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USEFUL FORMS OF THE HAMILTONIAN FOR ION-OPTICAL SYSTEMS

FORMES UTILES DE LA FONCTION DE HAMILTON POUR LES SYSTÈMES D'OPTIQUE IONIQUE

by

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RÉSUMÉ

La symbiose de l'algèbre différentielle et de la formulation algébrique de Lie de l'optique fournit un ensemble de moyens très puissants qui permettent d'analyser et de comprendre la dynamique orbitale dans les accélérateurs complexes, l'augmentation de la perturbation atteignant des ordres très élevés. Afin de pouvoir employer ces moyens efficacement, il est généralement nécessaire d'exprimer la fonction de Hamilton dans le système de coordonnées approprié. Dans ce rapport, on tire la fonction relativiste de Hamilton en coordonnées curvilignes (le système de coordonnées fondamental pour l'optique ionique), coordonnées cartésiennes et coordonnées polaires, formes convenant pour résoudre des problèmes en optique ionique et physique des accélérateurs avec et sans l'aide de l'algèbre différentielle.

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ABSTRACT

The symbiosis of differential algebra and the Lie-algebraic formulation of optics provides a set of very powerful tools for analyzing and understanding the orbit dynamics of complex accelerators up to very high orders. In order to use these tools effectively it is usually necessary to express the Hamiltonian in the appropriate coordinate system. In this report, the relativistic Hamiltonian is derived in curvilinear (the fundamental coordinate system for ion-optics), Cartesian and polar coordinates, in forms suitable for solving problems in ion optics and accelerator physics both with and without the help of differential algebra.

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1. Introduction

The development of differential algebra (DA) [1] coupled with the Lie-algebraic formulation of optics [2] has revolutionized our ability to compute and analyze ion-optical systems up to very high order. In particular, these methods provide us with a very powerful way of computing and analyzing the orbits both in beam lines and in circular accelerators such as synchrotrons, storage rings, and the superconducting cyclotron. These methods are especially well suited to the analysis of resonances.

The Lie-algebra formulation is intimately connected with Hamiltonian mechanics and as a consequence requires that the coordinates be truly canonical, a condition that is not satisfied in formulations that use the position and its derivative as coordinates, for example (x,x'), or (x,θ) etc. (such as the code TRANSPORT). Thus, it is best to integrate Hamilton's equations directly.

The generation of the high-order Taylor-series map (the usual aberration expansion) is very efficiently computed from Hamilton's equations with differential algebra, but the Lie map is not. Fortunately, DA provides, through its ability to compute high-order derivatives with high accuracy, a powerful tool for converting the Taylor-series map into a Lie map when necessary. Finally, for DA techniques to be used, the equations of motion and the electromagnetic potentials must be in analytic form.

In order to solve problems in optics, and especially if we want to use the Lie-algebraic formulation, it is necessary to express the Hamiltonian in the coordinates most suitable to the problem. Furthermore, the coordinate system is different if we are solving the equations directly in terms of Lie polynomials or via the Taylor series with the help of DA. To this end, the relativistic Hamiltonian is derived in several different forms, specifically in curvilinear (the fundamental coordinate system for ion-optics), Cartesian and polar coordinates, that are suitable for solving problems in ion optics and accelerator physics.

The equations of motion of a relativistic charged particle moving in an electromagnetic field are obtained most elegantly by expansion of the relativistic Hamiltonian in a curvilinear coordinate system [3]. The Hamiltonian, as a function of the time, t, in a Cartesian coordinate system, expressed in MKS units, is:

$$H = e\varphi + c\{m^2c^2 + (\mathbf{p}-e\mathbf{A})^2\}^{1/2} \tag{1}$$

where φ and $\mathbf{A}$ are the scalar and vector potentials of the electromagnetic field respectively and e is the charge of the particle; m is the particle mass and $\mathbf{p}$ the momentum vector. In a circular accelerator such as a synchrotron or cyclotron, φ could describe the RF accelerating voltage. The magnetic field is [4]

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{2}$$

and the electric field is

$$\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t} . \tag{3}$$

In ion-optical and accelerator systems, the Hamiltonian is transformed such that the independent variable is "s", the distance along the central ray, rather than the time, t, (see Fig. 1) because the positions and properties of the focusing elements are logically a function of s rather than t. It is also usual to use a curvilinear coordinate system as shown in Fig. 1. Here the radius of curvature ρ is not necessarily constant and the local coordinate system is defined in terms of the local radius of curvature.

2. Curvilinear Coordinates

Curvilinear coordinates are the natural coordinate system for optics because the map has a standard form with a standard interpretation. The curvilinear coordinate system based on the central trajectory can be defined by [5,6]

$$\mathbf{r} = \mathbf{r}_0(s) \ . \tag{4}$$

A local orthogonal coordinate system can be defined by unit vectors found by differentiating the reference vector (4). Thus

$$\hat{\alpha}(s) = \frac{d\mathbf{r}_0}{ds} \tag{5}$$

where $\hat{\alpha}(s)$ is the unit vector tangent to the curve at . , and

$$\frac{d\hat{\alpha}(s)}{ds} = -\kappa(s)\hat{\beta}(s) \tag{6}$$

where $\kappa(s)$ is the curvature of the central trajectory and $\hat{\beta}(s)$ is the unit vector perpendicular to $\hat{\alpha}$, called the principal normal [6]. Here we define the curvature, κ, in such a manner that it points along the radius vector. This is opposite to the usual definition used in differential geometry, but is consistent with the definition used almost universally in ion-optics. A third unit vector $\hat{\gamma}(s)$, orthogonal to both $\hat{\alpha}$ and $\hat{\beta}$, can be defined as

$$\hat{\gamma}(s) = \hat{\alpha}(s) \times \hat{\beta}(s) \tag{7}$$

which completes the coordinate system. The plane defined by $\hat{\alpha}$ and $\hat{\beta}$ is called the osculating plane. Eq. (6) is the first of three differential relations, called the *Frenet-Serret formulas* [6.5], which are given by:

$$\frac{d\hat{\alpha}(s)}{ds} = -\kappa(s)\hat{\beta}(s) \tag{8}$$

$$\frac{d\hat{\beta}(s)}{ds} = \omega(s)\hat{\gamma}(s) + \kappa(s)\hat{\alpha}(s) \tag{9}$$

$$\frac{d\hat{\gamma}(s)}{ds} = -\omega(s)\hat{\beta}(s) \tag{10}$$

where $\omega(s)$ is the torsion of the curve (again with a sign convention that is opposite to that used in differential geometry). For a plane curve $\omega(s)$ vanishes. The radius of curvature, ρ, and the radius of torsion, τ, are related to κ and ω by

$$\rho = 1/\kappa \text{ and } \tau = 1/\omega \ . \tag{11}$$

The position of any point in space, not too far from the central or reference trajectory, is given by

$$\mathbf{r}(s,x,y) = \mathbf{r}_0(s) + x\hat{\beta}(s) + y\hat{\gamma}(s) \ . \tag{12}$$

The point defined by (12) is seen from Fig. 1 to be unique for points whose distance from the central trajectory is less than ρ.

We now use a canonical transformation of the type [3]

$$F_3(\mathbf{P},\mathbf{q},t) = \sum_l P_l Q_l(s,\mathbf{q}) \equiv \mathbf{P}\cdot\mathbf{r}(s,x,y) \tag{13}$$

where $\mathbf{P}$ is the momentum vector in Cartesian coordinates, $\mathbf{q}$ is the position vector in curvilinear coordinates and t is the time. From (12) and (13), we see immediately that

$$F_3(\mathbf{P},\mathbf{q}) = \mathbf{P}\cdot\left[\mathbf{r}_0(s) + x\hat{\beta}(s) + y\hat{\gamma}(s)\right] \ . \tag{14}$$

Hence the desired canonical momenta in curvilinear coordinates are, by virtue of (14) and the relation [3],

$$p_n = \frac{\partial F_3}{\partial q_n} = \sum_m P_m \frac{\partial Q_m}{\partial q_n} \ , \tag{15}$$

given by

$$p_s = \frac{\partial F_3}{\partial s} = \mathbf{P}\cdot\left[\frac{\partial \mathbf{r}_0(s)}{\partial s} + x\,\frac{\partial\hat{\beta}(s)}{\partial s} + y\,\frac{\partial\hat{\gamma}(s)}{\partial s}\right]$$

$$= \mathbf{P}\cdot\left[[1 + \kappa(s)x]\hat{\alpha}(s) + \omega(s)[x\hat{\gamma}(s) - y\hat{\beta}(s)]\right] \tag{16}$$

$$p_x = \frac{\partial F_3}{\partial x} = \mathbf{P}\cdot\hat{\beta} = p_\beta \tag{17}$$

$$p_y = \frac{\partial F_3}{\partial y} = \mathbf{P}\cdot\hat{\gamma} = p_\gamma \ . \tag{18}$$

Note that

$$\mathbf{P}^2 = P_x^2 + P_y^2 + P_z^2 = p_\alpha^2 + p_\beta^2 + p_\gamma^2 \tag{19}$$

and

$$(1 + \kappa(s)x)p_\alpha = p_s + \omega(s)(yp_\beta - xp_\gamma) \tag{20}$$

where p_α is the component of momentum in the $\hat{\alpha}$ direction. In a similar manner, we transform the components of the vector potential **A**. We obtain by inspection the results:

$$A_s = \mathbf{A}\cdot\left[(1 + \kappa(s)x)\hat{\alpha}(s) + \omega(s)[x\hat{\gamma}(s) - y\hat{\beta}(s)]\right] \tag{21}$$

$$A_x = \mathbf{A}\cdot\hat{\beta} \tag{22}$$

$$A_y = \mathbf{A}\cdot\hat{\gamma} \tag{23}$$

If we impose midplane symmetry, then $\omega(s)\equiv 0$ which simplifies (16) and (21) considerably. The Hamiltonian in terms of the new coordinates is found from the transformation [3]

$$H = H + \frac{\partial F_3}{\partial t} = H \tag{24}$$

since F_3 is independent of t. Hence, the new Hamiltonian is just the old Hamiltonian (1) in terms of the new variables:

$$H = e\varphi + c\left\{m^2c^2 + \frac{1}{(1+\kappa x)^2}\left[p_s - eA_s + \omega y(p_x - eA_x) - \omega x(p_y - eA_y)\right]^2 + (p_x - eA_x)^2 + (p_y - eA_y)^2\right\}^{1/2} . \tag{25}$$

3. Change of Independent Variable

The variational principle [3], from which the canonical transformations are derived, states that

$$\delta\int\left[\sum_{1}^{N} p_n dq_n - H\,dt\right] = 0\ . \tag{26}$$

If we introduce the notation

$$q_0 \equiv t \tag{27}$$

$$p_0 \equiv -H \tag{28}$$

then (26) becomes

$$\delta\int\sum_{0}^{N} p_n dq_n = 0 \tag{29}$$

and the apparent asymmetry between t and the coordinates q has been removed. Clearly, we may now define any coordinate, say q_m, to be the independent variable; then $-p_m$ becomes the new Hamiltonian. As was stated in the introduction, it is logical to use the distance, s, along the central trajectory as the independent variable. If we assume midplane symmetry ($\omega\equiv 0$) and solve (25) for p_s we obtain

$$\mathcal{H} = -p_s = -eA_s - [1+\kappa x]\left\{\left[\frac{p_0+e\varphi}{c}\right]^2 - m^2c^2 - \left[p_x - eA_x\right]^2 - \left[p_y - eA_y\right]^2\right\}^{\frac{1}{2}}. \tag{30}$$

Here, and in the development to follow, we have chosen the sign of the radical such that the "time" is positive. Hamilton's equations in terms of the new variable, s, become

$$\left.\begin{aligned} t' &= \frac{\partial\mathcal{H}}{\partial p_0}\ , & p_0' &= -\frac{\partial\mathcal{H}}{\partial t} \\ x' &= \frac{\partial\mathcal{H}}{\partial p_x} & p_x' &= -\frac{\partial\mathcal{H}}{\partial x} \\ y' &= \frac{\partial\mathcal{H}}{\partial p_y} & p_y' &= -\frac{\partial\mathcal{H}}{\partial y} \end{aligned}\right\} \tag{31}$$

where ′ stands for d/ds.

The advantage of this formulation in curvilinear coordinates is that an expansion of the Hamiltonian in a Taylor series automatically results in equations of motion that generate the "correct" form for the first order (paraxial approximation) as well as for the higher order aberrations: that is, they are relative to the central or reference trajectory. Furthermore, when it is applied to beam transport systems, synchrotrons, or storage rings, comprised of discrete elements, κ is usually either zero or constant, greatly simplifying the equations of motion. Finally, the magnetic field of dipoles, quadrupoles and higher multipoles is usually referenced to the optic axis, or design trajectory whether or not the sharp cutoff approximation (SCOFF), with or without fringe-field correction elements, is incorporated.

Unlike the canonically conjugate variables, (x,p_x) and (y,p_y), the variables (t,p_0) are not differential quantities, but represent the total time-of-flight and the total momentum of the particle, respectively. If we evaluate Hamilton's equations, (31), for the Hamiltonian (30) on the central trajectory, where by definition

$$\left.\begin{aligned} x = 0\ , \quad p_x = 0 \\ y = 0\ , \quad p_y = 0 \end{aligned}\right\} \tag{32}$$

and where we assume for the purposes of this discussion that **A** is time independent, but that φ may be time dependent, we find that

$$t' = -\frac{(1+\kappa x)}{\{\ \ldots\ \}^{1/2}}\left(\frac{p_0 + e\varphi}{c^2}\right) \tag{33}$$

$$p_0' = +\frac{(1+\kappa x)}{\{\ \ldots\ \}^{1/2}}\left(\frac{p_0 + e\varphi}{c^2}\right) e\,\frac{\partial\varphi}{\partial t} \tag{34}$$

where the quantities in $\{\ \ldots\ \}$ are just those given in (30) and the expressions are to be evaluated under conditions (32) with $p_0 = p_0^c$, the central or design energy. For situations where the particles are not accelerated ($\varphi=0$), we see that $p_0'=0$ and $p_0=$ constant. In this case

$$t' = \frac{dt}{ds} = 1/v^c \tag{35}$$

where v^c = constant is the velocity of the central trajectory.

$$v^c = c\beta^c = c\left\{1 - \frac{m^2c^4}{p_0^{c2}}\right\}^{1/2} . \tag{36}$$

This equation can be integrated directly with the result

$$t^c = s/v^c\ . \tag{37}$$

If $\varphi\neq 0$, then we must solve (33) and (34) for t^c and p_0^c, where p_0^c is no longer constant. Now we define a new set of variables

$$\left.\begin{aligned} \tau &= t - t^c, & p_\tau &= p_0 - p_0^c \\ \alpha &= x & p_\alpha &= p_x \\ \psi &= y & p_\psi &= p_y \end{aligned}\right\} . \tag{38}$$

This transformation to the new variables is canonical and can be obtained from a generating function of the type F_2 [3]:

$$F_2(q,\mathcal{P}) = x p_\alpha + y p_\psi + [t - t^c][p_\tau + p_0^c] \tag{39}$$

where q are the old coordinates and $\mathcal{P}$ are the new momenta. The relationship between the new and old coordinates is found from the general relations [3]:

$$q_i = \frac{\partial F_2}{\partial p_i} , \quad P_i = \frac{\partial F_2}{\partial q_i} \tag{40}$$

and the new Hamiltonian is found from

$$K = \mathcal{H} + \frac{\partial F_2}{\partial s} . \tag{41}$$

Thus one finds the relations

$$\tau = \frac{\partial F_2}{\partial p_\tau} = t - t^c \tag{42}$$

$$p_0 = p_\tau + p_0^c \tag{43}$$

and the new Hamiltonian becomes

$$K = -eA_s - [1+\kappa x]\left\{\left(\frac{p_0^c + p_\tau + e\varphi}{c}\right)^2 - m^2c^2 - \left[p_x - eA_x\right]^2 - \left[p_y - eA_y\right]^2\right\}^{\frac{1}{2}}$$

$$\underbrace{- \frac{\partial t^c}{\partial s}[p_\tau + p_0^c]} \tag{44}$$

$$\downarrow$$

$$- \frac{1}{v^c}[p_\tau + p_0^c] \text{ if } p_0^c = \text{constant},$$

where we have substituted the "old" coordinates p_x and p_y from (38). If differential algebra is used in the solution of the equations of motion, the transformation (38)

from the coordinates (t,p_0) to (τ,p_τ) is made automatically and we would use (30) rather than (44).

4. Scaling

It is a fairly common practice to scale some or all of the variables. A very common scaling, especially when $\varphi=0$, is as follows:

$$\left.\begin{aligned} \tilde{\tau} &= c\tau, \quad \tilde{p}_\tau = p_\tau/P^c c \\ \tilde{x} &= x, \quad \tilde{p}_x = p_x/P^c \\ \tilde{y} &= y, \quad \tilde{p}_y = p_y/P^c \end{aligned}\right\} \tag{45}$$

where [8]

$$P^c = eB\rho^c = \left[\frac{p_0^{c2}}{c^2} - m^2c^2\right]^{\frac{1}{2}} = \frac{1}{c}\sqrt{2mc^2E^c+E^{c2}} = mc\beta^c\gamma^c \tag{46}$$

and E^c is the kinetic energy of the central particle; P^c is clearly the mechanical momentum of the central trajectory and $\gamma^c = 1/\sqrt{(1-\beta^2)}$. The new Hamiltonian is found immediately by dividing (44) by P^c, where $\tilde{p}$ is defined in (45) and $\tilde{A}=A/P^c$. Hence

$$\tilde{K} = -\tilde{A}_s - [1+\kappa x]\left\{\frac{(p_0^c + p_\tau)^2 - m^2c^4}{c^2\,P^{c2}} - \left[\tilde{p}_x - \tilde{A}_x\right]^2 - \left[\tilde{p}_y - \tilde{A}_y\right]^2\right\}^{\frac{1}{2}} - \frac{1}{\beta^c}\left[\tilde{p}_0^c + \tilde{p}_\tau\right] . \tag{47}$$

Since $p_0^c = -H = mc^2\gamma^c$ (see (28)), we see that

$$\tilde{p}_0^c = -\frac{p_0^c}{cP^c} = -1/\beta^c \tag{48}$$

so that the first term in {...} (47) reduces to [9]

$$(1+\delta)^2 = 1 + 2\tilde{p}_0^c\,\tilde{p}_\tau + \tilde{p}_\tau^2 = 1 - \frac{2\tilde{p}_\tau}{\beta^c} + \tilde{p}_\tau^2 \tag{49}$$

where we have used the identity $\gamma^2(1-\beta^2)=1$. (Remember that H = the total energy, $K=-p_s$ and $\tilde{K}$ is dimensionless.) On substituting (49) into (47), we obtain the final form of the new Hamiltonian,

$$\tilde{K} = -\tilde{A}_s - [1+\kappa x]\left\{(1+\delta)^2 - \left[\tilde{p}_x - \tilde{A}_x\right]^2 - \left[\tilde{p}_y - \tilde{A}_y\right]^2\right\}^{\frac{1}{2}} - \frac{\tilde{p}_\tau}{\beta^c} + \frac{1}{\beta^{c2}} \quad . \tag{50}$$

Note that although p_τ is a canonical coordinate, δ is *not* canonical even though it is frequently used in accelerator physics; it provides a convenient short-hand notation but must be used with care. The last term in (50) can be neglected as it never enters into Hamilton's equations. That this scaling produces a new set of canonical variables (45), can be seen from the fact that

$$\sum p dq - K\, ds = P^c\left(\sum \tilde{p} d\tilde{q} - \tilde{K}\, d\tilde{s}\right) . \tag{51}$$

The variational principle [3] gives

$$\delta\int\left(\sum p dq - K\, ds\right) = 0 \tag{52}$$

with q, p and s fixed at the end points, and

$$\delta\int P^c\left(\sum \tilde{p} d\tilde{q} - \tilde{K}\, d\tilde{s}\right) = 0 \tag{53}$$

with $\tilde{q}$, $\tilde{p}$ and $\tilde{s}$ fixed at the end points. From (53) we have that

$$\frac{d\tilde{q}}{d\tilde{s}} = \frac{\partial\tilde{K}}{\partial\tilde{p}} , \quad \frac{d\tilde{p}}{d\tilde{s}} = -\frac{\partial\tilde{K}}{\partial\tilde{q}} \tag{54}$$

for each pair of canonical variables.

This scaling is not very useful if the particles are undergoing acceleration, except perhaps at the end point, where one would scale by the final momentum. Scaling by a constant is often used as a method of improving the accuracy of the results.

5. Cartesian Coordinates

In the fringing field region of dipoles, one usually works in Cartesian coordinates because the angle of bend through the fringe-field is usually very small. The equations of motion for a dipole can be written in Cartesian coordinates, in principle, for the whole magnet as well as just for the fringing field region.

It is clear from the discussion in the previous section that (30) and (44) are automatically valid in Cartesian coordinates if $\kappa=0$. Furthermore, if we restrict ourselves to cases such as a quadrupole or the fringe-field region of a dipole where the curvature is sufficiently close to zero, then (44) is in fact the correct final form of the equations. If the curvature is not zero, it is clear that (30) is still correct if we write

$$H = -P_Z = -eA_Z - \left\{\left(\frac{P_0 + e\varphi}{c}\right)^2 - m^2c^2 - \left[P_X - eA_X\right]^2 - \left[P_Y - eA_Y\right]^2\right\}^{\frac{1}{2}} \tag{55}$$

where **P** and **A** are now the momentum and vector potential, respectively, in general Cartesian coordinates, not necessarily referenced to the central trajectory; $P_0=-H$ as before and the independent variable is now Z.

As before, we are interested in trajectories in the vicinity of the design or reference trajectory. In order to obtain the equations of motion for these trajectories, we introduce the variables:

$$\left.\begin{aligned} t &= T - T^c, \quad p_t = P_0 - P_0^c \\ x &= X - X^c, \quad p_x = P_X - P_X^c \\ y &= Y - Y^c, \quad p_y = P_Y - P_Y^c \end{aligned}\right\} . \tag{56}$$

As for (38), the transformation to the new variables is canonical and is obtained from the generating function

$$F_2(Q,p) = (X-X^c)(p_x+P_X^c) + (Y-Y^c)(p_y+P_Y^c) + (T-T^c)(p_t+P_0^c) \tag{57}$$

with

$$q_i = \frac{\partial F_2}{\partial p_i}, \quad P_i = \frac{\partial F_2}{\partial Q_i} \tag{58}$$

where Q_i represent the old coordinates X, Y, T, and p_i the new momenta p_x, p_y, p_t. (*Note:* our use of Q,P for the old coordinates and q,p for the new coordinates in this instance is opposite to that used in Goldstein [3].) The new Hamiltonian is given by

$$\mathcal{H} = H + \frac{\partial F_2}{\partial Z} . \tag{59}$$

Hence,

$$\mathcal{H} = -eA_z - \left\{\left(\frac{p_t + P_0^c + e\varphi}{c}\right)^2 - m^2c^2 - \left[p_x + P_x^c - eA_x\right]^2 - \left[p_y + P_y^c - eA_y\right]^2\right\}^{\frac{1}{2}}$$

$$- \frac{\partial X^c}{\partial Z}(p_x + P_x^c) + x\frac{\partial P_x^c}{\partial Z}$$

$$- \frac{\partial Y^c}{\partial Z}(p_y + P_y^c) + y\frac{\partial P_x^c}{\partial Z}$$

$$- \frac{\partial T^c}{\partial Z}(p_t + P_0^c) + t\frac{\partial P_0^c}{\partial Z} \qquad (60)$$

where we note that the canonical coordinates of the central trajectory are Z dependent. The scalar and vector potentials are also expressed relative to the central trajectory so that

$$\varphi = \varphi(x + X^c,\ y + Y^c,\ t + T^c; Z) \qquad (61)$$

$$\mathbf{A} = \mathbf{A}(x + X^c,\ y + Y^c,\ t + T^c; Z)\ . \qquad (62)$$

The coordinates of the central trajectory are found by solving Hamilton's equations (see (31)) with the Hamiltonian (55). If DA is used to generate the map, this transformation to the coordinate system with its origin on the central trajectory is done automatically.

There are two important differences between (44) and (60). First, a solution of Hamilton's equations for (60) will not lead to the "correct" Taylor series if the curvature of the central trajectory is finite, because Z cannot normally be tangent to the central ray at both the initial and final points. A coordinate transformation will have to be applied to the results. Secondly, if the bending angle is sufficiently large, the solutions of (60) will be doubly or multiply valued--not a pleasant situation.

6. Cylindrical Coordinates

In a cyclotron, it is most natural to work in a cylindrical coordinate system because this best represents the symmetry of the magnetic field including the dominant error terms in the magnetic field. Furthermore, it is usual to represent the field in a Fourier series based on a polar coordinate system. As was the case for a Cartesian system, the canonical variables will not be in the "correct" optical coordinate system in the radial plane.

In cylindrical coordinates, we define the direction vectors of the orthogonal coordinate system as shown in Fig. 2. Although we could write down the relativistic Hamiltonian in cylindrical coordinates by analogy to the non-relativistic case [3], it is perhaps safest to derive the canonical momenta directly from the Lagrangian. The relativistic Lagrangian for a charged particle moving in an electromagnetic field is [3]

$$L = -mc^2\sqrt{1-\beta^2} - e\varphi + \mathbf{v}\cdot\mathbf{A} \tag{63}$$

where

$$\beta^2 = \frac{1}{c^2}\left[\dot{\rho}^2 + \rho^2\dot{\theta}^2 + \dot{z}^2\right] \tag{64}$$

and

$$v_\rho = \dot{\rho}\ , \quad v_\theta = \rho\dot{\theta}\ , \quad v_z = \dot{z}\ . \tag{65}$$

Hence we obtain the momenta canonical to ρ, θ and z:

$$p_\rho = \frac{\partial L}{\partial\dot{\rho}} = \frac{mc^2}{\sqrt{1-\beta^2}}\,\frac{\dot{\rho}}{c^2} + eA_\rho \tag{66}$$

$$p_\theta = \frac{\partial L}{\partial\dot{\theta}} = \frac{mc^2}{\sqrt{1-\beta^2}}\,\frac{\rho^2\dot{\theta}}{c^2} + e\rho A_\theta \tag{67}$$

$$p_z = \frac{\partial L}{\partial\dot{z}} = \frac{mc^2}{\sqrt{1-\beta^2}}\,\frac{\dot{z}}{c^2} + eA_z\ . \tag{68}$$

The Hamiltonian can now be written immediately as

$$H = e\varphi + c\left\{m^2c^2 + \left[p_\rho - eA_\rho\right]^2 + \left[p_\theta/\rho - eA_\theta\right]^2 + \left[p_z - eA_z\right]^2\right\}^{\frac{1}{2}}\ . \tag{69}$$

As in the previous cases, we want to change the independent variable, from t to θ in this case, because the magnetic field is to be represented as functions of ρ and θ. Using the methods of section 3, we find that

$$H = -p_\theta = -e\rho A_\theta - \rho\left\{\left(\frac{p_0 + e\varphi}{c}\right)^2 - m^2c^2 - \left[p_\rho - eA_\rho\right]^2 - \left[p_z - eA_z\right]^2\right\}^{\frac{1}{2}}\ . \tag{70}$$

This equation is the equivalent of (55) and would be suitable for finding the coordinates of the central or reference trajectory. If DA is used to solve the equations it is already the correct form of the Hamiltonian.

If DA is not used, we must once again transform to the local coordinate system. In order to obtain the equation for trajectories in the vicinity of the central trajectory we introduce the variables:

$$\left.\begin{aligned} \tau &= t - t^c, & p_\tau &= p_0 - p_0^c \\ x &= \rho - \rho^c, & p_x &= p_\rho - p_\rho^c \\ z &= Z & p_z &= p_Z \end{aligned}\right\} . \tag{71}$$

Here we have assumed midplane symmetry and placed the origin of z on the midplane. Following (57), we find that the generating function for the transformation is

$$F_2 = (\rho - \rho^c)(p_x + p_\rho^c) + Zp_z + (t - t^c)(p_\tau + p_0^c) \tag{72}$$

with the new Hamiltonian given by

$$\mathcal{H} = H + \frac{\partial F_2}{\partial \theta} . \tag{73}$$

Hence,

$$\mathcal{H} = -(x+\rho^c)\left\{eA_\theta \pm \left[\left[\frac{p_\tau + p_0^c + e\varphi}{c}\right]^2 - m^2c^2 - \left[p_x + p_\rho^c - eA_x\right]^2 - \left[p_Z - eA_Z\right]^2\right]^{\frac{1}{2}}\right\}$$

$$- \frac{\partial \rho^c}{\partial \theta}(p_x + p_\rho^c) + x\frac{\partial p_\rho^c}{\partial \theta} - \frac{\partial t^c}{\partial \theta}(p_\tau + p_0^c) + \frac{\partial p_0^c}{\partial \theta} . \tag{74}$$

As before, we must express the potentials relative to the central trajectory. They are of the form:

$$\varphi = \varphi(x + \rho^c, z, \tau + t^c; \theta) \tag{75}$$

$$\mathbf{A} = \mathbf{A}(x + \rho, z, \tau + t; \theta) . \tag{76}$$

The extension of (74) to the case where midplane symmetry is broken is trivial and follows directly from (60) and (61) and (62).

Once again it must be emphasized that although the variables in (74) are canonical, they are not in the correct curvilinear system in the radial plane and a coordinate transformation is required for the map to have the "correct" meaning. In a cyclotron, scaling of these equations by the momentum of the central trajectory is not very useful because of the acceleration (see section 4), except perhaps at the end point. Scaling by a constant could, of course, be used as a method of improving the accuracy of the results. Finally, if there is no acceleration (ρ^c is constant), we see that scaling by $1/\rho^c$ reproduces (44) with the appropriate change to the definition of A_θ.

7. Conclusions

The relativistic Hamiltonian for a charged particle travelling in an electromagnetic field has been derived in the usual curvilinear coordinate system used in ion-optics as well as in Cartesian and polar coordinates. In all cases, the Hamiltonian is expressed in a form in which the particles near the central or reference trajectory are expanded about the central trajectory. This is essential for the calculation of the Lie map or the Taylor series map, except when differential algebra techniques are used in the solution of the Hamiltonian. In the latter case, the DA automatically makes the transformation. The map must ultimately be expressed in curvilinear coordinates in order to have its "standard" interpretation. This can be done by a coordinate transformation. In a similar manner, the electromagnetic field must be expressed in analytic form in a way that can be expanded about the central trajectory if we are to use the DA techniques.

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References

1. M. Berz, Differential Algebraic Description of Beam Dynamics to Very High Orders, Part. Accel. 24(1989)109.
2. A.J. Dragt and É. Forest, Computation of nonlinear behavior of Hamiltonian systems using Lie algebraic methods, J. Math. Phys. 24(1983)2734.
3. H. Goldstein, Classical Mechanics, Addison-Wesley, Reading (1959).
4. W.K.H. Panofsky and M. Phillips, Classical Electricity and Magnetism, Addison-Wesley, Reading (1956).
5. E.D. Courant and H.S. Snyder, Ann. of Phys., 3(1958)1.
6. W.G. Davies, Ph. D. Thesis, unpublished (1966).
7. J.L. Synge, and B.A. Griffith, Principles of Mechanics, McGraw-Hill, New York (1959).
8. W.G. Davies, Introduction to First Order Optics, AECL Report, AECL-8053 (1983).
9. É. Forest and R.D. Ruth, Fourth Order Symplectic Integration, SLAC-PUB-5071 (1989).

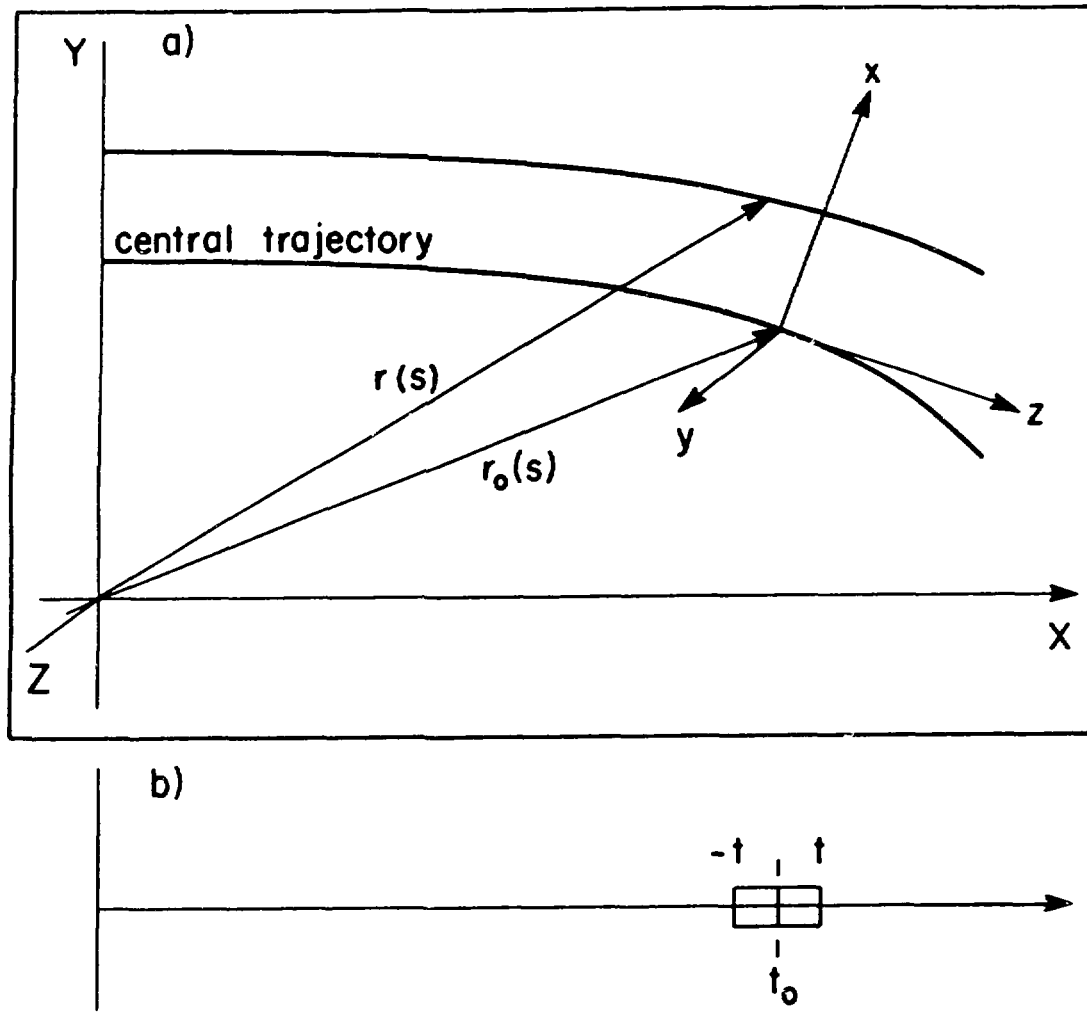

Fig. 1 *(a).* Curvilinear coordinate system used in computing ray trajectories. The local orthogonal coordinate system (x,y,z) is oriented such that (i) x is in the bending plane and directed along the local radius vector ρ, (ii) z is tangent to the central trajectory, and (iii) y is the upward-pointing vector perpendicular to the (x,z) plane. (Note the system can be either right-handed or left-handed, depending on the direction of the curvature.) The coordinate of the ray is given as a function of s, the distance along the central trajectory from the origin of the system to the local system. *(b)* Coordinates used to specify the propagation of a beam bunch of length 2τ through a section of the optical system; $\tau = t - t_o$, where t_o is the time of flight along the central trajectory and t is the time of flight of the "off-axis" particle.

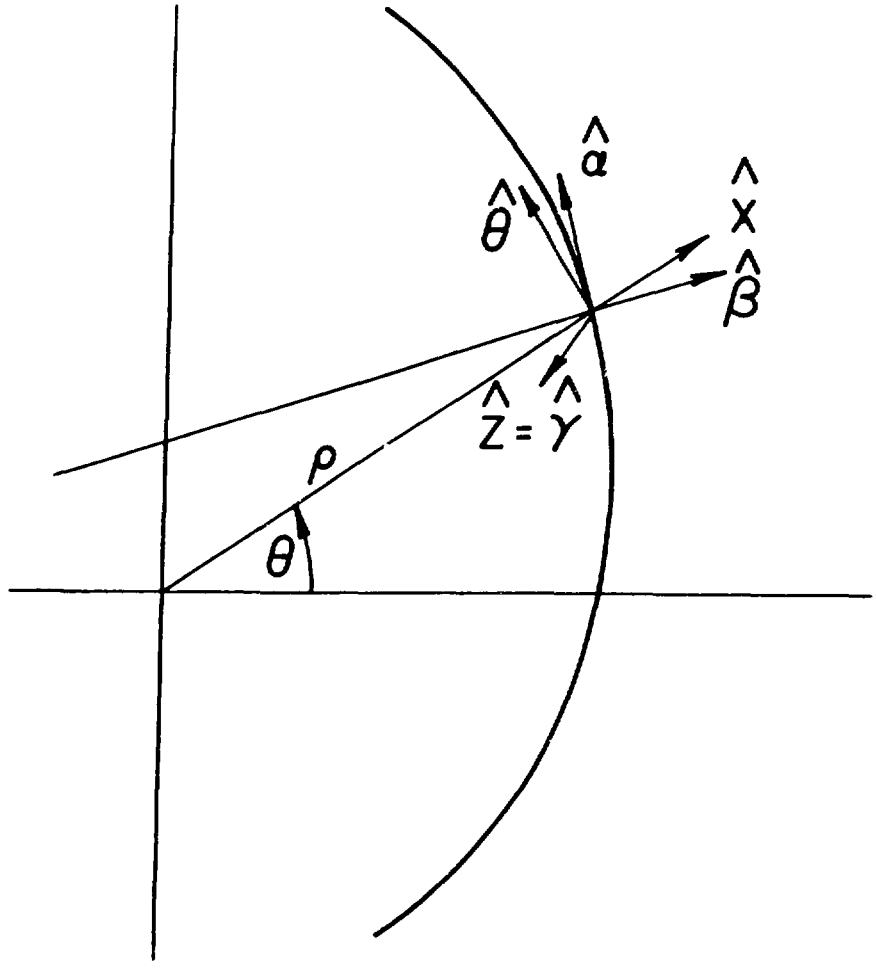

Fig. 2. Cylindrical coordinate system used to describe the orbit dynamics of a cyclotron and in some cases a dipole magnet. Here the local coordinate system is such that (i) $\hat{x}$ is in the bending plane and directed along the radius ρ from the origin; (ii) $\hat{\theta}$ is perpendicular to ρ^c but is not tangent to the central trajectory, and (iii) $\hat{z}$ is the upward-pointing vector perpendicular to the $(\hat{x},\hat{\theta})$ plane. (Note the system can be either right-handed or left-handed depending on the direction of θ, but is right-handed here). The coordinate of the ray is given as a function of θ, the total angle along the central trajectory from the origin of the system to the local system. Also shown are the unit vectors of the curvilinear system.

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