CALCULATION OF ABERRATION COEFFICIENTS UP TO SIXTH ORDER OF MULTIPOLE FOCUSING ELEMENTS*

N. Tsoupas, Brookhaven National Laboratory, Upton, NY 11973
H. A. Enge, Massachusetts Institute of Technology, Cambridge, MA 02139
E. Forest, Lawrence Berkeley Laboratory, Berkeley, CA 94720

Abstract

A method and a computer code have been developed to calculate the aberration coefficients, up to sixth order, for a focusing device consisting of magnetic or electric multipoles. The method is based on the calculation of the ray coordinates at the exit of a focusing device using the RAYTRACE[1] code which provides the magnetic and electric multipole fields necessary for the integration of the equation of motion of the charged particles moving into the focusing device. Subsequently, the exit ray coordinates are considered as a Taylor series expansion, about the origin, in terms of the ray coordinates at the entrance. The coefficients of expansion are the aberration coefficients. The method to calculate the aberration coefficients is discussed further in the text.

Introduction

A ray entering a focusing device can be characterized by the input (I) coordinates $x^{(I)}$, $\theta^{(I)}$, $y^{(I)}$, $\phi^{(I)}$ $\ell^{(I)}$, and $\delta^{(I)}$ (Fig. 1), where $\theta^{(I)}$ and $\phi^{(I)}$ are the angles formed by the z axis and the projection of the ray on the (x, z) and (y, z) planes respectively, $\ell^{(I)}$ is the beam pulse length, and $\delta^{(I)} = \delta p/p_0$ is the momentum deviation of the ray from the momentum p_0 of the central ray. Similarly, a ray can be characterized by the $x^{(O)}$, $\theta^{(O)}$, $y^{(O)}$, $\phi^{(O)}$, $\ell^{(O)}$, and $\delta^{(O)}$ coordinates at the exit coordinate system.

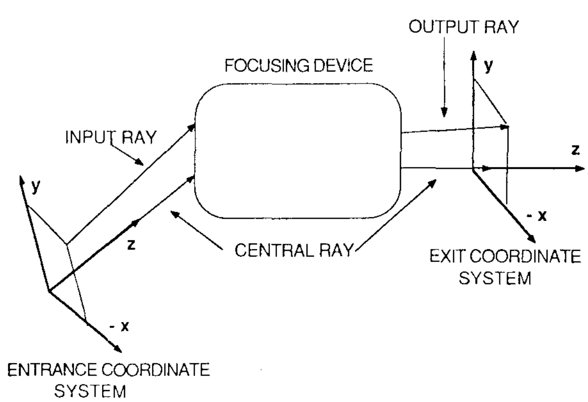

Fig. 1. Schematic of the entrance and exit coordinate system of a focusing device.

Any output ray coordinate can be considered as a function of the input ray coordinates, as in Eq. (1).

$$\chi_i^{(O)} = f\left(\chi_1^{(I)} \ldots \chi_6^{(I)}\right) \qquad i = 1 \ldots 6 \tag{1}$$

where the variables χ_1 to χ_6 correspond to the coordinates x, θ, y, ϕ, ℓ, and δ respectively.

The function in Eq. (1) can be expanded as a Taylor series (Eq. (2)) to the order desired. The central ray (Fig. 1) defines the origin about which the expansion is carried out.

$$\chi_i^{(O)} = \sum_{j=1}^{6} \frac{\partial \chi_i^{(O)}}{\partial \chi_j^{(I)}} \chi_j^{(I)} + \frac{1}{2!} \sum_{j,k} \frac{\partial^2 \chi_i^{(O)}}{\partial \chi_j^{(I)} \partial \chi_k^{(I)}} \chi_j^{(I)} \chi_k^{(I)}$$
$$+ \frac{1}{3!} \sum_{j,k,l} \frac{\partial^3 \chi_i^{(O)}}{\partial \chi_j^{(I)} \partial \chi_k^{(I)} \partial \chi_l^{(I)}} \chi_j^{(I)} \chi_k^{(I)} \chi_l^{(I)}$$
$$+ \text{(higher order terms)}. \tag{2}$$

All subindices run from 1 to 6.

By introducing the notation used in Ref. 2, Eq. (2) can be written more concisely as:

$$\chi_i^{(O)} = R_{ij} \chi_j^{(I)} + T_{ijk} \chi_j^{(I)} \chi_k^{(I)} + W_{ijkl} \chi_j^{(I)} \chi_k^{(I)} \chi_l^{(I)}$$
$$+ Z_{ijklm} \chi_j^{(I)} \chi_k^{(I)} \chi_l^{(I)} \chi_m^{(I)}$$
$$+ F_{ijklmn} \chi_j^{(I)} \chi_k^{(I)} \chi_l^{(I)} \chi_m^{(I)} \chi_n^{(I)}$$
$$+ S_{ijklmno} \chi_j^{(I)} \chi_k^{(I)} \chi_l^{(I)} \chi_m^{(I)} \chi_n^{(I)} \chi_o^{(I)} \tag{3}$$

where $j \le k \le l \le m \le n \le o$ and R, T, W, Z, F, and S are the first, second, and third order, etc. aberration coefficients. The summation is carried over the repeated indices. Equation (4) is an example of the concise notation used to designate the fourth order aberration coefficient.

$$Z_{ijklm} = \frac{\partial^4 \chi_i^{(O)}}{\partial \chi_j^{(I)} \partial \chi_k^{(I)} \partial \chi_l^{(I)} \partial \chi_m^{(I)}} \tag{4}$$

Method to Calculate Aberration Coefficients

In principle, the aberration coefficients appearing in Eq. (3) can be calculated by sending into the focusing system a number of rays with given coordinates $\chi_i^{(I)}$ at the entrance and calculating the ray coordinates $\chi_i^{(O)}$ at the exit, thus forming a set of n linear independent equations with m unknowns ($n \ge m$), the aberration coefficients. This set of equations can be solved by the least squares solution method.

Making no assumption about any symmetry in the multipole fields of the focusing system, the total number of aberration coefficients up to sixth order (not including the aberration coefficients with respect to (ℓ) coordinate) is 311 for each output beam coordinate $\chi_i^{(O)}$. Thus the matrix associated with the solution of the system of equations is at least 311 × 311 in dimension. Although the solution of such a system of equations is possible, not all computers can handle matrices of that size. Therefore, the following procedure was adopted for calculating the aberration coefficients corresponding to a particular exit coordinate $\chi_i^{(O)}$.

(All derivatives are taken with respect to the input (I) beam coordinates. Therefore, for the sake of clarity, the superscript (I) is omitted from Eqs. (5), (5a), and (5b).

By rearranging terms, Eq. (2) can be written

$$\chi_i^{(O)} = \sum \frac{\partial^{n_i}\chi_i^{(O)}}{\partial\chi_j^{n_i}}\,\chi_j^{n_i} + \sum \frac{\partial^{n_1+n_2}\chi_i^{(O)}}{\partial\chi_j^{n_1}\partial\chi_k^{n_2}}\,\chi_j^{n_1}\chi_k^{n_2}$$

$$+\sum \frac{\partial^{n_1+n_2+n_3}\chi_i^{(O)}}{\partial\chi_j^{n_1}\partial\chi_k^{n_2}\partial\chi_l^{n_3}}\,\chi_j^{n_1}\chi_k^{n_2}\chi_l^{n_3} + (\ldots) \qquad (5)$$

The terms under the first summation in Eq. (5) contain aberration coefficients with respect to one input coordinate only. Likewise, the terms under the second, third, etc. summation symbols contain aberration coefficients with respect to two coordinates, three coordinates, etc., respectively.

To proceed with the calculation of the aberration coefficients with respect to a single input beam coordinate, say $\chi_2^{(I)}$, we send through the device, few rays having all coordinates except one, say $\chi_2^{(I)}$, equal to zero. These rays reduce Eq. (5) to

$$\chi_i^{(O)} = \sum \frac{\partial^{n_1}\chi_i^{(O)}}{\partial\chi_j^{n_1}}\,\chi_j^{n_1} \qquad (5a)$$

The RAYTRACE code calculates the exit beam coordinates and then a least squares solution of a 6 $\times$ 12 (the number 6 corresponds to the aberration coefficients and the number 12 corresponds to the number of input rays) matrix equation provides all the aberration coefficients up to sixth order $\partial^n\chi_i^{(O)}/\partial\chi_j^n$, where $n = 1\ldots6$.

The aberration coefficients are then calculated with respect to two input beam coordinates, $\chi_j^{(I)}$ and $\chi_k^{(I)}$ ($j \neq k$), by sending rays having only two nonzero beam coordinates, say $\chi_1^{(I)}$ and $\chi_2^{(I)}$. These rays reduce Eq. (5) to

$$\chi_i^{(O)} = \sum \frac{\partial^{n_1}\chi_1^{(O)}}{\partial\chi_j^{n_1}}\,\chi_j^{n_1} + \sum \frac{\partial^{n_1+n_2}\chi_i^{(O)}}{\partial\chi_j^{n_1}\partial\chi_k^{n_2}}\,\chi_j^{n_1}\chi_k^{n_2} \qquad (5b)$$

The output beam coordinates are calculated from the RAYTRACE code. Then, taking into account the already known aberration coefficients ($\partial^n\chi_i^{(O)}/\partial\chi_j^n$), a set of linear equations is formed. This set of linear equations written in a matrix formalism involves a (15 $\times$ 24) matrix (15 corresponds to the number of aberration coefficients with respect to two input beam coordinates and 24 is the number of rays used). The least squares solution of the matrix equation provides the $\partial^{n+m}\chi_i^{(O)}/\partial\chi_j^n\partial\chi_k^m$ aberration coefficients ($n+m = 2\ldots6$ and $j < k$).

The same procedure is used to calculate the aberration coefficients with respect to three, four, five and six input beam coordinates. In Table I, the aberration coefficients are tabulated

Table I

ABERRATION COEFFICIENTS UP TO SIXTH ORDER TABULATED ACCORDING TO THE NUMBER OF INPUT RAY COORDINATES (Column 4)

Aberration Coefficient		Number of Aberration Coefficients	Number of Coordinates per Input Ray	Number of Rays Used for the Calculation
$\dfrac{\partial_1^{m}\chi_i^{(O)}}{\partial\chi_j^{(I)^{m_1}}}$	$m_1 = 1\ldots6$	6	1	12
$\dfrac{\partial^{m_1+m_2}\chi_i^{(O)}}{\partial\chi_j^{(I)^{m_1}}\partial\chi_k^{(I)^{m_2}}}$	$m_1+m_2 = 2\ldots6$ $j \neq k$	15	2	24
$\dfrac{\partial^{m_1+m_2+m_3}\chi_i^{(O)}}{\partial\chi_j^{(I)^{m_1}}\partial\chi_k^{(I)^{m_2}}\partial\chi_l^{(I)^{m_3}}}$	$m_1+m_2+m_3 = 3\ldots6$ $j \neq k \;\; k \neq l \;\; j \neq 1$	20	3	24
$\dfrac{\partial^{m_1+m_2+m_3+m_4}\chi_i^{(O)}}{\partial\chi_j^{(I)^{m_1}}\partial\chi_k^{(I)^{m_2}}\partial\chi_l^{(I)^{m_3}}\partial\chi_m^{(I)^{m_4}}}$	$m_1+m_2+m_3+m_4 = 4\ldots6$ j,k,l,m different from each other	15	4	20
$\dfrac{\partial^{m_1+m_2+m_3+m_4+m_5}\chi_i^{(O)}}{\partial\chi_j^{(I)^{m_1}}\partial\chi_k^{(I)^{m_2}}\partial\chi_l^{(I)^{m_3}}\partial\chi_m^{(I)^{m_4}}\partial\chi_n^{(I)^{m_5}}}$	$m_1+m_2+m_3+m_4+m_5 = 5\ldots6$ j,k,l,m,n all different from each other	6	5	12

with the number of input beam parameters and the number of rays used for the calculations. A more detailed description for the derivation of the aberration coefficients is given in Ref. 3.

Methods of Testing Aberration Coefficients

To test the aberration coefficients derived by the above method, the following procedures can be used.

a) Compare with aberration coefficients derived by MARYLIE,[4] TRANSPORT, or other existing codes.

b) Use the simplectic relation[5]

$$\tilde{M}JM = J$$

or

$$M_{i\alpha}J_{ij}M_{j\beta} = J_{\alpha\beta} \tag{6}$$

where $J_{\alpha\beta} = [\chi_\alpha^{(I)}, \chi_\beta^{(I)}]$ are the poisson brackets of the canonical variables $\chi_\alpha^{(I)}, \chi_\beta^{(I)}$ and $M_{i\alpha} = \partial\chi_i^{(O)}/\partial\chi_\alpha^{(I)}$ with $\chi_i^{(O)}$ given by Eq. (2).

Equation 6 yields the relationships that should be satisfied among the aberration coefficients. A few of the relationships which involve first, second, and third order aberration coefficients are given below.

$$R_{i\alpha}J_{ij}R_{j\beta} \;=\; J_{\alpha\beta} \tag{6a}$$

$$R_{i\alpha}J_{ij}T_{j\beta k'} \;+\; T_{i\alpha k}J_{ij}R_{j\beta} \;=\; 0 \tag{6b}$$

$$R_{i\alpha}J_{ij}W_{j\beta k'l'} \;+\; T_{i\alpha k}J_{ij}T_{j\beta k'}\; W_{i\alpha k\ell}J_{ij}R_{j\beta} \;=\; 0 \tag{6c}$$

The fact that the Eq. (6) is satisfied is not a proof that the aberration coefficients are correct. It is only a test to show that the aberration coefficients are wrong if the simplectic relation is not satisfied.

References

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