^2 / c^2}$ is the magnitude of the momentum.

INSTRUMENTAL FUNCTION OF AN ANALYZER AND TREATMENT OF MEASUREMENT DATA

Let us consider the motion of charged particles in an electrostatic analyzer. Let a particle enter the analyzer at a point with the coordinates (η , ξ) (the system of coordinates

coincides with the plane of the entrance electrode) in the direction assigned by the angles α and β with an energy $E = E_0/e$, where *e* is an elementary charge. The distribution of the field in the analyzer is assigned by the potentials U_i , where i = 1, ..., n, on the electrodes relative to the entrance electrode, which is at zero potential. At the *n*th or exit electrode of the analyzer the particle is at a point with the coordinates (η_1, ξ_1) (the coordinate system lies in the plane of the exit electrode).

The coordinates (η_1, ξ_1) are found by solving the equation of motion (3). Since the trajectory of the particle [Eq. (5)] remains unchanged as its energy and potential vary over the entire space by the factor *L*, the coordinates (η_1, ξ_1) remain unchanged when *E* and U_i , where $i=1, \ldots, n$, change simultaneously by the factor *L*. This condition holds only if the energy and the potentials appear in the functions of the coordinates (η_1, ξ_1) in the form of a ratio. Similarly, it can be shown that the charge and the energy also appear in the form of a ratio.

To find the relation between the output signal of the analyzer and the energy distribution function of the particles, we use the method described in Ref. 6. If the particles at the entrance to the analyzer have a distribution function with respect to the coordinates of the cross section of the beam formed by the surface of the entrance diaphragm, the angles, and the energy $f(\eta, \xi, \alpha, \beta, E)$, the number of particles which have an energy in the range from *E* to E + dE and emerge in the direction assigned by the angles α and β into a solid-angle element $d\Omega$ from an element dS_0 of the entrance diaphragm area per unit time equals

$$d^{3}I = I_{0}f(\eta,\xi,\alpha,\beta,E)d\Omega dS_{0}dE,$$
(8)

where

$$I_0 = \int \int \int \frac{d^3I}{dEdS_0 d\Omega} d\Omega dS_0 dE$$

is the number of particles passing through the hole in the entrance diaphragm per unit time.

To find the number of particles *I* passing through the hole in the exit diaphragm per unit time, Eq. (8) must be integrated over all the trajectories passing through the hole in the exit electrode. For this purpose we express the angles α and β in terms of the coordinates (η_1, ξ_1) of the coordinate system of the exit diaphragm

$$\alpha = \alpha \left(\eta, \xi, \eta_1, \xi_1, \frac{qU_1}{E}, \dots, \frac{qU_n}{E} \right),$$

$$\beta = \beta \left(\eta, \xi, \eta_1, \xi_1, \frac{qU_1}{E}, \dots, \frac{qU_n}{E} \right),$$
(9)

and substituting these expressions into (8), we integrate over the energy and the areas of the entrance and exit apertures

$$I = I_0 \int_0^{+\infty} \int_{S_0} \int_{S_1} f\left(\eta, \xi, \eta_1, \xi_1, \frac{qU_1}{E}, \dots, \frac{qU_n}{E}, E\right)$$
$$\times J(\alpha, \beta, \eta_1, \xi_1) \sin \alpha \, dS_1 dS_0 dE, \tag{10}$$

where

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

is the Jacobian of the transformation .

We assume that the energy distribution in the beam being analyzed does not depend on the distribution with respect to the cross section and the angles

$$f(\eta,\xi,\alpha,\beta,E) = f_1(\eta,\xi,\alpha,\beta)f_2(E).$$
(11)

Using such a function, we can represent expression (10) in the form

$$I = I_0 \int_0^{+\infty} A\left(\frac{qU_1}{E}, \dots, \frac{qU_n}{E}\right) f_2(E) dE, \qquad (12)$$

where

$$A\left(\frac{qU_1}{E}, \dots, \frac{qU_n}{E}\right)$$
$$= \int_{S_0} \int_{S_1} f_1\left(\eta, \xi, \eta_1, \xi_1, \frac{qU_1}{E}, \dots, \frac{qU_n}{E}\right)$$
$$\times J(\alpha, \beta, \eta_1, \xi_1) \sin \alpha \, dS_1 dS_0.$$

The function $A(qU_1/E_0, \ldots, qU_n/E_0)$ is the instrumental function of the analyzer, since it expresses the dependence of the output signal of the analyzer on the electrode potentials for a monoenergetic beam of particles. It should be noted that the instrumental function of the analyzer will be a function of the ratios of the electrode potentials to the particle energy, even if the condition of a one-to-one correspondence between the angles α and β at the entrance to the analyzer and the exit coordinates (η_1, ξ_1) is not satisfied, since the instrumental function is the integral over all the trajectories passing through the hole in the exit diaphragm, and each trajectory in the analyzer is a function of the ratios of the electrode potentials to the particle energy, for example, when the beam is focused on a point.

It is not difficult to show that convolution equation (1) is incompatible with Eq. (12) and is, thus, inapplicable to analyzers operating in the spectrometer regime. In fact, if it is assumed that the instrumental function simultaneously satisfies (1) and (12), the condition

$$W - E = F(qU_1/E, \dots, qU_n/E)$$
(13)

must be satisfied, i.e., the difference between the tuning energy of the analyzer and the energy of the particles must be a function of the ratios between the electrode potentials and the energy. On the other hand, the tuning energy W of an electrostatic analyzer should not depend on the energy E with which the particle enters the analyzer, in contradiction with condition (13).

In order that the instrumental function of the analyzer would have the form A(W/E), when the energy of the particles changes by a factor of L, the electric fields must vary by the same factor over the entire trajectory of the particles. This condition is strictly satisfied only if the similarity condition for the electric field holds in the entire space of the analyzer. Therefore, in this case the potentials on the electrodes should be linearly related:



$$\frac{U_2}{U_1} = \lambda_2; \dots; \frac{U_n}{U_1} = \lambda_n, \qquad (14)$$

FIG. 1. Results of the reconstruction of an energy distribution. a: solid curve — true distribution; dotted curve — distribution obtained by dividing the output signal by the energy; dashed curve — distribution [from Eq. (20) to within a correction associated with the second derivative] based on the known output signal (dashed curve in Fig. 1b) and the instrumental function (solid curve in Fig. 1b) (the full width of the true energy distribution at half-maximum is equal to the full width of the instrumental function at half-maximum).

where $\lambda_2, \ldots, \lambda_n$ are constants.

Then the tuning energy and the potential on one of the electrodes, in terms of which the current of the particles at the entrance to the analyzer is measured, will be related by the expression

$$W = k U_1, \tag{15}$$

where k = const is the analyzer constant.

In this case the relation between the current at the analyzer exit and the energy distribution function of the particles is described by the equation

$$I(U_1) = I_0 \int_0^{+\infty} A\left(\frac{q U_1}{E}, \lambda_2, \dots, \lambda_n\right) f(E) dE.$$
(16)

The solution of Eq. (16) for the energy distribution function of the particles can be found in an integral form using the Mellin transform³

$$f(k\breve{U}) = \frac{1}{I_0} \frac{1}{2\pi i} \int_{x_0 - i\cdot\infty}^{x_0 + i\cdot\infty} \frac{I_{x-1}}{A_{x-1}} (k\breve{U})^{-x} dx,$$
(17)

where

$$I_{x-1} = \int_{0}^{+\infty} I(U_1) U_1^{x-2} dU_1,$$

$$A_{x-1} = \int_{0}^{+\infty} A\left(\frac{qU_1}{E}\right) \left(\frac{U_1}{E}\right)^{x-2} d(U_1/E).$$
 (18)

The expression obtained is not convenient for practical use; therefore, we find the solution of the equation in the form of a series. For this purpose, we assume that $I(U_1)$ is infinitely differentiable and can be expanded into a Taylor series in the vicinity of the point \check{U} :

$$I(U_1) = \sum_{n=0}^{+\infty} \frac{I^{(n)}(\breve{U})(U_1 - \breve{U})^n}{n!}.$$
(19)

Substituting expression (19) into integral (18) and assuming, for simplicity, that $\check{U}>0$ and $U_1>0$, for Eq. (17) we obtain

$$f(k\breve{U}) = \frac{1}{I_0} \sum_{n=0}^{+\infty} I^{(n)}(\breve{U})\breve{U}^{n-1} \frac{1}{2\pi i n!}$$
$$\times \int_0^{+\infty} \int_{x_0 - i \cdot \infty}^{x_0 + i \cdot \infty} \frac{(U_1/\breve{U} - 1)^n}{A_{x-1}k^2} \left(\frac{U_1}{kU}\right)^{x-2} dx d(U_1/\breve{U})$$

or

$$f(k\breve{U}) = \frac{1}{I_0} \sum_{n=0}^{+\infty} B_n I^{(n)}(\breve{U}) \breve{U}^{n-1},$$
(20)

where $I^{(n)}(\check{U})$ is the *n*th derivative of the current at the analyzer exit with respect to \check{U} , and the B_n are constants.

We express the coefficients B_n in terms of the moments of the instrumental function. For this purpose, after expanding $I^{(n)}(\breve{U})$ into a Taylor series and substituting expression (20) into Eq. (16), we obtain the equation

$$I(U_1) = \sum_{n=0}^{+\infty} \sum_{m=0}^{+\infty} \frac{B_n C_{nm}}{m! k^{n+m-1}} I^{(n+m)}(U_1) U_1^{n+m}, \qquad (21)$$

where

$$C_{nm} = \int_0^{+\infty} z^{n-1} (z-k)^m A(q/z) dz.$$
 (22)

Since Eq. (21) holds for any function $I(U_1)$, the coefficient in front of $I^{(n+m)}(U_1)$ for n=0 and m=0 equals unity, and the sum of the coefficients in front of the remaining derivatives equals zero. Then

$$B_0 = \frac{1}{kC_{00}}, \quad B_n = -\frac{1}{C_{n0}} \sum_{i=0}^{n-1} B_i \frac{C_{i(n-i)}}{(n-i)!}.$$
 (23)

The analyzer constant can be expressed so as to satisfy the condition $B_1=0$; in that case it equals

$$k = \frac{C_{10}}{C_{00}}.$$
 (24)

Therefore, the correction associated with the first derivative $I'(U_1)$ can be eliminated by adjusting the analyzer constant. This allows us to assume, in contrast to the results obtained in Ref. 3, that the first derivative of the current has little influence on the shape of the energy distribution. Figure



FIG. 2. Dependence of $f_{\rm max}/f_{\rm 0max}$ and Δ/Δ_E on $\Delta_E/\Delta_{\rm instr}$, where $f_{\rm max}$ is the height of the reconstructed spectrum, $f_{\rm 0max}$ is the height of the true distribution, Δ is the full width of the reconstructed spectrum at half-maximum, Δ_E width of the true distribution, and $\Delta_{\rm instr}$ is the width of the instrumental function: solid curve – with consideration of the correction associated with the second derivative; dashed curve – for spectra obtained by simple division by the energy.

1 shows examples of the processing of the spectrum in a first approximation and with the correction associated with the second derivative of the current. The normal Gaussian distribution was employed as a trial function for the true distribution function. It can be concluded on the basis of the results obtained (Fig. 2) that the correction associated with the second derivative makes a significant contribution to the distribution function in the case in which the width of the true distribution function is of the order of the width of the instrumental function. In this case the energy distribution obtained with the correction is considerably closer to the true distribution than are the distributions obtained without it. In addition, it is not difficult to show that the distribution function thus obtained satisfies the normalization condition.

Using the normalization condition for f(E), it is not difficult to show that $I(U_1)$ tends to zero when $U_1 \rightarrow 0$ and $U_1 \rightarrow \infty$. Taking this into account, we find that

$$\int_{0}^{+\infty} I^{(n)}(U_1) U_1^{n-1} dU_1 = 0, \qquad (25)$$

where $n \ge 1$.

Expression (25) makes it possible to compare the intensities of two currents with quasimonoenergetic energy distribution functions of the particles having a width of the order of the width of the instrumental function without refining the form of the distribution function. It is noteworthy that a simple comparison of the current maxima at the analyzer exit gives an incorrect result:

$$\frac{I_{10}}{I_{20}} = \frac{\int_{0}^{+\infty} I_1(U)/UdU}{\int_{0}^{+\infty} I_2(U)/UdU} \neq \frac{I_{1\max}}{I_{2\max}},$$
(26)

where I_{10} and I_{20} are the particle currents at the entrance to the analyzer, and $I_{1\text{max}}$ and $I_{2\text{max}}$ are the maximum values of the particle currents $I_1(U)$ and $I_2(U)$ at the analyzer exit.

Let us now consider a magnetic analyzer of charged particles operating in the spectrometer regime. Assuming that the magnetic field in the analyzer is created by magnetooptical elements and that the strengths of fields created by these elements are linearly related, for a particle which has the coordinates (η , ξ) at the entrance diaphragm of the analyzer and emerges in the direction assigned by the angles α and β with the momentum *p*, from the equations of motion we obtain the coordinates of the particle at the exit diaphragm of the analyzer

$$\eta_1 = \eta_1(\eta, \xi, \alpha, \beta, qH/p), \quad \xi_1 = \xi_1(\eta, \xi, \alpha, \beta, qH/p),$$
(27)

where H is the magnetic field strength at an arbitrarily selected fixed point.

The distribution function of the particles with respect to the magnitude of the momentum, which does not depend on the distribution with respect to the angles and the cross section, and the number of particles passing through the hole in the entrance diaphragm per unit time are related by an expression similar to the expression for electrostatic analyzers

$$I(H) = I_0 \int_0^{+\infty} A(qH/p) f_2(p) dp.$$
 (28)

The momentum corresponding to tuning of the analyzer and the magnetic field strength H are related by the expression

$$p_1 = kH. \tag{29}$$

For a distribution function whose value varies weakly across the width of the instrumental function, the approximate solution of Eq. (28) will have the form

$$f_2(kH) \approx \frac{I(H)}{CI_0 H},\tag{30}$$

where $C = \int_0^{+\infty} A(q/z) dz$ is a constant and z = p/H.

CONCLUSIONS

Let us briefly review the main results of this work.

1. It has been shown in this work that for all electrostatic analyzers operating in the spectrometer mode, the energy distribution function of the charged particles at the entrance to the analyzer and the number of particles passing through the aperture in the exit electrode per unit time depend on the ratio between the electrode potentials and the particle energy and are related by Eq. (12). It should be noted that the expressions (12) and (16) obtained above for describing the relationship between the current at the analyzer exit and the energy distribution function of the particles remain valid when the stray electrostatic fields caused by the actual geometry of the electrodes are taken into account.

2. A detailed analysis shows that the convolution equation (1) previously proposed¹ for describing the relationship between the particle current at the analyzer exit and the energy distribution function of the particles is not applicable to an analyzer operating in the spectrometer mode.

3. Under the condition of a linear relationship between the potentials on the analyzer electrodes, the particle current at the analyzer exit and the energy distribution function of the particles are related by Eq. (2), in which the instrumental function is a function of the ratio of the tuning energy W to the particle energy E. For a magnetic analyzer operating in the spectrometer mode, the momentum distribution function of the particles and the particle current at the analyzer exit are related by an analogous equation (28) provided the fields created by the magnetooptical elements are linearly related.

4. Solution (20) in the form of a series in derivatives of the current at the analyzer exit, which was obtained for an arbitrary continuous energy distribution function of the particles, and recurrence relations (23) for the coefficients in the series permit the reconstruction of energy spectra with a width of the order of the width of the instrumental function.

5. Since the distribution function of the beam with respect to the coordinates of the cross section formed by the entrance diaphragm and the angles appears in expression (12) for the instrumental function, the monoenergetic particle beam used to calibrate an analyzer must have a distribution function with respect to the cross section and angles that is close to the spectra which are to be measured by the analyzer. For example, if the analyzer is intended for investigating particles reflected or emitted from a surface and the surface area "visible" to the analyzer is smaller than the emission area, and the angular distribution function of the particles varies weakly within the angular aperture of the analyzer, it is best to employ a broad monoenergetic particle beam with an angular distribution that is quasi-isotropic within the angular aperture of the analyzer to calibrate the latter.

6. Preliminary retardation of the particles is often used to improve the resolving power of a dispersion analyzer. As a rule, analyzers with preliminary retardation operate in two regimes:¹ in one regime the retarding potential remains constant, and the spectrum is scanned by varying the potential on the deflecting electrodes. One deficiency of this regime is that it is unsuitable for treating the results of measurements of broad spectra. In the other regime the potential difference on the deflecting electrodes remains constant, and the scanning is performed by varying the retarding potential. One deficiency of this regime is that the angular distribution function of the particles varies after the retardation system, making the ensuing treatment of the spectra difficult. The deficiencies just enumerated can be avoided by using an analyzer operating in a regime in which the retarding potential and the potentials on the deflecting electrodes are linearly related by Eq. (14). The use of a retarding potential permits improvement of the resolving power of the analyzer. On the other hand, the particle current at the analyzer exit and the energy distribution function are related by Eq. (16), and thus the treatment of the spectrum reduces, in a first approximation, to division of the signal by the energy.

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