Nuclear Instruments and Methods in Physics Research A258 (1987) 402–406
North-Holland, Amsterdam

COSY 5.0 – THE FIFTH ORDER CODE FOR CORPUSCULAR OPTICAL SYSTEMS

M. BERZ *, H.C. HOFFMANN and H. WOLLNIK

II. Physikalisches Institut, Universität Giessen, 6300 Giessen, FRG

COSY 5.0 is a new computer code for the design of corpuscular optical systems based on the principle of transfer matrices. The particle optical calculations include all image aberrations through fifth order. COSY 5.0 uses canonical coordinates and exploits the symplectic condition to increase the speed of computation.

COSY 5.0 contains a library for the computation of matrix elements of all commonly used corpuscular optical elements such as electric and magnetic multipoles and sector fields. The corresponding formulas were generated algebraically by the computer code HAMILTON. Care was taken that the optimization of optical elements is achieved with minimal numerical effort. Finally COSY 5.0 has a very general mnemoniç input code resembling a higher programming language.

1. The particle optical elements in COSY

The program HAMILTON [1] was used to determine the analytic solution of the equations of motion for the particle optical elements used in COSY. HAMILTON generates these formulas in the form of a FORTRAN subroutine fully compatible with the program COSY.

In particle optics the motion is usually described relative to the motion of a reference particle, the trajectory of which is called the optic axis. The set of coordinates used for the description of the movement is the following:

$$r_1 = x, \tag{1a}$$

$$r_2 = a = \frac{p_x}{p_0}, \tag{1b}$$

$$r_3 = y, \tag{1c}$$

$$r_4 = b = \frac{p_y}{p_0}, \tag{1d}$$

$$r_5 = 1 = v_0(t - t_0), \tag{1e}$$

$$r_6 = d = \frac{K - K_0}{K_0}, \tag{1f}$$

$$r_7 = g = \frac{m - m_0}{m_0}, \tag{1g}$$

Here x and y are the horizontal and vertical distances to the optic axis, respectively. The quantities p_0, v_0, K_0 and m_0 denote momentum, velocity, kinetic energy and mass of the reference particle, whereas p, v, K and m stand for the same quantities of the particle under consideration.

The values of the coordinates in eqs. (1) at the end of a particle optical device are now expressed in terms of the values at the beginning in the following form

$$r_i^{(\mathrm{f})} = \sum_{j=1}^{7} r_j \left\{ (r_i, r_j) + \sum_{k=j}^{7} r_k \left\{ (r_i, r_j r_k) + \sum_{l=k}^{7} r_l \{ \cdots \} \right\} \right\}, \; i = 1,7 \tag{2}$$

Using the program HAMILTON, we determined analytic formulas for the expansion coefficients or matrix elements (r_i, r_j), $(r_i, r_j r_k)$, $\cdots$ through fifth order. Thus COSY allows much more accurate calculations than other commonly used programs [2–4] which can only handle aberrations through third order. Since HAMILTON is not limited to fifth order, COSY could even be expanded to still higher orders if desired. At the moment, the following particle optical elements are available:

- field free drift,
- magnetic multipoles (quadrupole through dodecapole),
- superposition of magnetic multipoles,
- electric multipoles (quadrupole through dodecapole),
- homogeneous magnetic bending fields,
- inhomogeneous magnetic bending fields, and
- inhomogeneous electrostatic bending fields.

If desired, this library of subroutines can be expanded by additional routines quite easily. As soon as the field expansion of the electric and magnetic fields are known, one can use HAMILTON to determine the corresponding subroutine.

Besides these main elements, COSY is able to handle fringing fields in two different manners. The first method is an approximation for sharp cutoff fringe fields. In

* Work done in partial fulfillment of the requirements for the doctor's degree, University of Giessen, FRG.

0168-9002/87/$03.50 © Elsevier Science Publishers B.V.
(North-Holland Physics Publishing Division)

this case, one obtains a δ-function-like field perpendicular to the field boundary for which a solution of the equations of motion can be found. This leads to a kick of the particle trajectory only. Alternatively, arbitrary fringing fields can be handled using the method of power series tracking [5]. An implementation of this very versatile method for the special requirements of fringe fields is under development.

2. The conditions of symplecticity and its exploitation

The motion of charged particles in electromagnetic fields is governed by the Hamiltonian equations of motion having the form

$$\begin{bmatrix} \mathrm{d}q_1/\mathrm{d}s \\ \mathrm{d}p_1/\mathrm{d}s \\ \mathrm{d}q_2/\mathrm{d}s \\ \mathrm{d}p_2/\mathrm{d}s \\ \mathrm{d}q_3/\mathrm{d}s \\ \mathrm{d}p_3/\mathrm{d}s \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \partial H/\partial q_1 \\ \partial H/\partial p_1 \\ \partial H/\partial q_2 \\ \partial H/\partial p_2 \\ \partial H/\partial q_3 \\ \partial H/\partial p_3 \end{bmatrix} \tag{3}$$

where q_t and p_t are canonical variables describing the particle motion, and s is the independent variable. Note that by choosing $a = p_x/p_0$ instead of p_x/p_z as in GIOS [3] or TRANSPORT [2], the coordinates x, a and y, b are canonical up to a scaling factor. Since l and d describe the time-of-flight and the particle energy up to scaling factors, these quantities are also canonical. This choice of variables has the result that the full Hamiltonian theory can be applied directly. One consequence thereof is the condition of symplecticity. For its derivation let us first collect the q_t and p_t to one vector

$$\boldsymbol{r} = (r_1, r_2, r_3, r_4, r_5, r_6) = (q_1, p_1, q_2, p_2, q_3, p_3),$$

and then rewrite Hamilton's equations of motion (eq. (3)) as

$$\boldsymbol{r}' = J\frac{\partial H}{\partial \boldsymbol{r}}, \tag{4}$$

where J is the matrix of eq. (3), prime denotes differentiation with respect to the independent variable s and $\partial H/\partial \boldsymbol{r}$ denotes the gradient of H.

Let now $\boldsymbol{T}(s_0 \to s)$ be the transfer map describing the motion from position s_0 to position s (see eq. (2)), i.e.,

$$\boldsymbol{r}(s) = \boldsymbol{T}[\boldsymbol{r}(s_0)] \tag{5}$$

and let $M(s_0 \to s)$ be the Jacobian of $\boldsymbol{T}$; i.e.,

$$M(s_0 \to s) = \frac{\partial \boldsymbol{T}(s_0 \to s)}{\partial \boldsymbol{r}} = \frac{\partial \boldsymbol{r}(s)}{\partial \boldsymbol{r}(s_0)}. \tag{6}$$

Then we can infer the relations

$$\boldsymbol{r}(s)' = M(s_0 \to s)\boldsymbol{r}(s_0)'$$

and

$$\frac{\partial H}{\partial \boldsymbol{r}(s_0)} = M^{\mathrm{t}}(s_0 \to s)\frac{\partial H}{\partial \boldsymbol{r}(s)}. \tag{7}$$

Using now eqs. (4) and (7) one obtains:

$$\begin{aligned} J\frac{\partial H}{\partial \boldsymbol{r}(s)} &= \boldsymbol{r}(s)' = M(s_0 \to s)\boldsymbol{r}(s_0)' \\ &= M(s_0 \to s)J\frac{\partial H}{\partial \boldsymbol{r}(s_0)} \\ &= M(s_0 \to s)JM^{\mathrm{t}}(s_0 \to s)\frac{\partial H}{\partial \dot{\boldsymbol{r}}(s)}. \end{aligned} \tag{8}$$

Comparing the beginning and the end of eq. (8), we thus obtain

$$J\frac{\partial H}{\partial \boldsymbol{r}(s)} = M(s_0 \to s)JM^{\mathrm{t}}(s_0 \to s)\frac{\partial H}{\partial \boldsymbol{r}(s)}. \tag{9}$$

We now extend the Hamiltonian H beyond s in the following way:

$$H_e(\tilde{s}) = \begin{cases} H & \text{for} \qquad\qquad \tilde{s} \leqslant s, \\ r_1 & \text{for} \quad s \quad < \tilde{s} \leqslant s + \Delta s, \\ r_2 & \text{for} \quad s + \Delta s < \tilde{s} \leqslant s + 2\Delta s, \\ \vdots & \qquad\qquad\qquad\quad \vdots \\ r_6 & \text{for} \quad s + 5\Delta s < \tilde{s} \leqslant s + 6\Delta s, \end{cases} \tag{10}$$

where Δs is an arbitrary positive number. From eq. (10) we can infer

$$\frac{\partial H_e}{\partial \boldsymbol{r}} = \begin{cases} e_1 = (1, 0, 0, 0, 0, 0) & \text{for } s < \tilde{s} \leqslant s + \Delta s, \\ e_2 = (0, 1, 0, 0, 0, 0) & \text{for } s + \Delta s < \tilde{s} \leqslant s + 2\Delta s, \\ \vdots & \quad \vdots \\ e_6 = (0, 0, 0, 0, 0, 1) & \text{for } s + 5\Delta s < \tilde{s} \leqslant s + 6\Delta s, \end{cases} \tag{11}$$

and thus according to eq. (9)

$$Je_t = M(s_0 \to s + i\Delta s)JM^{\mathrm{t}}(s_0 \to s + i\Delta s)e_i$$

$$\text{for } i = 1 \cdots 6. \tag{12}$$

Since $\boldsymbol{T}$ is continuous, we can infer $M(s_0 \to s + i\Delta s) = \partial \boldsymbol{T}(s_0 \to s + i\Delta s)/\partial \boldsymbol{r} \to M(s_0 \to s)$ if $\Delta s \to 0$. Note further that the vectors e_t in eq. (11) form a basis of the six-dimensional space. Taking the limit $\Delta s \to 0$, thus, eq. (12) yields

$$J = M(s_0 \to s)JM^{\mathrm{t}}(s_0 \to s). \tag{13}$$

This relationship holds for all Jacobians derived from Hamiltonian transfer maps and thus is of global importance [6]. The relationship presents a restriction of the freedom a transfer map can have as soon as it is created by a Hamiltonian system.

Consider now the case where the transfer map is expanded in a power series of the initial coordinates. Inserting these power series into the condition of symplecticity produces a set of relationships among the expansion coefficients [7]. To first order one obtains the well-known results [8]:

$$(x|x)(a|a)-(x|a)(a|x)=1$$

and

$$(y|y)(b|b)-(y|b)(b|y)=1$$

as well as

$$(l|x)=k\{(x|x)(a|d)-(x|d)(a|x)\}$$

and

$$(l|a)=k\{(x|a)(a|d)-(x|d)(a|a)\}. \qquad (14)$$

Here k is a scaling factor. Note that the symplectic condition implies that there is some redundancy in the description of the transfer matrix.

This probably was the primary reason that led to the development of the code MARYLIE [4] in which the transfer map is represented by a standard time development operator of the form

$$M=\exp(:P:), \qquad (15)$$

Here exp is a function acting on the Lie algebra developed from the vector space of functions of the phase space coordinates where "multiplication" is introduced as the Poisson bracket.

The explicit derivation of the symplectic equations through higher orders seems hardly possible without the help of a computer. For this reason we wrote the FORTRAN program SYMPLI that analytically derives all symplectic conditions with or without midplane symmetry through any given order. Through fifth order, the order of matrix elements handled in COSY, we obtain a total of 617 symplectic equations, not all of which, however, are independent.

These symplectic equations present a perfect means of checking the validity and accuracy of a given program determining matrix elements. However, inspecting these conditions more closely shows that they can be actually solved for individual matrix elements. This implies that the matrix elements can be separated in genuine matrix elements and symplectically dependent matrix elements. Thus it suffices to actually compute the genuine matrix elements and then determine the symplectically dependent matrix elements in the much simpler way of using the symplectic condition. COSY exploits this advantage in its concatenation routine and in doing so saves about 25–30% in computer time.

3. The command language of COSY

Besides the ability to compute the quantitites of interest for charged particle optical systems, a very general instruction code and also fitting capabilities are desirable for the design of particle optics systems. For this reason COSY has a quite general input language involving use of variables, arbitrary arithmetic, logical structures and loops. Furthermore, COSY allows the fitting of any of the used variables or matrix elements by changing the values of other variables.

COSY input somewhat resembles a programming language like BASIC, upgraded for transfer matrix features and fitting capabilities. This approach permits a very general use and gives the user freedom to design the input to satisfy his needs. However, for the average user the utmost degree of generality is often not necessary, but a system very easy to use is desirable. This is why a second, slightly different input language is being designed now to allow a faster setup and treatment of standard problems [9]. We give a brief description of the commands already available in COSY input. For a full description of the commands available see ref. [10].

The first set of commands available in COSY enables the definition of beam properties and computation modes. Among these commands are ones defining the kinetic energy, mass and charge of the reference particle and the shape and size of the phase space occupied by a particle beam. Furthermore, maximum energy and mass spreads are defined. Finally the desired calculation order and the amount of detail to be given in the output are specified. The next set of commands involves particle optical elements and determines whether the transfer matrix of the given element is to be concatenated with the previously existing transfer matrix. The particle optical elements include drift lengths, magnetic and electric multipoles, bending magnets and condensers including inhomogeneities and fringe fields. Furthermore, a command that sets the current transfer map to unity is available.

Besides the concatenation of transfer maps, usual floating point algebra is available. The operands include constants, previously defined variables and matrix elements. The syntax follows FORTRAN syntax including the proper hierarchy of operations and parentheses. Besides the usual five operations: addition, multiplication, subtraction, division and exponentiation, six logical operators are available. The supported functions include all of the standard FORTRAN functions plus a few more, like factorials and logarithms to the bases 2 and 10.

Also interactive computations are possible. If this is desired, the control is returned to the user who can interactively input a floating point algebra command compatible with the form described above. After the command is put in, it is analyzed and executed using the values of the internal variables.

The next group of commands allows for structured logical decisions. They enable execution of a block of commands only if a certain key variable has a certain value. This allows both the simulation of block if structures and loops where in the latter case the key variable is changed within the block. Similar to the structured logical command is the fitting command. It entails that a certain block is executed over and over again, changing some previously picked variables such that the values of other variables approach previously chosen values. This action is carried on until a certain termination criterion is met.

Finally there are output commands. First of all there are print commands, very similar to the ones in FORTRAN or BASIC, allowing the output of any variables and even text strings both to the terminal and to an output file. Besides these commands there are print commands, which dump the entire transfer matrix to the terminal or the output file.

We conclude this section with an example of a COSY input file and explanation of the commands. The example of the input file is shown in table 1.

The command REFERENCE PARTICLE defines the energy, mass and charge of the reference particle to be 1 MeV, 4 amu and 2 elementary charges. With PHASESPACE X-DIRECTION and PHASESPACE Y-DIRECTION, the initial beam diameter and divergence are both set to 0.02 m and 0.01 rad, respectively. The following commands give the desired order of calculation and set some variables to start values.

The command WHILE BEGIN entails a logical decision. As long as the variable IWHILE is greater than zero, the block ending at the WHILE END of the same level is executed until the value of IWHILE becomes negative or zero. IWHILE can be set to zero in the very helpful command INTERACTIVE COMPUTATION which returns control to the user and allows arithmetic operations and changing the values of variables.

The FIT BEGIN command marks the beginning of a section which is run through over and over again, where the variables after the FIT BEGIN are changed. The FIT END command denotes the end of this section and gives the name of a variable to be minimized (IMAGO), the accuracy to which the minimization is to be done (ITOL), and the maximum number of iteration steps (NANZ).

With the UNITY MATRIX (U M) command the total transfer matrix is first set to unity. Then an optical system is defined starting with a field free drift length (D L) of length 0.1 m followed by a magnetic quadrupole (M Q) of length 0.1 m, pole flux density B_1 and aperture 2 of 0.01 m. The next command (D L) entails that a field free drift length of length L be included, then follow another quadrupole and another drift length.

IFIT is a variable counting the iterations. Whenever it is divisible by 10, IP will be set to 1, otherwise to zero.

Table 1
An example of a COSY input file

```
REFERENCE PARTICLE 1 4 2;
PHASESPACE X-DIRECTION .02 .01;
PHASESPACE Y-DIRECTION .02 .01;

CALCULATION ORDER 5;
L = .1;
B1 = .01; B2 = -.01;
NANZ = 100; ITOL = 1E-5;

IWHILE = 1;
WHILE BEGIN IWHILE;
   IFIT = 0;
   FIT BEGIN L B1 B2;

      U M; D L .1; M Q .1 B1 .01; D L L; M Q .1 B2 .01; D L .1;

      IFIT = IFIT + 1
      IMAGO = SQRT((X, A)*(X, A) + (Y, B)*(Y, B)); IFIT = IFIT + 1;
      IP = INT(IFIT/10) EQ IFIT/10;
      WHILE BEGIN IP; PRINT SCREEN IFIT IMAGO; WHILE END;

   FIT END IMAGO ITOL NANZ;

   INTERACTIVE COMPUTATION;

WHILE END;

COSY END;
```

Thus the following while block will be only executed on every tenth iteration. In this case it prints to the screen the values of IFIT and IMAGO.

The command INTERACTIVE COMPUTATION allows a selection of new start values in the case the first fit has not converged. In case the fit has converged, the variable IWHILE can be set to zero and the major while block will be terminated. The last command terminates the program COSY.

References

[1] M. Berz and H. Wollnik, Nucl. Instr. and Meth., in press.

[2] K.L. Brown, SLAC-Rep. 91, Stanford (1970).

[3] H. Wollnik, J. Brezina, M. Berz and W. Wendel, Proc. AMCO-7, GSI-Rep. THD-26 (1984) 679; Nucl. Instr. and Meth., in press.

[4] A.J. Dragt, L.M. Healy, F. Neri and R. Ryne, IEEE Trans. Nucl. Sci. NS-3 (5) (1985).

[5] M. Berz, Nucl. Instr. and Meth., in press.

[6] A.J. Dragt, 1981 Fermilab Summer School, AIP Conf. Proc. Vol. 87 (1982).

[7] H. Wollnik and M. Berz, Nucl. Instr. and Meth. A238 (1985) 127.

[8] H. Wollnik, Optics of Charged Particles (Academic Press, New York, 1986).

[9] H.C. Hoffmann, Thesis, University of Giessen (1987) unpublished.

[10] M. Berz, Thesis, University of Giessen (1986) unpublished.