SYNTHESIS OF OPTIMAL NANOPROBE (NONLINEAR APPROXIMATION)

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Abstract

This paper is a continuation of the paper devoted to synthesis of optimal nanoprobe in linear approximation. Here the main goal is the optimization of nanoprobe including nonlinear aberrations of different nature up to third order. The matrix formalism for Lie algebraic methods is used to account for nonlinear aberrations. This method gives a possibility to consider nonlinear effects separately. Here we mean that a researcher can start or remove different kind of nonlinearities. This problem is separated into several parts. On the first step, we consider possibilities of additional optimization for some structures, selected on the step of linear approximation. The most of aberrations have harmful character, and their effect must be maximally decreased. Therefore, on the next steps, some we use analytical and numerical methods for generation of nonlinear corrected elements. The matrix formalism allows reducing the correction procedure to linear algebraic equations for aberration coefficients. Some examples of corresponding results are given.

INTRODUCTION

In this paper we consider some problems of nonlinear effects in a nanoprobe with high value of demagnification parameter (less than 0.01). In the paper [1] there are described procedures of optimal variants of a nanoprobe based on researcher demands to system characteristics. Strong requirements to the demagnification parameter, to beam spot shape, beam emittance lead us to necessity of very careful analysis of selected variants for a linear model of the nanoprobe. The goal of similar analysis is to select the most appropriate variants of nanoprobes. In case of need a necessary procedure of unwanted nonlinear aberrations using correcting multipoles, for example of correcting sextupole or/and octupole lenses.

MATHEMATICAL BACKGROUNDS AND MODELS

A Model of the Beam Line System for Nanoprobe

Similar to the paper [1] our consideration is based on so called “russian quadruplet” [1, 2], which allows forming high quality beams. According to [1] the optimal variants are based on the following demands:

1) focusing condition “point-to-point”;
2) values of optimal lens gradients are belong to load curves.

For the nonlinear model the base criterion of a beam quality — linear demagnification — DMl = |Rl1| should be replaced on its nonlinear variant

$$\text{DM}_n = \left(\sup_{x,y} (x^2 + y^2) \right) \left(\sup_{x_0,y_0} (x_0^2 + y_0^2) \right),$$

where $x, y \in \mathbb{M}, x_0, y_0 \in \mathbb{M}_0$, (1)

where $\mathbb{M}_0, \mathbb{M}$ — input and output phase manifolds of a beam.

Nonlinear Motion Equations for Beam Particles

For the necessity computation we use the Lie algebraic methods [3], which allows to design a nonlinear propagator $\mathcal{M}(s|s_0)$ in accordance to the following formulae:

$$\frac{d\mathcal{M}(s|s_0)}{ds} = \mathcal{L}(s) \circ \mathcal{M}(s|s_0),$$

where $\mathcal{L}(s|s_0)$ — a Lie operator of a dynamical system [3], defined by the following nonlinear motion equations

$$\frac{d\mathbf{Z}}{ds} = \mathbf{F}(\mathbf{Z}, s), \quad \mathbf{Z} = (x, x', y, y')^\ast.$$ (3)

Under the assumption of monochromaticity of the beam (in this case we have $\delta p = 0$) eq. (3) is generated by the following scalar equations

$$x'' + kxx' = -\frac{3}{2}kxx' - \frac{1}{2}kxy'^2 + kx'y'y + k'y'yy' + \frac{1}{12}k''x^2y^2 + \frac{k''}{4}x^3y^2 + \mathcal{O}(5),$$

$$y'' - kxx' = \frac{3}{2}kyy' + \frac{1}{2}kyy'^2 - k'y'xx' - k'y'xx' = k'y'xx' - \frac{1}{12}k''y^3 - \frac{1}{4}k''y^3 + \mathcal{O}(5),$$

where $k$ is a reduced gradient.

In eq.(4) nonlinear terms describe nonlinear geometrical effects. Restricted to nonlinearities up to the third order the eq.(4) can be written in the form

$$\frac{d\mathbf{Z}}{ds} = \mathbb{P}^{11}(s)\mathbf{Z} + \mathbb{P}^{13}(s)\mathbf{Z}[3],$$ (5)

According to the matrix formalism for Lie algebraic tools [4, 5] the solution of eq. (5) may be written in the following form

$$\mathbf{Z}(s) = \mathbb{R}^{11}(s|s_0)\mathbf{Z}_0 + \mathbb{R}^{13}(s|s_0)\mathbf{Z}_0^{[3]},$$ (6)

where $\mathbf{Z}_0^{[3]}$ — a Kronecker power for the phase vector $\mathbf{Z}$ of the third order, $s$ — a length, measured along of a beam line.

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optical axis, \( s_0 \) — its initial value (for example, \( s_0 = 0 \)). Here nonlinear aberrations of the third order are collected in the corresponding matrix \( \mathbb{R}^{13}(s|s_0) \) — the matrix of the third order geometrical aberrations.

For quadrupole focusing systems the forth-dimensional equation (6) it be convenient to rewritten as two-dimensional equations

\[
X(s) = \mathbb{R}^{12}(s|s_0)X_0 + \mathbb{R}^{13}(s|s_0)X_0^{[3]}, \\
Y(s) = \mathbb{R}^{11}(s|s_0)Y_0 + \mathbb{R}^{13}(s|s_0)Y_0^{[3]},
\]

(7)

For the partial matrices \( \mathbb{R}^{11}_x, \mathbb{R}^{11}_y \) and \( \mathbb{R}^{13}_x, \mathbb{R}^{13}_y \) there are evenly the group properties in the recurrent form (for example, for \( \mathbb{R}^{13}_x \))

\[
\mathbb{R}^{11}_x(s|s_0) = \mathbb{R}^{11}_x(s_{j+1}|s_j)\mathbb{R}^{11}_x(s_j|s_0), \\
\mathbb{R}^{13}_x(s|s_0) = \mathbb{R}^{13}_x(s_{j+1}|s_j)\mathbb{R}^{13}_x(s_j|s_0) + \mathbb{R}^{13}_x(s_j|s_0)\mathbb{R}^{13}_x(s_j|s_0),
\]

(8)

where \( \mathbb{R}^{33}_x = (\mathbb{R}^{11}_x)^{[3]} \). It should be mentioned that among these aberrations the main role play so called spherical aberrations, which are described the following elements of \( \mathbb{R}^{13}_x \): \( R_{14} \) under \( x^3 \), \( R_{10} \) under \( x^2 \), and for \( \mathbb{R}^{13}_y \): \( R_{14} \) under \( y^3 \), and \( R_{10} \) under \( y^2 \).

**Motion Equation for Beam Matrix Envelope**

It is known that for the linear motion equations we can use the so called envelope matrix — \( \sigma \)-matrix:

\[
\sigma^{env} = \{ \sigma_{ik} \}, \quad i, k = 1, 4.
\]

In this paper we use two variants of this matrix. The first can be defined according to equalities

\[
\sigma^{env}_{ik} = z_i(k - \max(\mathfrak{M})) z_k(i - \max(\mathfrak{M})),
\]

where \( z_i(k - \max(\mathfrak{M})) \) — an \( i \)-th component of the phase vector \( Z \) with maximal \( k \)-th component on the beam transverse manifold \( \mathfrak{M} \). The second case for \( \sigma \)-matrix is well known rms-envelope matrix

\[
\sigma^{rms}(s) = \int_{\mathfrak{M}(s)} f(Z, s) ZZ^* dZ,
\]

(9)

where \( f(Z, s) \) is a distribution function.

For the linear beam line model the propagation of \( \sigma \)-matrix is defined by following equation (both for \( \sigma^{env} \) and \( \sigma^{rms} \))

\[
\sigma(s) = \mathbb{R}(s|s_0)\sigma(s_0)\mathbb{R}^*(s|s_0),
\]

(10)

In the nonlinear case we can use the nonlinear variant of the equality (10) (see, for example, [5])

\[
\sigma^{11}(s) = \sum_{i=1, k=1}^{\infty} \mathbb{R}^{11}(s|s_0)\sigma^{ik}(s_0) (\mathbb{R}^{1k}(s|s_0))^*,
\]

(11)

where “nonlinear components” of the \( \sigma \)-matrix — \( \sigma^{ik} \), \( i, k \leq 1 \) in (11) can be evaluated using the analogue of the equality (9)

\[
\sigma^{ik}(s) = \int_{\mathfrak{M}(s)} f(Z, s)Z^i Z^{k*} dZ,
\]

(12)

It is not difficult to see, that in the linear case for the demagnification parameter we have

\[
DM^2 = \left| \frac{\sigma^{out}_{11}}{\sigma^{in}_{11}} \right|^2 = |R_{11}|^2.
\]

(13)

For nonlinear case instead of \( DM \) we should use the new parameter \( DM_{nl} \), for which the equalities (1) and (11) allow to evaluate the demagnification in nonlinear case.

**Characteristics for Nonlinear Nanoprobes**

For the nonlinear nanoprobe there are some other distortions of optimal characteristics (see, [6]). Indeed, in the case of nonlinear beam dynamics we should use the condition \( \sigma_{11} = \sigma_{22} \) instead of \( R_{11} = R_{22} \) the load curves change their configuration. If we take into consideration only spherical aberrations (see above) the circular symmetry for linear case should be replaced by symmetry relative to turn over \( \pi/2 \) (see Fig. 1). As it can be shown from this image, similar symmetry of the output beam spot guarantees the equality \( \sigma_{11} = \sigma_{44} \) (i.e. \( \sup x^2 = \sup y^2 \)). The main contribution of nonlinear aberrations of third order leads to increasing of the beam size and changes the circular symmetry (compare the corresponding images on the Fig. 1).

![Figure 1: Comparison of the beam spot for linear and nonlinear models.](image-url)

For focusing systems with critical characteristics the spread for beam spot may become too big. That is why in this case we have to put to use special correctors. In the case of geometrical aberrations these are octupole lenses. These lenses can be used either as separate elements (between quadrupole lenses) or both as combined lenses, which are quadrupole and octupole lenses at the same time. Here one can use two approaches. Beam spot after correction (this procedure is presented on Fig. 1 as black dashed lines) could be like on Fig. 1 as red line.

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A Problem of Correction of Undesirable Aberrations

The first of the used method is based on usual nonlinear programming methods. Here we use a combination of a Monte-Carlo method and the flexible tolerance method [7]. For this approach one should form an objective function $f(U)$, $U = n$ and derating in the form of equalities and inequalities:

$$\begin{align*}
\mathbf{H}(U) &= 0, \quad \dim \mathbf{H} = m < n, \\
\mathbf{G}(U) &\leq 0, \quad \dim \mathbf{G} = p,
\end{align*}$$

(14)

where $U$ is a vector of variable parameters. In is necessary to point that these parameters (non-dimensional) have to reduce to a single scale. For our problem for the objective function we can use $f(U) = \mathbf{DM}_{nl}(U)$, see eq. (1). As an equality constraint we can use $\mathbf{H}(U) = (\sigma_{11}(U) - \sigma_{44}(U))^2$. At last the inequalities constraints describe the range of variation of required parameters — components of $U$.

Let us describe the second approach [8]. The “nonlinear part” of the matrix $\mathbf{R}^{13}$ can be presented as a product $\mathbf{R}^{13} = \mathbf{R}_{\text{quad}}^{13} \mathbf{C} + \mathbf{R}_{\text{oct}}^{13} \mathbf{C}$, where $\mathbf{C}$ is a vector of octupole forces $C_j$, $j = 1, \ldots, NO$, where NO is a number of correcting octupole lenses. For the introduced matrix $\mathbf{R}^{13}$ we can write in the form (6)

$$Q^{13} = Q_{\text{quad}}^{13} + \sum_{j=1}^{NO} C_j \int_{s_j}^{s_{j+1}} R^{11}(s_0|\tau) R^{13}_{\text{oct}}(\tau) R^{33}(\tau|s_0) d\tau.$$

Here the intervals $[s_j, s_{j+1}]$ enclose only one control element (one of multipole lenses), and the matrices $R_{\text{oct}}^{13}$ is a matrix, calculated under the condition $C_j = 1$, $C_k = 0$, $\forall k \neq j$.

Consider as an example the problem of spherical aberration correction. In this case we can include in the focusing system four correctors — octupole lenses. In this case eq. (corrector 1) can be write the following equation

$$\mathbf{X}(s_t) = \mathbf{R}^{11}(s_t|s_0) \left( \mathbf{X}_0 + \left[ Q_{\text{quad}}^{13}(s_t|s_0) + \sum_{j=1}^{NO} Q_{\text{oct}}^{13}(s_t|s_0) \right] \mathbf{X}_0 \right),$$

where

$$Q_{\text{oct}}^{13}(s_j|s_{j-1}) = C_j \int_{s_{j-1}}^{s_j} R^{11}(s_0|\tau) R^{13}_{\text{oct}}(\tau) R^{33}(\tau|s_0) d\tau.$$

For the spherical aberrations it is quite enough to use four octupole lenses as correctors. The forces of these lenses can be found form the following linear algebraic equation

$$A \mathbf{C} = \mathbf{B}_{\text{quad}}.$$

where the matrix $A$ consists of the $R^{13} = R^{11}Q^{13}(s_t|s_0)$ elements $R_{16}$ and $R_{12}$, calculated under the following conditions: the $k$-th column calculated under $C_k = 1$, $C_j = 0$, $\forall j \neq k$. The vector $\mathbf{B}_{\text{quad}}$ consists of the same matrix elements, but calculated under $C_j = 0$, $\forall j$.

The analogue procedure can be applied for a non-monochromatic beam (see, for example, [9]). But in this case we should use sextupole lenses.

The above described approach can be simplified. For this we can use minor number of correctors. In this case we have to use the first of above mentioned approach, based on nonlinear programming methods. But here we can not to obtain so essential decreasing the for beam spot.

Usage of the described approach we can minimize the beam spot, which generate “nonlinear focusing system” (see Fig. 1). For some variants we succeeded in beam spot size contraction up to 6 times. But it should be mentioned that similar correction procedure can be realized in the case of all beam line parameters setup. Unfortunately many of appropriate variants have property of high sensitivity with respect to parameters deviation.

CONCLUSION

As above described, the nonlinear aberrations (both geometrical and chromatic) lead to modification of the form and increasing of beam spot size. The corresponding correction procedures help to reduce the beam size on the target. But it should be mentioned that the described correction procedures depend on the value of the selected beam parameters set. Here we mean that basic beam characteristics could be very sensitive to possible deviations from optimal parameters (see, i. e. [6]).

REFERENCES