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THE PROGRAM HAMILTON FOR THE ANALYTIC SOLUTION OF THE EQUATIONS OF MOTION THROUGH FIFTH ORDER

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HAMILTON is a computer code performing all algebraic operations necessary for an analytic determination of the power series of the Hamiltonian equations of motion in the electromagnetic fields with at least one plane of symmetry. It is written entirely in FORTRAN in order to achieve fast machine performance, a requirement which is essential due to the complexity of the equations of motion in higher orders. HAMILTON is considerably faster than common more versatile formula manipulators and uses noticeably less storage.

Besides the mere solution of the equations of motion, HAMILTON also produces FORTRAN code compatible with the program COSY 5.0 allowing the computation of matrix elements of individual optical elements and their concatenation. The produced FORTRAN code is highly optimized and on average requires only 30% of the execution time of a handwritten comparable code.

1. Introduction

In the mathematical description of particle optics systems, two major approaches have been used in the past. In the first approach the equations of motion describing the system under consideration are integrated numerically for a set of characteristic particles, and the desired information is extracted from the final coordinates of these particles [1–5]. In the second approach, coefficients of the Taylor expansion of the map describing the system are computed analytically [5–10]. This is done for all particle optical elements of interest, and the results are programmed as a library of subroutines for all individual elements. Even though the mathematics required for the derivation of these formulas does not require any advanced techniques, the procedure is very cumbersome in higher orders due to an enormous complexity of the occurring expressions. Thus the problem is well-suited for computer formula manipulation.

In this paper we present a new formula manipulator specifically designed for the power series solution of the equations of motion of charged particles in piecewise constant electromagnetic fields with at least one plane of symmetry. Due to a special procedure in performing elementary operations, the method used here for the solution of the different equations is very fast and efficient. In order that the results of Hamiltonian theory can be used directly, the equations of motion will be derived in a set of coordinates which up to scaling factors is symplectic.

2. The equation of motion in particle optical coordinates

Particle optical systems are usually not described in Cartesian coordinates. Instead, all quantities are determined relative to the trajectory of a reference particle, called the optic axis. The independent variable here is the arc length s along the optic axis. Since all commonly used particle optical fields have at least one plane of symmetry, one can assume that the optic axis always lies in one plane, the reference plane. If $h(s)$ denotes the momentary curvature, i.e., the reciprocal of the momentary radius of curvature $\rho_0(s)$ of

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the optic axis at the position s, the following set of seven coordinates describes the properties of an arbitrary particle trajectory completely

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

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

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

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

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

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

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

Here x is the distance between the optic axis and the projection of the particle's position into the reference plane, y is the distance to the reference plane, p_x the momentum component in the reference plane and p_y the momentum component perpendicular to the reference plane. K is the particle's kinetic energy, v its velocity, t its flight time to the momentary position and m its mass. The charge of the particle is assumed to have the same value for all particles. p_0, K_0, v_0, t_0 and m_0 are momentum, energy, velocity, flight time and mass of the reference particle, respectively.

Note that in this set of coordinates, $a = p_x/p_0$ and $b = p_y/p_0$ are used instead of $x' = p_x/p_z$ and $y' = p_y/p_z$ as in refs. [5–7]. Firstly, this implies some simplifications. Secondly, the coordinates x, a, y, b, l and d are canonical coordinates up to a scaling factor. Thus many of the advantages of Hamiltonian theory can be exploited [11,12], in particular the fact that Hamiltonian systems produce symplectic maps [8].

In order to derive the equations of motion in the particle optical coordinates of eqs. (1) we start with the equations of motion in Cartesian coordinates

$$\frac{\mathrm{d}}{\mathrm{d}t}P_x = F_x, \qquad \frac{\mathrm{d}}{\mathrm{d}t}P_y = F_y, \qquad \frac{\mathrm{d}}{\mathrm{d}t}P_z = F_z. \tag{2}$$

Integrating these equations with respect to the independent variable s transforms the differential equations to integral equations

$$P_x(s) = P_x(s_0) + \int_{t(x_0)}^{t(s)} F_x(t)\,\mathrm{d}t = P_x(s_0) + \int_{s_0}^{s} F_x(s)t'\,\mathrm{d}s, \tag{3a}$$

$$P_y(s) = P_y(s_0) + \int_{t(s_0)}^{t(s)} F_y(t)\,\mathrm{d}t = P_y(s_0) + \int_{s_0}^{s} F_y(s)t'\,\mathrm{d}s, \tag{3b}$$

$$P_z(s) = P_z(s_0) + \int_{t(s_0)}^{t(s)} F_z(t)\,\mathrm{d}t = P_z(s_0) + \int_{s_0}^{s} F_z(s)t'\,\mathrm{d}s, \tag{3c}$$

with $t' = \mathrm{d}t/\mathrm{d}s$. Note here that on the way from s_0 to s, the reference trajectory was bent by the angle

$$\alpha = \int_{s_0}^{s} h\,\mathrm{d}s. \tag{4}$$

Transforming the momentum components P_x, P_y, P_z of the initial coordinate system into the new

reference system at s, one obtains the components p_x, p_y, p_z of the transformed momentum from eqs. (3) and (4)

$$p_x(s) = \cos\left(\int_{s_0}^{s} h\,\mathrm{d}s\right)\left(P_x(s_0) + \int_{s_0}^{s} F_x(s)t'\,\mathrm{d}s\right) + \sin\left(\int_{s_0}^{s} h\,\mathrm{d}s\right)\left(P_z(s_0) + \int_{s_0}^{s} F_z(s)t'\,\mathrm{d}s\right), \tag{5a}$$

$$p_y(s) = \left(P_y(s_0) + \int_{s_0}^{s} F_y(s)t'\,\mathrm{d}s\right), \tag{5b}$$

$$p_z(s) = -\sin\left(\int_{s_0}^{s} h\,\mathrm{d}s\right)\left(P_x(s_0) + \int_{s_0}^{s} F_x(s)t'\,\mathrm{d}s\right) + \cos\left(\int_{s_0}^{s} h\,\mathrm{d}s\right)\left(P_z(s_0) + \int_{s_0}^{s} F_z(s)t'\,\mathrm{d}s\right). \tag{5c}$$

Differentiating the expressions in eqs. (5) with respect to s yields the equations of motion in the system relative to the optic axis with s being the independent variable:

$$p_x' = F_x t' + h p_z, \tag{6a}$$

$$p_y' = F_y t', \tag{6b}$$

$$p_z' = F_z t' - h p_x, \tag{6c}$$

As above, here the primes denote differentiations with respect to s. With eqs. (6), the general form of the equations of motion in particle optical coordinates can be determined by representing all expressions in eqs. (6) in terms of particle optical coordinates. First note that in cylindrical coordinates one has

$$\frac{p_x}{p_z} = \frac{\rho_0}{\rho_0 + x} \lim_{\mathrm{d}s \to 0} \frac{\mathrm{d}x}{\mathrm{d}s} = \frac{x'}{1 + hx}, \tag{7}$$

with $h = 1/\rho_0(s)$ and thus

$$x' = (1 + hx)\frac{p_x}{p_z}, \qquad y' = (1 + hx)\frac{p_y}{p_z}. \tag{8}$$

The derivative of the particle's path length with $\mathrm{d}L = [\mathrm{d}s^2(1 + hx)^2 + \mathrm{d}x^2 + \mathrm{d}y^2]^{1/2}$ is simply:

$$L' = \left((1 + hx)^2 + x'^2 + y'^2\right)^{1/2} = (1 + hx)\left(1 + \frac{p_x^2 + p_y^2}{p_z^2}\right)^{1/2}. \tag{9}$$

With the definition of the particle optical coordinates a and b (eq. (1)) one obtains

$$\frac{p_x}{p_z} = \frac{p_x}{p_0}\frac{p_0}{p_z} = a\frac{p_0}{\left(p^2 - p_x^2 - p_y^2\right)^{1/2}} = a\frac{p_0}{p}\left(1 - \left(\frac{p_0}{p}\right)^2 (a^2 + b^2)\right)^{-1/2} \tag{10}$$

and from the relativistic relations

$$v = \frac{p}{m}\left(1 + \frac{p^2}{m^2c^2}\right)^{-1/2}$$

and

$$p = (2mK)^{1/2}\left(1 + \frac{K}{2mc^2}\right)^{1/2}:$$

$$\frac{v_x}{v_0} = \frac{p_x}{p_0}\frac{m_0}{m}\frac{\left(1 + \dfrac{p_0^2}{m_0^2c^2}\right)^{1/2}}{\left(1 + \dfrac{p^2}{m^2c^2}\right)^{1/2}} = a\frac{m_0}{m}\frac{\left(1 + 2\dfrac{K_0}{m_0c^2}\left(1 + \dfrac{K_0}{2m_0c^2}\right)\right)^{1/2}}{\left(1 + 2\dfrac{K}{mc^2}\left(1 + \dfrac{K}{2mc^2}\right)\right)^{1/2}} = a\frac{m_0c^2 + K_0}{mc^2 + K}. \tag{11}$$

Analogously to eqs. (10) and (11), one finds

$$\frac{p_y}{p_z} = b\frac{p_0}{p}\left(1-\left(\frac{p_0}{p}\right)^2(a^2+b^2)\right)^{-1/2}, \tag{12}$$

$$\frac{v_y}{v_0} = b\frac{m_0c^2+K_0}{mc^2+K}. \tag{13}$$

Thus one obtains from eqs. (8)–(12) for x' and y' as well as for the derivative of the l of eq. (1e):

$$x' = a(1+hx)\frac{p_0}{p}\left(1-\left(\frac{p_0}{p}\right)^2(a^2+b^2)\right)^{-1/2}, \tag{14a}$$

$$y' = b(1+hx)\frac{p_0}{p}\left(1-\left(\frac{p_0}{p}\right)^2(a^2+b^2)\right)^{-1/2}, \tag{14b}$$

$$l' = v_0\frac{\mathrm{d}t}{\mathrm{d}s} = \frac{v_0}{v}\frac{\mathrm{d}L}{\mathrm{d}s} = (1+hx)\frac{v_0}{v}\left(1-\left(\frac{p_0}{p}\right)^2(a^2+b^2)\right)^{-1/2} \tag{14c}$$

and from eqs. (6a) and (6b) one obtains for the derivatives of the coordinates a and b:

$$\begin{aligned} a' &= \left(\frac{p_x}{p_0}\right)' = \frac{1}{p_0}(F_x t' + hp_z) = \left(\frac{ze}{p_0v_0}E_x + \frac{ze}{p_0}\left(\frac{v_y}{v_0}B_z - \frac{v_z}{v_0}B_y\right)\right)l' + h\left(\frac{p^2}{p_0^2} - a^2 - b^2\right)^{1/2} \\ &= \left(\frac{1}{\chi_e}E_x + \frac{1}{\chi_m}b\frac{m_0c^2+K_0}{mc^2+K}B_z - \frac{1}{\chi_m}\frac{v}{v_0}\left(1-\left(\frac{v_0}{v}\right)^2\left(\frac{m_0c^2+K_0}{mc^2+K}\right)^2(a^2+b^2)\right)^{1/2}B_y\right)l' \\ &\quad + h\frac{p}{p_0}\left(1-\left(\frac{p_0}{p}\right)^2(a^2+b^2)\right)^{1/2}, \end{aligned} \tag{14d}$$

$$b' = \left(\frac{1}{\chi_e}E_y - \frac{1}{\chi_m}a\frac{m_0c^2+K_0}{mc^2+K}B_z + \frac{1}{\chi_m}\frac{v}{v_0}\left(1-\left(\frac{v_0}{v}\right)^2\left(\frac{m_0c^2+K_0}{mc^2+K}\right)^2(a^2+b^2)\right)^{1/2}B_x\right)l'. \tag{14e}$$

here ze is the charge of the particle and $\chi_e = p_0v_0/ze$, $\chi_m = p_0/ze$ are the electric and magnetic rigidities, respectively. In the last step the terms p_0/p, v_0/v and $(m_0c^2+K_0)/(mc^2+K)$ must be expressed in particle optical coordinates. Note here that the kinetic energy K of a particle consists of the reference energy times the factor $(1+d)$ [see eq. (1f)] plus the additional energy the particle obtains by virtue of the electric potential V_e:

$$K = K_0(1+d) - zeV_e(s, x, y) = K_0(1+d-\phi V_e(s, x, y)), \tag{15}$$

with $\phi = ze/K_0$. Considering $m = m_0(1+g)$ [eq. (1g)] and using $\eta = K_0/m_0c^2$ one obtains with eq. (15)

$$\frac{1+\dfrac{K}{mc^2}}{1+\dfrac{K_0}{m_0c^2}} = 1+\frac{\eta}{1+\eta}\left(\frac{d-\phi V_e-g}{1+g}\right), \tag{16a}$$

$$\frac{\left(1+\dfrac{K_0}{2m_0c^2}\right)^{1/2}}{\left(1+\dfrac{K}{2mc^2}\right)^{1/2}} = \left(\frac{1+\eta/2}{1+\left(\dfrac{1+d-\phi V_e}{1+g}\right)\dfrac{\eta}{2}}\right)^{1/2} = \left(1+\frac{1}{2}\frac{\eta}{1+\eta/2}\left(\frac{d-\phi V_e-g}{1+g}\right)\right)^{-1/2}. \tag{16b}$$

From

$$p = 2(mK)^{1/2}\left(1 + \frac{K}{2mc^2}\right)^{1/2}$$

and

$$v = \left(2\frac{K}{m}\right)^{1/2}\left(1 + \frac{K}{2mc^2}\right)^{1/2} \Big/ \left(1 + \frac{K}{mc^2}\right)$$

(see above eq. (11)), we thus can infer with eqs. (16a) and (16b)

$$\frac{p_0}{p} = \left(\frac{K_0}{K}\right)^{1/2}\left(\frac{m_0}{m}\right)^{1/2} \frac{\left(1 + \frac{K_0}{2m_0c^2}\right)^{1/2}}{\left(1 + \frac{K}{2mc^2}\right)^{1/2}}$$

$$= (1+g)^{-1/2}(1 + d - \phi V_e)^{1/2}\left(1 + \frac{1}{2}\frac{\eta}{1+\eta/2}\left(\frac{d - \phi V_e - g}{1+g}\right)\right)^{-1/2} \tag{17}$$

$$\frac{v_0}{v} = \left(\frac{K_0}{K}\right)^{1/2}\left(\frac{m}{m_0}\right)^{1/2} \frac{\left(1 + \frac{K_0}{2m_0c^2}\right)^{1/2}}{\left(1 + \frac{K}{2mc^2}\right)^{1/2}} \frac{1 + \frac{K}{mc^2}}{1 + \frac{K_0}{m_0c^2}}$$

$$= (1+g)^{1/2}(1 + d - \phi V_e)^{-1/2}\left(\left[1 + \frac{1}{2}\frac{\eta}{1+\eta/2}\left(\frac{d - \phi V_e - g}{1+g}\right)^{-1/2}\right]\left[1 + \frac{\eta}{1+\eta}\left(\frac{d - \phi V_e - g}{1+g}\right)\right]\right). \tag{18}$$

Inserting eqs. (17) and (18) into eq. (14) yields the differential equations in particle optical coordinates. Note that the four constants describing the reference particle are χ_e, χ_m, ϕ and η where for nonrelativistic systems η vanishes. Note also that if desired, ϕ can be expressed in terms of χ_e, χ_m, and η.

In the following part we describe how the electric and magnetic fields can be expressed in x and y. Since, contrary to a and b, these quantities are the same as in previous derivations of the particle optics equations of motion, we just give a brief summary of those results. First note that both $\nabla \times \boldsymbol{E}$ and $\nabla \times \boldsymbol{B}$ are zero due to time independence. Thus there are scalar potential V_e and V_m to the magnetic and electric fields. They satisfy Laplace's equation which in particle optical coordinates has the form [13,14,6]

$$\nabla^2 V = \frac{1}{1+hx}\frac{\partial}{\partial x}\left((1+hx)\frac{\partial V}{\partial x}\right) + \frac{\partial^2 V}{\partial y^2} + \frac{1}{1+hx}\frac{\partial}{\partial s}\left(\frac{1}{1+hx}\frac{\partial V}{\partial s}\right) = 0. \tag{19}$$

Assuming that the electric or magnetic potential can be written as a power series expansion in x and y

$$V = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} A_{ij}\frac{x^i}{i!}\frac{y^j}{j!}$$

and inserting this power series into Laplace's equation, one obtains after some arithmetic

$$\begin{aligned} A_{i,j+2} = &-A_{i+2,j} - (3i+1)hA_{i+1,j} - i(3i+1)h^2A_{i,j} - i(i-1)^2h^3A_{i+1,j} - 3ihA_{i-1,j+2} \\ &- 3i(i-1)h^2A_{i-2,j+2} - i(i-1)(i-2)h^3A_{i-3,j+2} - A''_{ij} - ihA''_{i-1,j} + ih'A'_{i-1,j}. \end{aligned} \tag{20}$$

As above, primes denote differentiation with respect to s and it is understood that all coefficients with

negative indices are zero. Eq. (20) represents a recursion formula to compute all field expansion coefficients $A_{i,j}$ for $j \geqslant 2$ from those with $j = 0$ and $j = 1$. This means that Maxwell's equations determine the potential in the whole space once its first two y-derivatives in the horizontal plane are known.

3. A general algorithm for the solution of the equations of motion

Inspecting the equations of motion (eqs. (14)) one sees that they can be written as

$$x' = a + f_x(x, a, y, b, g, d), \quad a' = k_x^2 x + f_a(x, a, y, b, g, d) \tag{21a}$$

$$y' = b + f_y(x, a, y, b, g, d), \quad b' = k_y^2 y + f_b(x, a, y, b, g, d) \tag{21b}$$

$$l' = f_l(x, a, y, b, g, d). \tag{21c}$$

Here the functions f_x, f_a, f_y and f_b are free of linear terms in x, a, y and b; however, they may contain linear terms in g and d. Expanding the transfer map describing the motion from s_0 to s in a power series in the coordinates at s_0 and collecting orders, one obtains

$$\begin{aligned} x(s) &= \sum_{i=1}^{\infty} x^{(i)}(s), \quad a(s) = \sum_{i=1}^{\infty} a^{(i)}(s), \quad y(s) = \sum_{i=1}^{\infty} y^{(i)}(s), \\ b(s) &= \sum_{i=1}^{\infty} b^{(i)}(s), \quad l(s) = \sum_{i=1}^{\infty} l^{(i)}(s), \end{aligned} \tag{22}$$

where $x^{(i)}$, $a^{(i)}$, $y^{(i)}$, $b^{(i)}$ and $l^{(i)}$ are polynomials consisting of monomials of exact degree i in the phase space coordinates at s_0. In a similar way one expands the functions f from eq. (21) and collects orders:

$$f_x = \sum_{i=1}^{\infty} f_x^{(i)}, \quad f_a = \sum_{i=1}^{\infty} f_a^{(i)}, \quad f_y = \sum_{i=1}^{\infty} f_y^{(i)}, \quad f_b = \sum_{i=1}^{\infty} f_b^{(i)}, \quad f_l = \sum_{i=1}^{\infty} f_l^{(i)}. \tag{23}$$

According to eqs. (21), the linear terms of f_x, f_a, f_y, and f_b do not contain x, a, y and b, but may contain g and d. Inserting eqs. (22) in (23) and collecting orders yields the following set of differential equations for the different orders:

$$x^{(i)\prime} = a^{(i)} + F_x^{(i)}, \quad a^{(i)\prime} = k_x^2 x^{(i)} + F_a^{(i)}, \tag{24a}$$

$$y^{(i)\prime} = b^{(i)} + F_y^{(i)}, \quad b^{(i)\prime} = k_y^2 y^{(i)} + F_y^{(i)}, \tag{24b}$$

$$l^{(i)\prime} = F_l^{(i)}. \tag{24c}$$

Here $F_x^{(i)}$, $F_a^{(i)}$, $F_y^{(i)}$ and $F_b^{(i)}$ do not contain $x^{(i)}$, $a^{(i)}$, $y^{(i)}$ and $b^{(i)}$ any more since the f in eq. (23) are free of the corresponding linear terms. This implies that the eqs. (24a) and (24b) allow the iterative determination of $x^{(i)}$, $a^{(i)}$, $y^{(i)}$, $b^{(i)}$ in every order i since $F_x^{(i)}$, $F_a^{(i)}$, $F_y^{(i)}$ and $F_b^{(i)}$ only contain already computed quantities. Once the terms $x^{(i)}$, $a^{(i)}$, $y^{(i)}$ and $b^{(i)}$ are computed, $l^{(i)}$ can be determined from eq. (24c) by a mere integration since $F_l^{(i)}$ does not contain l.

Since the transfer function from position s_0 to position s is the identical map, one obtains for the initial conditions

$$x^{(i)}(s = s_0) = x_0 \delta_{i,1}, \tag{25a}$$

$$a^{(i)}(s = s_0) = a_0 \delta_{i,1}, \tag{25b}$$

$$y^{(i)}(s = s_0) = y_0 \delta_{i,1}, \tag{25c}$$

$$b^{(i)}(s = s_0) = b_0 \delta_{i,1}, \tag{25d}$$

$$l^{(i)}(s = s_0) = l_0 \delta_{i,1}, \tag{25e}$$

where δ represents Kronecker's symbol. In order to obtain a solution of order i, one first determines the "homogeneous solution" of the two systems:

$$x^{(i)\prime} = a^{(i)}, \qquad y^{(i)\prime} = b^{(i)}, \tag{26a}$$

$$a^{(i)\prime} = k_x^2 x^{(i)}, \qquad b^{(i)\prime} = k_y^2 y^{(i)}. \tag{26b}$$

With the abbreviations

$$c_x = \cosh(k_x s), \qquad s_x = \frac{1}{k_x}\sinh(k_x s), \qquad c_y = \cosh(k_y s), \qquad s_y = \frac{1}{k_y}\sinh(k_y s) \tag{27}$$

one of course obtains for the general solution of the homogeneous system

$$x^{(i)} = A_x c_x + B_x s_x, \qquad a^{(i)} = B_x c_x + k_x^2 A_x s_x, \tag{28a}$$

$$y^{(i)} = A_y c_y + B_y s_y, \qquad b^{(i)} = B_y c_y + k_y^2 A_y s_y, \tag{28b}$$

where A_x, B_x, A_y, and B_y are constants determined by the initial conditions.

In order to obtain a solution of the inhomogeneous differential equation (eqs. (24a) and (24b)), one uses the well-known method of variation of constants. One makes a guess of the form of eqs. (28a) and (28b), except that the quantities A_x, B_x, A_y, and B_y now are viewed as s-dependent. Differentiating these expressions with respect to s and comparing with the system of differential equations (eqs. (24)), one obtains

$$A_x' c_x + B_x' s_x = F_x^{(i)}, \qquad B_x' c_x + k_x^2 A' s_x = F_a^{(i)}, \tag{29a}$$

$$A_y' c_y + B_y' s_y = F_y^{(i)}, \qquad B_y' c_y + k_y^2 A' s_y = F_b^{(i)}. \tag{29b}$$

Solving this system of equations for A' and B' and integrating finally yields

$$A_x = \int\left(c_x F_x^{(i)} - s_x F_a^{(i)}\right), \qquad B_x = \int\left(-k_x^2 s_x F_x^{(i)} + c_x F_a^{(i)}\right), \tag{30a}$$

$$A_y = \int\left(c_y F_y^{(i)} - s_y F_b^{(i)}\right), \qquad B_y = \int\left(-k_y^2 s_y F_y^{(I)} + c_y F_b^{(i)}\right). \tag{30b}$$

Inserting these expressions into eqs. (28) and choosing the integration constants such that the initial conditions are satisfied yields the solution of the inhomogeneous system of differential equations ((eqs. (24)).

4. The storage of the data in the program HAMILTON

According to the algorithm described in section 3 which is used by HAMILTON, the general solution of any order consists of polynomials in the phase-space coordinates. Each monomial in the phase-space coordinates has the following standard form:

$$M = \frac{N}{D} \cdot x^{n_x} a^{n_a} y^{n_y} b^{n_b} g^{n_g} d^{n_d} \cdot s^{n_s} s_x^{n_{s_x}} c_x^{n_{c_x}} s_y^{n_{s_y}} c_y^{n_{c_y}} \cdot k_x^{n_{k_x}} k_y^{n_{k_y}} \cdot k_1^{n_{k_1}} \cdots k_{32}^{n_{k_{32}}} \cdot d_1^{n_{d_1}} \cdots d_{24}^{n_{d_{24}}}. \tag{31}$$

Here N and D are integers (numerator and denominator), x, a, y, b, g and d are the phase-space coordinates, s is the independent variable, s_x, c_x, s_y, c_y are the functions defined in section 3. The k_x and k_y are the frequencies in x- and y-direction as defined in section 3, k_1 through k_{32} can hold problem-related constants like quantities describing the reference particle (χ_c, χ_m, η and ϕ) or multipole strengths, the curvature of the optic axis, magnetic and electric rigidities, etc. d_1 through the d_{24} are

Table 1
Contents of 12 integer variables

Number	Contents	Number	Contents
1	Numerator (factor N)	7	$10^0 n_{k_9} \cdots 10^7 n_{k_{16}}$
2	Denominator (factor D)	8	$10^0 n_{k_{17}} \cdots 10^7 n_{k_{24}}$
3	$10^0 n_x + 10^1 n_a + 10^2 n_y + 10^3 n_b + 10^4 n_g + 10^5 n_d$	9	$10^0 n_{k_{25}} \cdots 10^7 n_{k_{32}}$
4	$10^0 n_{s_x} + 10^1 n_{c_x} + 10^2 n_{s_y} + 10^3 n_{c_y} + 10^4 n_s$	10	$10^0 n_{d_1} \cdots 10^7 n_{d_8}$
5	$1000100 + n_{k_x} + 10^4 n_{k_y}$	11	$10^0 n_{d_9} \cdots 10^7 n_{d_{16}}$
6	$10^0 n_{k_1} \cdots 10^7 n_{k_8}$	12	$10^0 n_{d_{17}} \cdots 10^7 n_{d_{24}}$

certain denominators that can occur when $s^l s_x^j c_x^k s_y^l c_y^m$ is integrated according to eqs. (3). These denominators have the form

$$\frac{1}{nk_x^2 - mk_y^2}, \qquad 2 <= n + m <= 8.$$

Note that if we restrict ourselves to less than tenth order, the exponents $n_x, \cdots, n_d$, $n_s, \cdots, n_{c_y}$, $n_{k_l}, \ldots, n_{k_{32}}$, $n_{d_1}, \ldots, n_{d_{24}}$ occurring in eq. (31) are all between 0 and 9, whereas the coefficients n_{k_x}, n_{k_y} can take positive and negative values.

All the information characterizing one monomial is now stored in 12 integer variables on the computer which contain the list presented in table 1. HAMILTON can store a maximum of about 50 000 of these monomials. Each polynomial is represented by a string of monomials stored consecutively in the stack where the monomials are sorted in ascending order.

5. Representation of the basic operations of polynomial addition, multiplication and integration

The addition of polynomials is performed such that the resulting polynomial is also in ascending order. To accomplish this the next monomials of each polynomial are compared. If all the exponents agree, a fraction addition of the numerator and denominators is performed, and the new numerator and denominator are stored together with the other integers representing the exponents. If the exponents do not agree, the monomial coming first is copied. This is repeated until all monomials of both polynomials have been treated.

The multiplication of polynomials is performed monomialwise with consecutive reordering of all resulting monomials. Note that the multiplication of two monomials is particularly simple since it just involves addition of the characteristic integers 3 through 12 (which contain the exponents of the possibly occurring quantities) and a fraction multiplication of the numerators and the denominators. Using the pattern described in section 2, one sees that any monomial whose phase-space coordinates have an order larger than the one which is just being treated can be neglected. This considerably reduces the size of the polynomials after multiplication and avoids an exponential growth of the sizes.

The integration of polynomials with respect to s uses a look up table containing all the integrals of the form

$$\int s^{i_s} \cdot s_x^{i_{s_x}} \cdot c_x^{i_{c_x}} \cdot s_y^{i_{s_y}} \cdot c_y^{i_{c_y}} \qquad \text{for} \quad i_s + i_{s_x} + i_{c_z} + i_{s_y} + i_{c_y} \leqslant 8. \tag{33}$$

Note that an integral of this form can always be written as a sum over expressions of exactly the same kind (with different exponents), where in addition some of the denominators d_1 through d_{24} can occur. Once a monomial must be integrated with respect to s, the monomial is copied for each term occurring on the right-hand side of the integral, and the characteristic integers 4, 10, 11, 12 are changed.

6. The input of HAMILTON and the internal flow

All command describing the differential equations are contained in a file. The first command describes the order to which matrix elements are to be computed. It has the form

ORDER = 5;

Next all problem-related constants have to be defined. Their exponents will eventually be stored in the characteristic integers 6, 7, 8, 9 (see table 1). They are defined in the following form

k_{28}: $(1/\rho_0)$, i.e., the reciprocal of radius of bend,

k_{27}: $(1/\chi_0)$, i.e., the reciprocal of magnetic rigidity,

k_{32}: η, i.e., the kinetic energy divided by mc^2,

and stored at positions 28, 27 and 32 of the 32 available places in the characteristic integers 6, 7, 8, 9. In the next step, those problem-related constants which are dependent on the just defined ones are declared together with the way they are computed. For instance, since one needs the expression $1/(1+\eta)$ and $1/(1+\eta/2)$ in the equations of motion, one must write in the input file

$k_{30} = 1/(1+k_{32})$,

$k_{31} = 1/(1+0.5k_{32})$,

so that the exponents of $1/(1+\eta)$ and $1/(1+1/2\eta)$ will be stored in positions 30 and 31, respectively, of the integers 6, 7, 8, 9.

Now the commands describing the equations of motion are given. This is done by introducing new variables step by step as well as rules to compute them from other variables. Here the variables occurring on the right-hand side are x, a, y, b, g and d or other previously defined variables. For instance, since in the equations of motion the expression a^2+b^2 occurs, one could write

AB = $+A * A + B * B$

and then use AB in the future. Finally, the variables XP, AP, YP, BP and LP must be defined. These variables have a predefined meaning since they stand for the derivation of the phase space coordinates in the differential equations of motion.

After the input is read, HAMILTON performs various consistency checks. For instance, it is checked that all variables used on the right-hand sides of assignments are either phase space variables or previously defined variables. In addition, it is checked if the equation of motion are really of the form of eqs. (31), since HAMILTON can handle only this specific form at the moment. After these checks are performed, HAMILTON finds out how the frequencies k_x and k_y can be computed from the problem-related constants. Then it determines the first-order solution of the form of eq. (27). Finally, order after order is computed following the pattern described in section 2. Each new order usually takes about a factor of 5 longer than the previous one due to the quick increase in the lengths of the polynomials. This is the main limit of the orders HAMILTON can computer. On a MICROVAX II, the maximum order which can be achieved with reasonable computer time is 5. Since at least the nominal operations in HAMILTON vectorize, it might be possible to determine even higher orders on a vector computer.

7. The output generated by HAMILTON

In order to avoid all extra programming effort, HAMILTON produces a complete FORTRAN subroutine which can compute numerically the matrix elements of the particle optical element under consideration. This subroutine is compatible with the program COSY [10]. The quantities passed to the subroutine are the problem-related constants defined in the input file. In the above example, k_{25}, k_{28} and k_{29} would stand in the argument list of the subroutine. Since it is not always necessary to compute the

matrix elements to the maximum order, also the order to which computation is to be executed is passed. Besides this FORTRAN routine, also a readable output is generated which can serve for checking purposes and documentation.

Great care is taken that the computation of the matrix elements is performed with the least amount of floating point operations. This entails that virtually all terms that occur more than once are determined in advance in a separate statement and stored in a temporary variable. This increases the length of the code, but leads to significantly faster machine performance. In order to achieve this property, first all combinations of k_x and k_y to different powers stored in the characteristic integer 5 are collected and computed first. Then all occurring combinations of the functions s, s_x, c_x, s_y and c_y are computed and stored in temporary variables and similarly all occurring combinations of problem-related constants as well as the 21 denominators. Then all occurring monomials are computed, where each monomial is assembled from the four previously computed parts described above, and finally the matrix elements are found by collecting the appropriate monomials and multiplying them with the proper numerators and denominators.

The savings in computer time due to this strategy is substantial. For example, considering matrix elements of fifth order, each individual monomial occurs about ten times on average at many different places. Also each of the four fragments of the monomials usually occurs about twenty times in different monomials.

Up to now HAMILTON has been used to create subroutines for the main field region of magnetic and electric quadrupoles, hexapoles, decapoles, and duodecapoles, as well as for inhomogeneous sector fields (see ref. [10]).

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