

Functional Dependence, Broad-Band Fitting, and Ancillary Conditions

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Abstract

The ability to make multiple passes through a charged particle optical system, as a single step in a mathematical procedure, opens up new computational capabilities. At the simplest level, the functional dependence of any transfer matrix of any order, or any beam phase-space parameter can be plotted as a function of any other parameter used to describe the optical configuration. Secondly, broad-band fitting can be done on aberrations, where all orders are considered simultaneously according to their importance on the final phase-space beam distribution. Finally, ancillary conditions may be imposed in the calculation of functional dependences. For example, the dependence of a matrix element on a beam line parameter may be calculated and plotted, subject to constraints imposed on other matrix elements. The computer program TRANSPORT now has these capabilities. Additional examples will be given.

1 INTRODUCTION

Functional dependence, broad-band fitting, and ancillary conditions are all useful concepts in a charged particle optical system. The computer program TRANSPORT [1] now has these three capabilities. In this section and the following we describe each of these three items, what they represent mathematically, and how to implement them with TRANSPORT.

The functional dependence can involve any of the parameters used to describe the physical beam line and any of the transfer matrix elements which can be calculated. One parameter can be stepped over an interval. As it is stepped, the values of the transfer- and beam- matrix elements will vary systematically. Plots can be made of any matrix element vs the stepped parameter, or of one matrix element vs another.

Ancillary conditions can be imposed in the form of constraints on the matrix elements. With constraints, a fitting process is carried out for each value of the stepped parameter. The constraint will now make the stepped parameter affect the value of any parameters which are varied or calculated from parameters which are varied. Now there will be functional dependence between parameters, and plots can be made of one parameter vs another. The plots will be made with the values of the fitted parameters at the end of the fitting process.

In broad-band fitting, there is no longer a separate fitting procedure for each value of the stepped parameter. Rather, the entire set of values of the stepped parameter are included in a single fitting procedure. Broad-band fitting is useful for eliminating aberrations. In broad-band fitting, aberrations

are not separated into orders, but minimized as they actually occur in a charged particle optical system.

In the following sections, we will give examples of the three capabilities: functional dependence, broad-band fitting, and ancillary conditions. Functional dependence and ancillary conditions will be treated together in the next section since they are strongly related. Broad-band fitting will be treated in a separate section.

2 FUNCTIONAL DEPENDENCE AND ANCILLARY CONDITIONS

Consider a symmetric quadrupole triplet. The pole-tip fields are varied so as to obtain a first-order focus in both transverse planes. The triplet is placed so that its longitudinal midpoint is two meters upstream of the longitudinal midpoint of the beam line.

Now the triplet is treated as a rigid body and slid forward and backward. The triplet continues to be symmetric. At each location the pole-tip magnetic fields are adjusted to give foci in the two transverse planes at the end of the beam line.

We define a parameter DS which indicates the longitudinal displacement of the triplet from the point two meters before the midpoint of the beamline. If DS is decreased, then the triplet moves toward the beginning of the beam line. If DS is increased, then the triplet moves toward the end.

Figure (1) is a plot of the two pole-tip magnetic fields of the symmetric triplet vs the longitudinal displacement DS . Note that the fields are minimized when the parameter DS is 2.0 meters. At that point the configuration is longitudinally symmetric. The triplet is equidistant from the beginning and the end of the beam line.

The plot shown is made with TRANSPORT [1] and TOPDRAWER [2]. The entire process of making the plot is automated. Starting with a data file for TRANSPORT and a skeleton data file (all instructions except the data), the plots are produced by invoking a single procedure.

The functional dependence of the pole-tip fields is shown clearly. The ancillary conditions are embodied in the requirement that there be a focus in both transverse planes at the end of the beam line.

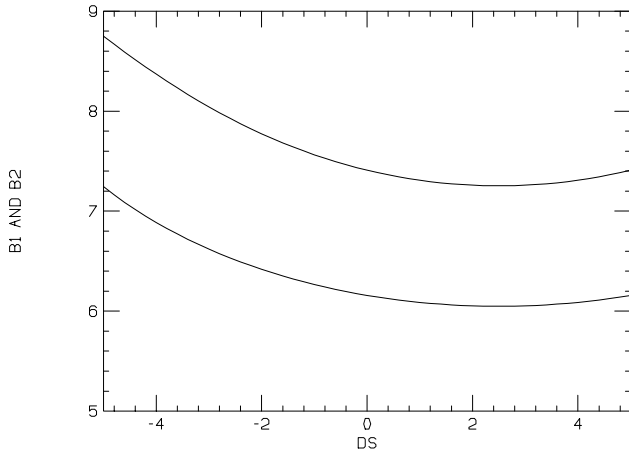


Figure (1): The dependence of the two pole-tip magnetic fields of a symmetric triplet on the longitudinal position of the triplet.

3 OFF-MOMENTUM TRANSFER MATRICES

In the theory of charged-particle optics, the action of an optical system on a charged particle is represented by a matrix expansion. The final coordinates $X_i(1)$ are given in terms of the initial coordinates $X_i(0)$ by the expression [3] [4]:

$$\begin{aligned} X_i(1) &= \sum_j R_{ij} X_j(0) \\ &+ \sum_{jk} T_{ijk} X_j(0) X_k(0) \\ &+ \sum_{jkl} U_{ijkl} X_j(0) X_k(0) X_l(0) , \end{aligned} \quad (1)$$

The three quantities R , T , and U represent respectively the first-, second-, and third-order matrices of the Taylor-series expansion. The six beam coordinates are taken to be $(x, x', y, y', \ell, \delta)$. Here δ is defined as $\Delta p/p_0$, the fractional deviation from the central momentum. When we speak of the displacement of a trajectory, we include a displacement in δ , even though the term “displacement” sounds like a geometric consideration and δ is a kinematic quantity. A trajectory which follows the axis of a quadrupole channel can still have a displacement in δ if the trajectory momentum is different from the reference momentum.

Let us now shift our reference to a trajectory which is displaced from the original reference trajectory. The new reference trajectory is denoted as X_r , and the difference between an arbitrary trajectory and the new reference trajectory is given by ΔX . In terms of these new quantities, equation (1) can now be rewritten as:

$$\begin{aligned} X_{1r} + \Delta X_1 &= X_{1s} + R(X_{or} + \Delta X_o) \\ &+ T(X_{or} + \Delta X_o)(X_{or} + \Delta X_o) \\ &+ U(X_{or} \Delta X_o)(X_{or} + \Delta X_o)(X_{or} + \Delta X_o) \end{aligned} \quad (2)$$

Subtracting the equation for the reference trajectory, we derive

$$\begin{aligned} \Delta X_1 &= R \Delta X_o + T(2X_{or} \Delta X_o + \Delta X_o \Delta X_o) \\ &+ U(3X_{or} X_{or} \Delta X_o + 3X_o \Delta X_o \Delta X_o \\ &\quad + \Delta X_o \Delta X_o \Delta X_o) \\ &= (R + 2TX_{or} + 3UX_{or} X_{or}) \Delta X_o \\ &+ (T + 3UX_{or}) \Delta X_o \Delta X_o + U \Delta X_o \Delta X_o \Delta X_o \end{aligned} \quad (3)$$

From equation (3), we can define new first- and second-order transfer matrices by

$$\begin{aligned} R^* &= R + 2TX_{or} + 3UX_{or} X_{or} \\ T^* &= T + 3UX_{or} \end{aligned} \quad (4)$$

These redefined matrices for each element can then be accumulated to produce transfer matrices for the entire magnetic optical system. The transformation of a particle trajectory through the system can now be represented by a transformation similar in appearance to equation (1).

$$X_1 = X_{1r} + R(t)X_o + T(t)X_o X_o + U(t)X_o X_o X_o \quad (5)$$

Here the matrices $R(t)$, $T(t)$, and $U(t)$ are calculated as products of the matrices R^* , T^* , and U , as defined in equation (4). They are expressed relative to the transformed original reference trajectory X_{1r} . The original reference trajectory is transformed through the system using equation (1) on an element-by-element basis.

The off-axis expansion can be used to explore chromatic effects. If a nonzero δ is specified, the first-order transfer matrix will be with respect to the off-momentum centroid. If there is dispersion in the system, the centroid will, at some point, be displaced from the reference trajectory. The result from an off-axis expansion can differ substantially from that of an on-axis calculation. The effect of many orders higher than second or even third can be seen.

Let us consider the example of a very long focusing system, with many intermediate foci. The value of the R_{12} matrix element at the end of such a system is shown in figure (2). First, we use the traditional procedure and accumulate the transfer matrices about the original reference trajectory. Then, at the end, we use equation (4) to define a new momentum-dependent first-order transfer matrix for the entire system. The value of the R_{12} matrix element is given by the straight line (labeled simply “2nd order”), passing through the origin. The inclusion of third order makes no visible difference.

For an exact calculation, with a ray tracing program, the behavior is quite different. For a slight deviation from the reference momentum, the value of R_{12} will, as before, grow linearly with the value of δ . As the momentum deviation continues to increase, one of the intermediate foci will move downstream and the system will once again be focusing.

We can also calculate the off-momentum first-order transfer matrix for each element using equation (4). If we

then accumulate these off-momentum R matrices over the entire beam line, then we get the two curves shown in figure (2). Both curves are labelled “SBA”, which means shift before accumulating. The curve labelled “2nd order” includes only the second-order terms in equation (4). The curve labelled “3rd order” also includes the third-order term in equation (4). Since the third-order curve is indistinguishable from the exact calculation, no higher orders in the expansion are necessary.

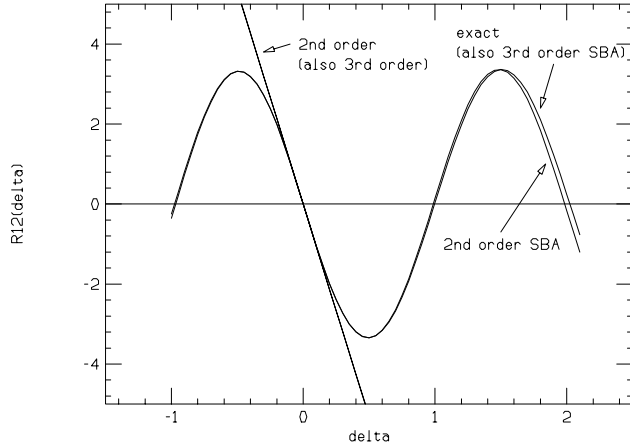


Figure (2): The magnitude of the sinelike trajectory, as a function of relative momentum deviation δ , at the end point of a long beam line. The various meanings of the curves in the figure are explained in the text.

4 BROAD-BAND FITTING

Broad-band fitting resembles the combination of functional dependence with ancillary conditions in a very simple way. Both involve fitting, and both involve stepping of a parameter over an interval. With functional dependence with ancillary conditions, the fitting loop is inside the stepping. In other words, there is a separate fitting procedure for each value of the stepped parameter.

With broad-band fitting, there is a single fitting procedure which includes all the values of the stepped parameter. The chi-squared for the the configuration is equal to the sum of the individual chi-squareds for the different values of the stepped parameter. In the example given above, the stepped parameter is the relative momentum deviation δ .

A broad-band fitting procedure then imposes a constraint over an interval in δ . The example given is a constraint for a point-to-point focus. The off-momentum transfer matrix, according to equation (4), contains contributions from the higher-order matrix elements. Therefore a broad-band constraint on the first-order matrix elements R_{12} and R_{34} is simultaneously a constraint on all higher-order chromatic matrix elements affecting the focusing.

To effect the broad-banded fitting in TRANSPORT, one need do only three things. First, one must indicate that a first-order fit is to be made on the matrix elements R_{12} and R_{34} . Secondly, one must specify that the parameter δ is to be stepped, and also give the limits of the interval and the

step size. Finally, one must include a line in the data which has on it the word BROAD, indicating that the fit is to be broad-banded.

TRANSPORT can then optimize the chromatic characteristics of the beam line by adjusting the strength of sextupoles, octupoles, and any other optical element influencing higher-order terms. The optimization will be imposed uniformly across the entire momentum interval specified, instead of favoring the origin, as one does when one fits the different orders separately.

5 REFERENCES

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