MODELING AND OPTIMIZATION CODES FOR MASS-SEPARATOR DESIGN

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Abstract

In this report we suggest an approach to design optimal mass-separators. In the beginning for linear approximation we build some hypersurfaces in the corresponding parameters space, described desired characteristics. For this purpose we use computer algebra codes with necessary visualization procedures. Particularly, for solenoids as focusing elements these hypersurfaces demonstrated a very complicated behaviour. Secondly, we investigate found optimal regimes in allowed domains in the parameters space including nonlinear aberrations both for separate elements and for total beam line. Such approach should lead to a better understanding of the influence of different parameters in charged particle optical systems. The corresponding computer codes demonstrate effectiveness of this approach.

1 INTRODUCTION

The design process of such systems as focusing systems, mass- and other types of separators and so on can be presented as a manipulation with some finite number of steering modules (drifts, focusing and deflecting elements). But the designer have to remember that such systems have complex behaviour in a parameters space. Moreover, the optimization procedure should be realized taking into consideration multicriteria character of such problems. In this paper we suggest an approach based on two levels of investigation. The first level consists symbolic manipulation both linear and nonlinear models of designed systems. The second one consists numerical investigation using modular presentation of both the system and using methods [1]. As a basic mathematical method we use the matrix formalism for Lie algebraic tools [2].

2 STATEMENT OF A PROBLEM

The suggested approach is based on symbolic presentation of transfer matrices for all sections along the systems used for formulating physical demands to the system under study. This allows to give the designer a powerful analytical tools for investigation the problem. On this step the designer create some sequence of criteria as a vector function $\mathbf{F}^*(\mathbf{A}) = (f_1(\mathbf{A}), \dots, f_p(\mathbf{A}))$ of system parameters $\mathbf{A}^* = (a_1, \dots, a_m)$:

$$\mathbf{F}(\mathbf{A}) = \mathbf{G}\left(\left\{\mathbf{M}^{11}(z_k|z_0;\mathbf{A})\right\}\right),\tag{1}$$

where p is a number of criteria, m – a number of the system parameters, $\mathbf{M}^{11}(z_k|z_0; \mathbf{A})$ is the transfer matrix (in linear approximation) corresponding to a part of the system from the initial point z_0 up to a current point z_k , $\mathbf{G}(\cdot)$ is a auxiliary vector function. Its form depends on a presentation form for formulated criteria set. Here $\{\cdot\}$ denotes a set of a argument ".". For the current phase vector X(z) one can write

$$X(z) = \mathbf{M}^{11}(z|z_0) \cdot X_0 + E_v(z|z_0) \cdot \delta_v + E_{MQ}(z|z_0)) \cdot \delta_{MQ},$$

where $\mathbf{M}^{11}(z|z_0) = \mathbf{M}^{11}(z|z_0; \mathbf{A})$ is the current transfer (4×4) matrix describing the beam line action from the initial point z_0 up to a current point z, X_0 is a initial phase vector, $X_0 \in \mathfrak{M}_0, \mathfrak{M}_0 = \mathfrak{M}(z_0)$ is an initial phase set, $E_v = E_v(z|z_0; \mathbf{A})$ and $E_{MO} = E_{MO}(z|z_0; \mathbf{A})$ are vectors describing corresponding dispersion properties in different points along of the mass-spectrometer and at last δ_v and $\delta_{M/Q}$ are corresponding relative deviations. As for achromatic condition one can note that this problem is treated in different ways. For example, one can choose to vanish corresponding coefficients attached to the fractional deviation of velocity δ_v : $\{E_v(z_{\text{fin}}|z_0)\}_k$, for k = 1, 3 and simultaneously to increase the corresponding coefficients attached to the deviation δ_{MQ} of the ratio mass/charge: $\{E_{MQ}(z_{fin}|z_0)\}_k = \alpha_k$, where α_k are constants describing partial (in X- and Y-planes) of the mass-spectrometer and $z_{\rm fin}$ is the terminate point corresponding to transmitters location. This coefficient defines the mass dispersion D of the mass-spectrometer and the value 1 corresponds to the requirement 10 mm /%.

3 BRIEF DESCRIPTION OF MODELING PROCESS

For choosing a parameters set for the mass-spectrometer we create computer algebra codes (using, for example, (MAPLE V), which allow to build some 2D- and 3Dpictures for significance parameters. These parameters are separated in two groups: a set of geometrical parameters and force parameters. In turn the first type of parameters are separated in two groups also: the distances between focusing and deflecting elements (lengths of drifts and the lengths of these elements). The last parameters should be varied on some discrete set of values. Obviously this set must be selected from technological reasons. The lengths of drifts can be found from described criteria. These criteria have the form of algebraic equations according to these parameters and can be solved easy. But it should be noted that these solutions are functions of the second groups of parameters and characteristics of the initial phase

beam portrait. Appropriate solutions of these equations can be chosen using visual presentation of corresponding dependencies these parameters on parameters describing stirring elements (both force and geometrical parameters). We should note that for achromatic system creation there are two ways: the corresponding distance d_2 is calculated from the total system achromatic condition (see above) and this distance is calculated from truncated system achromatic condition when we are not consider terminal solenoid and drift. The corresponding dependence d_2 on the system parameters has different forms. For the total system there is a ravine on a smooth slope (see the left picture on the Fig.1). Using computer algebra codes allows to proceed parameters choosing flexible and suitable for passage from one model to another. These tools are based on symbolic formulae and corresponding visual interpretations. This approach is more flexible than pure numerical modeling. The Fig.1 and Fig.2 demonstrate complex dependencies of d_2 and D on the system parameters A. As one can see from these pictures there are some problems attached to choosing of the final variant of the mass-spectrometer with solenoids as focusing systems. Moreover such choosing procedure should lead to a set of variants, which should be investigated including high order aberrations. From these pictures a designer should select an appropriate range of solenoid field B_{s_2} for some desired value of the distortion parameter D. The first phase of similar modeling process is finished by formation of a set of parameters ranges for next investigation and optimization. From the truncated system condition we obtained the same smooth slope, without the ravine. This ravine point the B_{s2} values should be avoided for stability of the system working. The character of such dependence is similar for quadrupole and solenoid as the central focusing element. We should note that the similar behavior there is for the mass-spectrometer with quadrupole doublets as focusing systems (compare with [4]). For similar system the beam has a crossover in center of the system only in the deflection plane. The achromatism condition is one of possible conditions which can be imposed on the system. For the designed system we also consider different additional (besides main conditions for achromatism and mass-dispersion) conditions (for example, aperture conditions). This is necessary for next investigations including high order aberrations. The made investigations show that the system with desired characteristics exists. As an example we consider the variant when there is a crossover in the center of the system. For the mass-spectrometer with solenoids as focusing systems we have the crossover in both planes. The corresponding envelopes in these systems are demonstrated on the pictures (see the Fig.3 and 4). On these pictures one can see the beam spots on the detectors plane for the corresponding structures also. We must note that the some magnification of the beam spot in the second case is induced by essential enlargement of entrance solid angle (approximately in 10 times). Correspondingly the rotation of the second spot is caused by using of solenoid as a focusing system.

4 COMPUTER CODES FOR MASS-SPECTROMETER MODELING

As we mentioned above there is a set of problems which must be solved on the first phase of modeling: the phase of linear approximating model. Complexity of similar problems leads to necessity of creation of effective computer codes for solution these problems. For this purpose we suggest two groups of codes: computer algebra codes (using MAPLE V) and numerical codes created using RAD Delphi. The symbolic manipulation allows to study the parameter space very carefully. Than we use the numerical codes with necessary graphical support both on the phase of mass-spectrometer grouping and overlooking of results. For high order investigation we use numerical codes similar [?]. These codes will be included to whole package. For this the matrix formalism for Lie algebraic tools is used.

5 SOME RESULTS ON HIGH ORDER ABERRATIONS INVESTIGATION

The influence of high order aberrations we consider step by step: beginning from second order aberrations in a separate element and finishing by third order aberrations for the total system.

5.1 Second Order Aberrations

On the first step of the investigation we consider the influence of the second order aberrations (geometrical and chromatic) separately for the every structure element and compare their influences. The geometrical and chromatic aberrations of the second order in the electrostatic deflector lead to the shift of the picks from the center. In particular, geometrical aberrations lead to the shift of the central pick is equal 7.2 mm and chromatic aberrations leads to the same shift and distortion of the first and second picks widths approximately up to three times. The influences of the geometrical and chromatic aberrations in the bending magnets are studied without aberrations induced by the ED. Separately these types of aberrations lead to the following distortions: for geometrical aberrations: the central pick is the same and the neighboring pick width grows in two times. for chromatic aberrations: the grow of the both picks widths has the factor 3/2. All aberrations influence without and with chromatic aberrations in magnetic and electric deflectors demonstrates the necessity of using correction elements (for example, sextupoles). These pictures in the full measure demonstrate the influence of second order aberrations in the mass-spectrometer. Certainly it is necessary to study these influences more detailed for some selected variants of the system.

5.2 Third Order Aberrations

Third order aberrations should be separated into two parts: 1) Geometrical aberrations in *focusing* elements (in the

solenoids and the quadrupole). Only chromatic aberrations induced by these elements we investigate in all order; 2) Chromatic and geometric aberrations in *deflecting* elements: electrostatic and magnetic elements. In particular, geometrical aberrations of the third order in the solenoids lead to the grow of the first pick width in 1.2 times. For the quadrupole geometrical aberrations the first pick has the same width but the second pick width has the factor 1.1.

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Figure 1: Two variant of hypersurfaces in the parameters space $d_2 = d_2(B_{s_2}, \omega)$. The left picture corresponds to the focusing systems with solenoids. The right picture corresponds to the focusing systems with doublets of quadrupoles.



Figure 2: The dependence of distortion parameter D on the terminal solenoid field B_{s_2} .



Figure 3: The envelopes in X- and Y- planes and beam spots and distributions for mass-spectrometer with quadrupole focusing systems.



Figure 4: The envelopes in X- and Y- planes and beam spots and distributions for mass-spectrometer with solenoid focusing systems.