

ADVANTAGES OF USING DIFFERENTIAL ALGEBRA AND  
LIE ALGEBRA IN THE ORBIT DYNAMICS OF CYCLOTRONS

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ABSTRACT

There have been significant developments during the past few years in both numerical and analytic tools for computing and understanding the orbit dynamics of accelerators. In particular, differential-algebraic techniques can result in unprecedented accuracy in computing the nonlinear behaviour of accelerators. In addition, Lie-algebraic techniques provide powerful methods of simplifying and understanding this behaviour. The application of these techniques to the design and analysis of cyclotrons should improve their quality, predictability and ease of operation.

1. INTRODUCTION — THE TRADITIONAL METHOD

Traditionally, calculations of the orbit dynamics of cyclotrons have been done by numerically integrating the relativistic equation<sup>1)</sup>

$$\mathbf{F} = \frac{d}{dt} \frac{m\mathbf{v}}{\sqrt{1-\beta^2}}; \quad \beta = \frac{|\mathbf{v}|}{c} \quad (1)$$

with a Runge-Kutta integrator, where the Lorentz force is  $\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ ; here  $\mathbf{E}$  is the electric field,  $\mathbf{B}$  the magnetic field,  $c$  is the speed of light and  $q$ ,  $m$ , and  $\mathbf{v}$  are the charge, the mass and the velocity of the particle, respectively. Also, the usual practice is to interpolate the measured midplane field component,  $B_z$ , by, for example, Aitken's method or some combination of Fourier analysis and interpolation; we shall see that such interpolation schemes restrict both the order and the accuracy of higher derivatives of the field, which are explicitly and/or implicitly required for the analysis of the nonlinear behaviour and resonances. Finally, extrapolation of the magnetic field off the midplane is achieved by expanding  $B_z$  in a Taylor series and using Maxwell's equations plus midplane symmetry to determine the coefficients as follows: assume  $\mathbf{B}$  may be derived from a magnetic scalar potential  $\Phi(r, \theta, z)$  via  $\mathbf{B} = -\nabla\Phi$ ; from  $\nabla \cdot \mathbf{B} = 0$  we see that  $\Phi$  satisfies Laplace's equation,  $\nabla^2\Phi = 0$ . In cylindrical coordinates, the Laplacian may be split into "transverse" and  $z$ -pieces,  $\nabla^2 = [\nabla_{\perp}^2 + \partial_z^2]$  where  $\nabla_{\perp}$  and  $\partial_z$  commute. Since  $B_z = \partial_z\Phi$ , it therefore follows that  $\nabla^2 B_z = 0$  also. Assuming midplane symmetry, we expand  $B_z$  about the midplane as a Taylor series in  $z$ ,

$$B_z(r, \theta, z) = \sum_m \frac{1}{(2m)!} B_{2m}(r, \theta) z^{2m}. \quad (2)$$

The  $B_{2m}$  may be determined by substituting Eq. 2 into Laplace's equation and setting like powers of  $z$  to zero. We find that  $B_2 = -\nabla_{\perp}^2 B_z|_{z=0}$ ,  $B_4 = +\nabla_{\perp}^4 B_z|_{z=0}$ , etc.; in other words, we must take high-order derivatives of the interpolated midplane field  $B_z$ . Since differentiation of interpolated data rapidly results in total loss of numerical significance, we are in practice limited to  $m = 0, 1$ , i.e., expansion of the field only to sextupole order. Furthermore, we see why we must require midplane symmetry: it is impossible to infer  $\partial_z B_z|_{z=0}$  if given only  $B_z$  on the single plane  $z = 0$ .

With this approach, it is very difficult to analyse resonances with much accuracy. Typically, the determinant of the 1<sup>st</sup> order transfer matrix obtained by differencing the principal rays is only accurate to about 5%, and higher order maps will be much less accurate. Thus the *symplectic condition* is violated, and hence *Liouville's theorem* is not satisfied and phase-space is not preserved.

2. DIFFERENTIAL ALGEBRA — THE NEW METHOD

The limitations discussed above can be overcome with the use of *differential algebra* ( $DA$ )<sup>2)</sup>, which allows us to accurately calculate the high order behaviour. The advantage of  $DA$  is that it automatically generates a Taylor series expansion of Eq. 1, or the Hamiltonian of the system, about any point in space. The derivatives in the expansion are computed to *machine precision*; there is no *truncation error*. Also, an arbitrary number of variables with derivatives to arbitrary order can be accommodated.

However, for  $DA$  to be used, the electromagnetic fields must be expressed in terms of analytic functions. This has pros and cons. Extrapolation of an interpolated magnetic field off the midplane does not allow us to accurately calculate high order effects in any case, so a better approach is needed even without  $DA$ . Unfortunately, a realistic and analytic magnetic (and RF) field model is in general difficult to achieve and will be much more computationally intensive than the traditional approach. Fortunately, use of a Bulirsch-Stoer<sup>3)</sup> integrator wins back much of this 'lost time' plus the bonus of much greater numerical accuracy than can be achieved with the

traditional Runge-Kutta integrator.\* At Chalk River, we have developed accurate 3-dimensional models of the magnetic and RF fields<sup>1)</sup> for the TASC superconducting cyclotron, which do not require midplane symmetry; the midplane field data is only needed to fix parameters of the model.

## 2.1. How DA Works

$DA^2)$  is a special algebra that replaces ordinary multiplication with a new kind of vector multiplication designed to achieve automatic differentiation. Space does not permit an extensive exposition of  $DA$ , so the rudiments will be illustrated by the following example; the interested reader is referred to ref. 2 for details. A  $DA$  of order  $n$  in  $v$  variables is denoted  ${}_nD_v$  and the  $DA$  vector  $Df = (f_0, f_1, f_2, \dots, f_n)$ , where  $f_0$  denotes the scalar value of  $f = f(\mathbf{x})$  at  $\mathbf{x} = \mathbf{x}_0, (\mathbf{x} \in \mathbf{R}^v)$ . The  $f_1, f_2, \dots, f_n$  are themselves sub-vectors containing the  $1^{st}, 2^{nd}$ , and  $n^{th}$  order derivatives of  $f$ , respectively. The *unit element* of the algebra is  $(1, 0, \dots, 0)$  and the *unit differentials* are  $d_i = (0, \delta_i^1, \delta_i^2, \dots, 0)$  where  $i = 1 \dots v$  and  $\delta_i^j$  is the Kronecker  $\delta$ . For  $2^{nd}$  derivatives of functions of one variable,  ${}_2D_1$ , the rules of the algebra are:

$$A + B = (A_0 + B_0, A_1 + B_1, A_2 + B_2) \quad (3)$$

$$A * B = (A_0 B_0, A_0 B_1 + B_0 A_1, A_0 B_2 + A_1 B_1 + A_2 B_0). \quad (4)$$

We see that  $d = (0, 1, 0)$ ,  $d^2 = (0, 1, 0) * (0, 1, 0) = (0, 0, 1)$  and  $d^3 = (0, 1, 0) * (0, 1, 0) * (0, 1, 0) = (0, 0, 0)$ ; i.e. the algebra is *nilpotent* at order  $n$ . Thus if  $f(\mathbf{x}) = \mathbf{x}^2$  at  $\mathbf{x} = 5$ , we obtain  $(5, 1, 0) * (5, 1, 0) = (25, 5 \cdot 1 + 1 \cdot 5, 5 \cdot 0 + 1 \cdot 1 + 0 \cdot 5) = (25, 10, 1)$ , but

$$Df = (25, 10, 1) \equiv \left( f(\mathbf{x}), \frac{df(\mathbf{x})}{d\mathbf{x}}, \frac{1}{2} \frac{d^2 f(\mathbf{x})}{d\mathbf{x}^2} \right)_{\mathbf{x}=5} \quad (5)$$

which are the coefficients of a Taylor series to  $2^{nd}$  order about  $\mathbf{x} = 5$ . Note: only one function evaluation was needed.

## 2.2. Application of DA to Cyclotrons

As we wish to preserve the symplectic condition, canonical coordinates must be used, and it is convenient to use the Hamiltonian formulation. The relativistic Hamiltonian in cylindrical coordinates, the “natural” coordinate system for cyclotrons, is<sup>5)</sup>

$$H = -erA_\theta - r \left\{ \left( \frac{p_0 + \varphi}{c} \right)^2 - m^2 c^2 - [\mathbf{P}_\perp - \mathbf{A}_\perp]^2 \right\}^{1/2} \quad (6)$$

\*In our tests Bulirsch-Stoer was from 3 to 5 times faster than Runge-Kutta and  $10^6$  times more accurate.  $B-S$  is ideal for integrating  $DA$  problems because all the functions are analytic.

where  $H$  is the momentum in the azimuthal direction,  $\theta$  is the independent variable,  $r$  is the radius of curvature,  $p_0$  is the total energy,  $\varphi$  is the electromagnetic scalar potential, and  $\mathbf{P}_\perp$  and  $\mathbf{A}_\perp$ , are the transverse components of the momentum and the electromagnetic vector potential, respectively;  $A_\theta$  is the azimuthal component of the vector potential. We make a  $DA$  expansion of the Hamiltonian

$$H \Rightarrow (H, H_r, H_{P_r}, H_Z, H_{P_Z}, \dots) = \sum_{s=0}^N \frac{1}{s!} \frac{\partial^{|s|} H}{\partial q^s} dq^s \quad (7)$$

where  $q^s = r^i P_r^j Z^k P_Z^l T^m P_T^n$ ,  $|s| = i + j + k + l + m + n$  and  $s! = i!j!k!l!m!n!$ . In this expansion, the derivatives are with respect to the canonical coordinates,  $\mathcal{Z} = (\tau, P_r, Z, P_Z, T, P_T)$ , of the fundamental cylindrical coordinate system. The differential quantities  $dq^s$  are monomials of the  $DA$  basis vectors which represent the monomials  $\zeta^s$  appearing in the usual expansion of the Hamiltonian (see Eq. 10), where  $\zeta = (x, p_x, z, p_z, t, p_t)$  are the familiar differential canonical coordinates. Hamilton's equations in Poisson bracket form are

$$\mathcal{Z}' = -[H, \mathcal{Z}] \quad (8)$$

where the ‘ $'$ ’ denotes differentiation with respect to  $\theta$ . The usual form of Hamilton's equations are readily obtained from Eq. 8. The  $DA$  expansion of Hamilton's equations have the form

$$\begin{aligned} r' &= \frac{\partial}{\partial P_r} (H, H_r, H_{P_r}, H_Z, H_{P_Z}, H_T, H_{P_T} \dots) \\ &= (H_{P_r}, H_{P_r r}, H_{P_r P_r}, H_{P_r Z}, H_{P_r P_Z}, H_{P_r T}, H_{P_r P_T} \dots) \end{aligned} \quad (9)$$

for the  $r'$  equation and similarly for the other coordinates. The straightforward method of obtaining Eq. 9 is to differentiate the Hamiltonian “by hand” and evaluate the “right-hand-side” of Hamilton's equations in  $DA$ . The resulting  $DA$  vectors are integrated numerically. The result is the reference trajectory, along with the usual Taylor series map, or aberration expansion,

$$\zeta_i^{FIN} = R_{ij} \zeta_j^{IN} + T_{ijk} \zeta_j^{IN} \zeta_k^{IN} + U_{ijkm} \zeta_j^{IN} \zeta_k^{IN} \zeta_m^{IN} + \dots; \quad (10)$$

repeated indices are summed. The superscripts, IN and FIN, refer to the initial and final coordinates connected by the map. Since  $DA$  can expand functions to arbitrarily high order, unlike conventional “transfer-matrix” codes the order of the Taylor-expanded map Eq. 10 is not fixed, but may be freely chosen at run-time.

One might naively assume that it is easy to use  $DA$  to take the derivatives of the  $DA$ -Hamiltonian, Eq. 7, but this is not the case, because the  $\partial$ -operator in  $DA$  maps  ${}_nD_v$  onto  ${}_{n-1}D_v$ , so that expansion of the Hamiltonian to order  $n$  results in an expansion of Hamilton's

equations only to order  $n - 1$ . Thus the  $n^{th}$  order terms will be in error after the first integration step, the  $n - 1$  order terms are in error after the second step and so on. However, it can be shown (see Eq. 7 and 4) that if the first derivatives of  $H$  are zero then the problem is circumvented and we have a consistent algebra. We can make the derivatives zero by explicitly making the canonical transformation to the reference trajectory.<sup>9)</sup>

A further problem (and difference between  $DA$  and ordinary calculus) is that the  $\partial$ -operator in  $DA$  gives the *values* of the derivatives with respect to the expansion variables whereas the usual  $\partial$ -operator generates a *function* of the phase space variables at a general point. Because in our case the expansion variables are the phase space variables at the initial azimuth  $\theta_0$ , we do not directly obtain the derivatives needed for the standard form of Hamilton's equations. The Poisson bracket form, Eq. 8 allows us to circumvent this problem, because the map from initial to final phase-space variables is a canonical transformation, and the Poisson bracket is invariant under canonical transformations. Thus the penalty for generating Hamilton's equation with  $DA$  is that we must evaluate  $H$  to one order higher than the desired map, plus we must make a canonical transformation at each step, both of which increase the computation time.

Eq. 10 plus the reference trajectory are sufficient if we are interested only in the behavior of the reference trajectory, tunes or phase-space plots. For the study of the non-linear behavior, especially resonances, it is helpful to transform to a Lie-algebraic representation, which by presenting the dynamics in a simpler and more compact form greatly facilitates understanding. Furthermore, many powerful and elegant theorems of Lie algebras, symplectic groups and symplectic geometry<sup>10)</sup> are immediately applicable, aiding in the simplification, analysis and understanding of the problems under study.

### 3. LIE-ALGEBRAIC ANALYSIS

The Poisson bracket  $\{H, \mathcal{Z}\}$  in Hamilton's equations, Eq. 8, satisfies the requirements of a Lie algebra, namely, the commutation relation

$$A * B = (A, B) = AB - BA \quad (11)$$

and the Jacobi identity

$$(A, (B, C)) + (B, (C, A)) + (C, (A, B)) = 0. \quad (12)$$

Note: This algebra is *neither commutative nor associative*.

The Taylor series map Eq. 10, written as  $\zeta^{FIN} = \mathcal{M}\zeta^{IN}$ , can be transformed<sup>6)</sup> with the help of  $DA$  into an equivalent Lie-map

$$\mathcal{M} \Rightarrow \mathcal{M}_f, \quad \mathcal{M}_f = e^{:f:}; \quad :f:g = [f, g] \quad (13)$$

where

$$e^{:f:} \stackrel{\text{def}}{=} \sum_{n=0}^{\infty} \frac{:f:^n}{n!}; \quad :f:^0 = \mathcal{I} = \{\text{identity map}\}, \quad (14)$$

and  $[\cdot, \cdot]$  is the Poisson bracket<sup>7)</sup> with respect to the canonical coordinates  $(x, p_x, z, p_z, t, p_t)$ . The Lie-map,  $\mathcal{M}_f$ , can be factored<sup>6)</sup> into

$$\mathcal{M}_f = \mathcal{M}_1 \mathcal{M}_2 \mathcal{M}_3 \mathcal{M}_4 \dots = e^{:f_1:} e^{:f_2:} e^{:f_3:} e^{:f_4:} \dots \quad (15)$$

where  $\mathcal{M}_f$  and  $\mathcal{M}_n$  are *symplectic maps* and  $f_n$  are homogeneous polynomials of degree  $n$ .

In a circular accelerator, it is desirable that the reference orbit be a closed orbit (*i.e.* a "fixed point" of the one-turn map); this is, in fact, necessary for the transformation to normal form. If the reference trajectory is not a closed orbit, the map,  $\mathcal{M}_f$ , will have an  $\mathcal{M}_1$  factor. The closed orbit can be found from the map by solving for the fixed point given by the relation  $\zeta_* = \mathcal{M}_f \zeta_*$ . If the non-linearities are small and/or the initial conditions are not too far from the fixed point, the problem converges in one iteration. However, if the non-linearities in the map are large and we truncate the map (which we must invariably do), then the solution of the fixed point equation will not be exact, and the process must be repeated until convergence is obtained. Once the fixed point has been found, the map can be transformed by a canonical change of variables  $\tilde{\zeta} = \mathcal{A}\zeta$ , such that  $\tilde{\zeta}_* = \mathcal{A}\zeta_* = 0 \Rightarrow \tilde{\zeta}_* = \mathcal{A}\mathcal{M}_f\mathcal{A}^{-1}\tilde{\zeta}_* = \tilde{\mathcal{M}}_f\tilde{\zeta}_* = 0$  *i.e.*  $\tilde{\mathcal{M}}_f$  maps the origin onto itself.

The Lie-polynomials provide a much more compact representation of the map than Eq. 10, and preserve the symplectic nature of the map,  $\mathcal{M}$ , exactly, which Eq. 10, when truncated, does not do. With the help of  $DA$ , Eq. 15 can be transformed into *normal form*<sup>6)</sup> which provides a very powerful method for identifying and analysing non-linear behaviour and resonances in particle accelerators.

#### 3.1. Normal Form

The normal form is the transformation  $\mathcal{N} = \mathcal{A}\mathcal{M}\mathcal{A}^{-1}$  such that  $\mathcal{N}$  is in its "simplest" form;  $\mathcal{M}$  must be expanded about a "closed orbit" *i.e.* no  $H_1$  terms in  $H$ , which implies no  $\mathcal{M}_1$  terms in  $\mathcal{M}$ . The symplectic map  $\mathcal{A}$  is an  $n^{th}$  order canonical transformation that *isolates* the tune shifts and resonances to  $n^{th}$  order. Using the factored map or alternatively the Taylor map and  $DA$ , we can normalize  $\mathcal{M}$  order by order to obtain<sup>6)</sup>

$$\mathcal{N} = \mathcal{A}_n \dots \mathcal{A}_4 \left\{ \mathcal{A}_3 \left\{ \mathcal{A}_2 \mathcal{M} \mathcal{A}_2^{-1} \right\} \mathcal{A}_3^{-1} \right\} \mathcal{A}_4^{-1} \dots \mathcal{A}_n^{-1} \quad (16)$$

We proceed as follows: From the eigenvectors (they must be distinct) of  $R$ , Eq. 10, we get a canonical transformation that *rescales and block diagonalizes*  $R$ ;<sup>†</sup>

$$\mathcal{R} = \mathcal{A}_2 R \mathcal{A}_2^{-1} \Rightarrow \mathcal{R} = \begin{pmatrix} \mathcal{R}_1 & & 0 \\ & \mathcal{R}_2 & \\ 0 & & \mathcal{R}_3 \end{pmatrix} \quad (17)$$

where

$$\mathcal{R}_i = \begin{pmatrix} \cos(\mu_i) & \sin(\mu_i) \\ -\sin(\mu_i) & \cos(\mu_i) \end{pmatrix}, \begin{pmatrix} 1 & L_i \\ 0 & 1 \end{pmatrix}, \text{ or } \begin{pmatrix} 1 & 0 \\ a_i & 1 \end{pmatrix}.$$

Next, we normalize  $\mathcal{M}_3$

$$\begin{aligned} \mathcal{N} &= \mathcal{A}_3 \mathcal{A}_2 R e^{iJ_3} \dots \mathcal{A}_2^{-1} \mathcal{A}_3^{-1} = e^{iG_3} \mathcal{R} e^{iG_3} \dots e^{-iG_3} \\ &= \mathcal{R} \exp \left\{ -(I - \mathcal{R}^{-1})G_3 + g_3 : \right\} \dots \end{aligned} \quad (18)$$

A further simplification results if we expand  $(I - \mathcal{R}^{-1})$ , and  $g_3$  in a complex or ‘resonance’ basis as follows:  $h_{\pm} = \mathbf{x} \pm i\mathbf{p}_x$ ,  $v_{\pm} = z \pm ip_z$ . Hence,

$$(I - \mathcal{R}^{-1}) |n, m\rangle = \left[ 1 - \sum_{n+m=3} e^{i(n-m)\cdot\mu} \right] |n, m\rangle, \quad (19)$$

and

$$g_3 = \sum_{n+m=3} A_{nm} |n, m\rangle, \quad |n, m\rangle = h_+^{n_1} h_-^{m_1} v_+^{n_2} v_-^{m_2}; \quad (20)$$

$n, m, \mu$  are vectors with components  $(n_1, n_2)$  etc. Substituting Eq. 19 and Eq. 20 into Eq. 18 and solving for  $G_3$ , we obtain

$$G_3 = \sum_{n+m=3} \frac{A_{nm}}{\{1 - \exp[i(n-m)\cdot\mu]\}}. \quad (21)$$

All terms in  $g_3$  can be incorporated into  $G_3$  except when  $n - m = 0$ , or  $(n - m) \cdot \mu = 2\pi\ell$ ,  $\ell = \text{integer}$ ; *i.e.*  $(n_1 - m_1)\mu_x + (n_2 - m_2)\mu_z = 2\pi\ell$ ;  $\ell = 0, \pm 1, \pm 2 \dots$ . The integer  $\ell$  characterizes the resonance. In a similar fashion, we could proceed to find  $G_4$  etc.

<sup>†</sup>The matrix  $R$  is the evaluated representation of the Lie-map  $e^{iJ_2}$ . As is common in the literature we will use  $R$  to represent both the Lie-map and the matrix itself, the choice being determined from the context. In fact, if canonical coordinates are used, the matrix  $R$  obtained from the Lie-map is always identical with that obtained from the Taylor-series, Eq. 10, and satisfies the symplectic condition exactly (*i.e.*  $\det|R| = 1$ ).

A further transformation to *action-angle* variables,  $h_{\pm} = \sqrt{2J_x} e^{\mp i\varphi_x}$ ,  $v_{\pm} = \sqrt{2J_z} e^{\mp i\varphi_z}$ , leads to

$$\mathcal{N} = \exp : \left\{ (\mu_x + \mu'_x p_t + \mu''_x p_t^2 \dots) J_x + (\mu_z + \dots) J_z + a_x J_x^2 + a_z J_z^2 + \dots \right\} : \quad (22)$$

where we have assumed no acceleration and no explicit resonances;  $J_x$  and  $J_z$  are the *action invariants* with associated angles  $\varphi_x$  and  $\varphi_z$ ,  $\mu$  are the *phase advances*,  $\mu'$  etc. are the *chromaticities*, and all terms proportional to  $J^n$  are non-linear *tune shifts*. That we can incorporate all the other non-linearities into  $\mathcal{A}$  and ‘get rid of them’ makes the analysis of the tune-shifts and resonances much easier! If explicit resonances occur with  $(n - m) \cdot \mu = 2\pi\ell$ ;  $n, m, \ell = \text{integers}$ , these must be added to Eq. 22. Because  $[J_i^n, J_j^m] = 0$ , that is all powers of the actions commute, the transformation from factored to single-exponent form is straightforward in Eq. 22. However, if there are resonances in the system, the *Campbell-Baker-Hausdorff* formula<sup>7)</sup> or *DA* must be used to convert to single exponent form. Finally, the *normal form* has the remarkable property that

$$\mathcal{M}^n = \mathcal{A}^{-1} \mathcal{N}^n \mathcal{A} \quad (23)$$

where  $n$  is the number of times the map is concatenated with itself. Use of Eq. 23 results in an enormous saving of work when applicable.

#### 4. EXAMPLES AND DISCUSSION

Cyclotrons are only quasi-periodic and one should ideally work with accelerated maps, which our *DA* approach allows us to do. However, the dominant features of resonance topology can be studied using a simplified autonomous ( $\theta$ -independent) Hamiltonian.

In isochronous cyclotrons,  $\nu_x \simeq 1$ , and the azimuthally averaged (‘bulk’) field  $B_z \propto \gamma = (1 - \beta^2)^{-1/2}$  can be approximated as a constant plus a term proportional to  $r^2$ ; this generates radially increasing bulk-quadrupole and bulk-sextupole terms when the field is expanded about the reference trajectory. The bulk quadrupole term is defocusing in the  $z$ -plane and is overcome by increasing the spiral angle of the hills, which produces additional local quadrupole and sextupole terms near the hill edges (‘edge’ fields) which approximately compensate the defocusing effect of the bulk field radial variation. Expanded through 3<sup>rd</sup> order about the reference trajectory, the combined effects of the bulk and edge fields can be modelled by the vector potential

$$A_{\theta} = -\frac{x + r_0}{2} B_0 - \frac{1}{r_0} \left\{ Q_x x^2 + Q_z z^2 \right\} - \frac{S_x}{r_0} \left\{ \frac{x^3}{3} - x z^2 \right\} \quad (24)$$

where  $Q_x, Q_z, S_x$ , are the effective quadrupole and sextupole strengths, respectively. Inserting this vector potential into the Hamiltonian, Eq. 6, we will investigate the leading order nonlinearities and outline the analysis of the Walkinshaw or  $\nu_x = 2\nu_z$  coupling resonance, which occurs near extraction in many cyclotrons. As a final illustration of the power of this type of analysis, we will show the effect of an octupole field on the orbits in the vicinity of the “one-third integer” sextupole resonance in a 3-fold symmetric cyclotron.

Because Eq. 24 is independent of  $\theta$ , the Hamiltonian Eq. 6 has the solution

$$\mathcal{M}(\theta) = e^{-\theta \cdot H} \quad (25)$$

which can be factored into the form of Eq. 15. As we are neglecting acceleration, the energy of each particle is conserved and  $p_t = (E_0 - E)/P_0 c$ , where  $E$  is the particle energy, and  $E_0$  and  $P_0$  are the energy and momentum of the central trajectory, respectively.

#### 4.1. Non-resonant Non-linear Behaviour

We will now apply the normalization procedure described in section 3.1 to the map given by Eq. 25. Since we assume no explicit resonances, the normal form contains  $g_2 = -[\mu_x J_x + \mu_z J_z]$ , the Lie-generator of the “rotation matrix”  $\mathcal{R}$ , Eq. 17, and

$$\begin{aligned} g_3 = & \frac{(1 - \nu_x)}{4\nu_x\beta} J_x p_t + \frac{(1 - \nu_z)}{4\nu_z\beta} J_z p_t \\ & + \pi S_x \frac{k_x^2}{\nu_x\beta} J_x p_t - \pi S_x \frac{k_x k_z}{\nu_x\beta} J_z p_t \\ & + \pi k_x \frac{1 - \beta^2}{\nu_x\beta} p_t^3 + \pi S_x \frac{2k_x^3}{3\nu_x^3\beta^3} p_t^3 \quad (26) \end{aligned}$$

Eq. 26 has four *chromaticity* terms proportional to  $p_t$  and two time-of-flight aberration terms proportional to  $p_t^3$ . Here  $k_x = r_0/\nu_x$ ,  $k_z = r_0/\nu_z$ .

If, for the moment, we make  $\nu_x = 1$  (i.e. the system is resonant in the radial plane) then the first term in Eq. 26 vanishes. If we also adjust the spiral such that  $S_x = 0$  then all the *chromaticity* terms vanish except the second one involving  $(1 - \nu_z)$ . Under these circumstances  $\mathcal{R}_1 = \mathcal{R}_x = \mathcal{I}_x$ ,  $\mathcal{R}_2 = \mathcal{R}_z$ , and we find that

$$\begin{aligned} \mathcal{M} &= \{ \mathcal{A}_3^{-1} \mathcal{A}_2^{-1} \mathcal{N} \mathcal{A}_2 \mathcal{A}_3 \} = \{ \mathcal{A}_3^{-1} \mathcal{I}_x \mathcal{R}_z e^{i g_3} \mathcal{A}_3 \} \\ &= \hat{\mathcal{A}}_3^{-1} \mathcal{R}_z e^{i \hat{g}_3} \hat{\mathcal{A}}_3 \quad (27) \end{aligned}$$

where

$$\hat{g}_3 = \frac{(1 - \nu_z)}{4\nu_z\beta} J_z p_t + \pi k_x \frac{1 - \beta^2}{\nu_x\beta} p_t^3$$

and the  $\hat{\mathcal{A}}$  now contain only terms involving  $z$ ; i.e. all the non-linearities involving only the  $x$  coordinate cancel!

In reality,  $\nu_x \simeq 1$ ,  $S_x \simeq 0$  (at least on the average but not necessarily locally) and  $\nu_z \ll 1$  over most of the accelerating region. Hence there is a large vertical chromaticity term in the map as is well known, but all the radial plane nonlinearities will be small through  $3^{rd}$  order. What happens at  $4^{th}$  order is another story! However, as we pass (adiabatically) through the resonances in the horizontal and vertical plane, this cancellation will be punctuated by terms with small denominators which must be retained (locally) in the normal map. In particular, in a 3-sector cyclotron, the residual sextupole can excite the “one-third integer resonance” in the radial plane (see section 4.3). Similarly, a one-fourth integer resonance can be excited by the octupole field in a 4-sector cyclotron, but this is usually much weaker. This analysis demonstrates why a 4-sector cyclotron is less affected by non-linearities than a 3-sector machine.

#### 4.2. Walkinshaw Resonance

In the fringe-field region near the extraction radius, we have large sextupole and octupole strengths and the magnetic field is no longer isochronous. We will ignore the octupole component for the purposes of this discussion, but it can have a profound effect on the stability of the orbits. At the Walkinshaw resonance, where  $\nu_x = 2\nu_z$  (i.e.  $(\mathbf{n} - \mathbf{m}) \cdot \boldsymbol{\mu} = 2\pi\ell$  with  $\ell = 0$ ), we have a vanishing denominator in Eq. 21. This resonant term must be retained in the normal map. We can write the normal map, which now includes the resonance term, in factored form as follows:

$$\mathcal{N} = e^{i g_2} e^{i g_3} e^{i \alpha p_t^3} = e^{i g_2} e^{i g'_3} e^{i \hat{g}_3} e^{i \alpha p_t^3} \quad (28)$$

where  $g_2 = -\boldsymbol{\mu} \cdot \mathbf{J} = -[\mu_x J_x + \mu_z J_z]$  and  $g'_3 = \mu'_x p_t J_x + \mu'_z p_t J_z$ , the chromaticities, Eq. 26. The factorization of  $e^{i g_3}$  into  $e^{i g'_3} e^{i \hat{g}_3}$  can be done trivially because we restrict ourselves to  $3^{rd}$  order in the map. Because  $[J_i^n, J_j^m] = 0$ , we can easily combine  $g_2$  and  $g'_3$  into a single exponent as  $-\hat{\boldsymbol{\mu}} \cdot \mathbf{J} = -\boldsymbol{\mu} \cdot \mathbf{J} + p_t \boldsymbol{\mu}' \cdot \mathbf{J}$  where  $\hat{\boldsymbol{\mu}} = \boldsymbol{\mu} - p_t \boldsymbol{\mu}'$ , i.e. the new tune is energy dependent. The tune-shifted resonance occurs when  $(\mathbf{n} - \mathbf{m}) \cdot \hat{\boldsymbol{\mu}} = 0$ . The sextupole driving term,  $\hat{g}_3$  is given by

$$\begin{aligned} \hat{g}_3 = & -S_x \pi \frac{\sqrt{2k_x}}{4} k_z J_x^{1/2} [e^{i\varphi_x} + e^{-i\varphi_x}] \times \\ & J_z [e^{2i\varphi_z} + e^{-2i\varphi_z}]. \quad (29) \end{aligned}$$

In order to understand the topology of this resonance it is convenient to transform to the “co-moving” frame<sup>8</sup>. This transformation is defined by the expression

$$\phi_1 = \mathbf{k} \cdot \boldsymbol{\varphi}; \quad (\mathbf{n} - \mathbf{m}) = \lambda \mathbf{k}, \quad \lambda = \text{integer} \quad (30)$$

and

$$K_1 = \frac{\mathbf{k} \cdot \mathbf{J}}{\|\mathbf{k}\|^2}, \quad K_2 = \frac{\mathbf{a} \cdot \mathbf{J}}{\|\mathbf{a}\|^2} \quad (31)$$

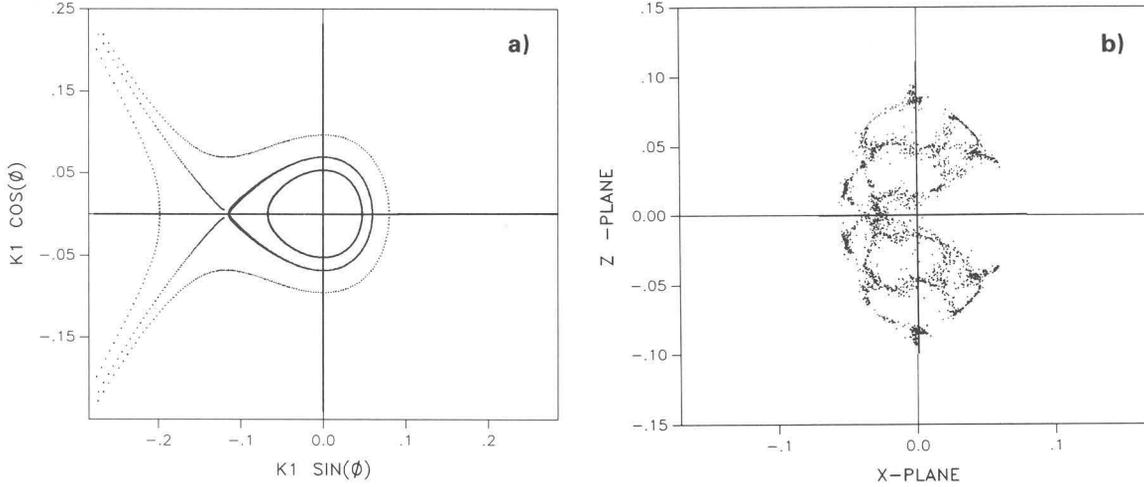


Figure 1. Phase-space plots for the  $\nu_x = 2\nu_z$  resonance where  $\hat{\nu}_x = 1.195$ ,  $\hat{\nu}_z = 0.6025$  and the normalized sextupole strength is 1.700 units;  $J_x = 0.0004$ ,  $J_z = 0.0025$ . a) shows the position of the fixed point at  $\phi_1 = \pi$ , the separatrix, and trajectories inside and outside the separatrix in order to illustrate the topology. b)  $x$  vs  $z$  projection in the original space. The parameters place the orbits very close to the separatrix.

where  $\mathbf{a}$  is orthogonal to  $\mathbf{k}$ , ( $\mathbf{k} \cdot \mathbf{a} = 0$ ). In our case  $\lambda = 1$ . Hence,

$$\phi_1 = \varphi_x - 2\varphi_z \text{ and } \phi_2 = 2\varphi_x + \varphi_z \quad (32)$$

where  $\mathbf{k} = (1, -2)$  and  $\mathbf{a} = (2, 1)$ . Thus,

$$K_1 = \frac{J_x - 2J_z}{5}, \quad K_2 = \frac{2J_x + J_z}{5}. \quad (33)$$

The transformation to the co-moving frame is effected by the transformation<sup>8)</sup>

$$\mathcal{N}_c = e^{i2\pi\ell K_1} \mathcal{N} = e^{i2\pi\ell K_1} e^{-i\hat{\mu} \cdot J} e^{i\tilde{g}_3} e^{i\alpha p_i^3} \quad (34)$$

where  $2\pi\ell = \mathbf{k} \cdot \boldsymbol{\mu}$ . In our case  $\ell = 0$ , and the transformation is the identity map. We want to expand about the resonance, that is we assume that we are not quite on resonance, and write  $\mathbf{k} \cdot \boldsymbol{\mu} = 2\pi(\nu_x - 2\nu_z) = \delta$ . Hence

$$\mathcal{N}_c = e^{-i\delta K_1 - i\mu \cdot \mathbf{a} K_2} e^{i\tilde{g}_3} e^{i\alpha p_i^3} \quad (35)$$

where  $\tilde{g}_3$  is in the co-moving coordinates;

$$\tilde{g}_3 = -S_x \pi k_z \frac{\sqrt{2k_x}}{2} [K_1 + 2K_2]^{1/2} \times [K_2 - 2K_1] [e^{i\phi_1} + e^{-i\phi_1}]. \quad (36)$$

We note that there is no  $\phi_2$  dependence. Thus we have reduced the apparently two-dimensional resonance into a one-dimensional form with parameter  $K_2$ . If we combine exponents in Eq. 34 so that

$$\mathcal{N}_c = e^{-i\delta K_1 - i\mu \cdot \mathbf{a} K_2} e^{i\tilde{g}_3} e^{i\alpha p_i^3} = e^{i h} e^{i\alpha p_i^3} \quad (37)$$

we obtain the ‘‘pseudo-Hamiltonian’’  $h$ . The fixed points of the resonance can be found in the usual way by setting  $\zeta = \mathcal{M}\zeta$ , which reduces to

$$\frac{\partial h}{\partial K_1} = 0 \text{ and } \frac{\partial h}{\partial \phi_1} = 0, \quad (38)$$

the usual condition for a fixed point if  $h$  were the real Hamiltonian. This leads to<sup>†</sup>

$$\tan(\phi_1) = -\frac{1 - \cos(\delta)}{\sin(\delta)} \simeq \frac{1}{2}\delta \ll 1 \quad (39)$$

and

$$\frac{2\pi k_z \sqrt{2k_x} S_x [6K_1 + 7K_2] - \delta \sqrt{K_1 + 2K_2}}{\sqrt{K_1 + 2K_2}} = 0 \quad (40)$$

which has the solutions

$$\phi_1 = \{0, \pi\} \text{ and } K_1 = \pm \frac{\delta \sqrt{15K_2}}{72\pi k_z \sqrt{k_x} S_x} - \frac{7K_2}{6} \quad (41)$$

where we have neglected terms of order  $\delta^2$  in the expansion of the trigonometric functions. The topology of this resonance is rather complicated, being a function of  $\delta$ ,  $S_x$ , and  $K_2$ . The *level sets* of the pseudo-Hamiltonian

<sup>†</sup>In the non-Lie-algebraic treatment one usually obtains a sine rather than a tangent; since  $\delta$  is assumed small the two results are equivalent to first order.

define the contours of normalized phase space and the level set that passes through the hyperbolic fixed point defines the *separatrix* of the resonance.

A phase-space plot for the  $\nu_x = 2\nu_z$  resonance where  $\hat{\nu}_x = 1.195$ ,  $\hat{\nu}_z = 0.6025$  is shown in Fig. 1;  $\hat{\nu}$  is the tune associated with the chromaticity-shifted phase advance  $\hat{\mu}$ . Fig. 1 shows the position of the fixed point at  $\phi_1 = \pi$  and the separatrix, along with trajectories inside and outside the separatrix in order to illustrate the topology. Here we are working in the Cartesian equivalent of  $K_1, \phi_1$  space. This plot was generated by iterating the map,  $\mathcal{M}$ , 3000 times, which is approximately equivalent to Eq. 23,

$$\mathcal{M}^n = \mathcal{A}^{-1} \mathcal{N}^n \mathcal{A} = \mathcal{A}^{-1} e^{in\hat{h}} \mathcal{A} \quad (42)$$

except that the iterated map generates higher order nonlinearities by “feed-up” which Eq. 42 does not do.

### 4.3. One-third Integer Resonance

In a 3-sector cyclotron, we have 3-fold symmetry in the magnetic field. Since  $\nu_x \simeq 1$ , the radial phase advance per cell is  $\mu_x \simeq 2\pi/3$  and we see from Eq. 21 that if  $n_1 - m_1 = 3$ , we will have a resonant condition. For the purposes of this discussion, we will treat the  $\theta$ -dependence of the sextupole and octupole fields in the “kick” approximation. In this approximation, the map for  $1/3$  of a turn can be written immediately in factored form as

$$\mathcal{M}(2\pi/3) = e^{if_2} e^{if_3} e^{if_4} \quad (43)$$

where

$$f_3 = \frac{S_x x^3}{3r_0} \quad \text{and} \quad f_4 = \frac{O_x x^4}{6r_0},$$

and  $O_x$  is the octupole strength; we assume that  $z = 0$ . If we transform  $\mathcal{M}(2\pi/3)$  into normal form, we obtain

$$\begin{aligned} g_3 &= S_x \frac{\sqrt{2}}{4} J_x^{3/2} [e^{3i\varphi_x} + e^{-3i\varphi_x}] \\ g_4 &= 4 [O_x + \kappa S_x^2] J_x^2 \end{aligned} \quad (44)$$

where  $\kappa$  is a factor that comes from “feed-up” from the iterated sextupole field (*i.e.* the generation of higher order nonlinearities or aberrations from the repeated passage through lower order non-linear elements). The octupole component has no resonant term for a 3-fold symmetric machine, but does generate a tune-shift term. Note also that the “feed-up” term is of order  $S_x^2$ . If we neglect the  $g_4$  component for the moment, and carry through the transformation to the co-moving frame as was done in section 4.2, we obtain the pseudo-Hamiltonian and the equations for the fixed points of the one-third integer resonance,

$$h \simeq \delta J_x - S_x \delta \frac{3\sqrt{2} \cos(3\varphi_x) \sin(3\delta)}{4(1 - \cos(3\delta))} + \mathcal{O}(S_x^2), \quad (45)$$

$$\frac{\partial h}{\partial \varphi_x} \simeq \sin(3\varphi_x) = 0,$$

$$\frac{\partial h}{\partial J_x} \simeq 1 - S_x \frac{9\sqrt{2} J_x \cos(3\varphi_x) \sin(3\delta)}{8(1 - \cos(3\delta))} = 0 \quad (46)$$

where  $\delta = 2\pi\ell - k \cdot \mu$  with  $\mathbf{k} = (3, 0)$ , and  $\ell = 1$ . (Here,  $K_1 = J_x$  and  $\phi_1 = 3\varphi_x$ , but it is convenient to work with the original variables) This has the well-known solutions

$$\varphi_x = \{\pi/3, 2\pi/3, 5\pi/3\}, \quad J_x = \left[ \frac{2\sqrt{2}\delta}{3S_x} \right]^2. \quad (47)$$

A phase space plot for the one-third integer resonance is shown in Fig. 2a, where we have truncated the map to third order, *i.e.* only the  $g_3$  term is included. Addition of the octupole component just adds the term  $a_x J_x^2 = 4[O_x + \kappa S_x^2] J_x^2$  to the pseudo-Hamiltonian,  $h$ , Eq. 45. This term is a “tune-shift with amplitude” term (see Eq. 22) and as can be seen from Fig. 2b has a profound effect on the stability of the orbits in this example. (The strength of the octupole was chosen to be very large in the example so as to clearly illustrate the effect.) It is clear from Eq. 46 that the angles of the fixed points are unchanged by addition of the octupole, but their actions are altered. The latter are given by

$$J_x = \frac{9S_x^2 + 32a_x \delta^2 - 3 |S_x| \sqrt{9S_x^2 + 64a_x \delta^2}}{64a_x^2 \delta^2}. \quad (48)$$

Equation 48 reduces to Eq. 47 as  $a_x \rightarrow 0$ . Although there are two solutions to the fixed point equation, Eq. 38, only one of them is physically meaningful.

In this section, we have used simplified models of the magnetic field of a cyclotron in order to illustrate the power of the Lie-algebraic method. In a real cyclotron,  $A_\theta$  is a complicated function of  $\theta$ ,  $r$  and  $z$ . However with  $DA$ , we can accurately calculate the non-linear behaviour to high order, and transform the Taylor series into normal form in the Lie-algebraic representation; this gives us precise values for the tune shifts and resonance driving terms. These terms along with the type of analysis discussed above allows us to analyse and understand the effects of the nonlinearities on the orbit dynamics of the machine in a very sophisticated manner.

## 5. CONCLUSIONS

In conclusion, we believe that the symbiosis of differential algebra and the Lie-algebraic methods provides a box of very powerful tools for analyzing and understanding the orbit dynamics of cyclotrons up to very

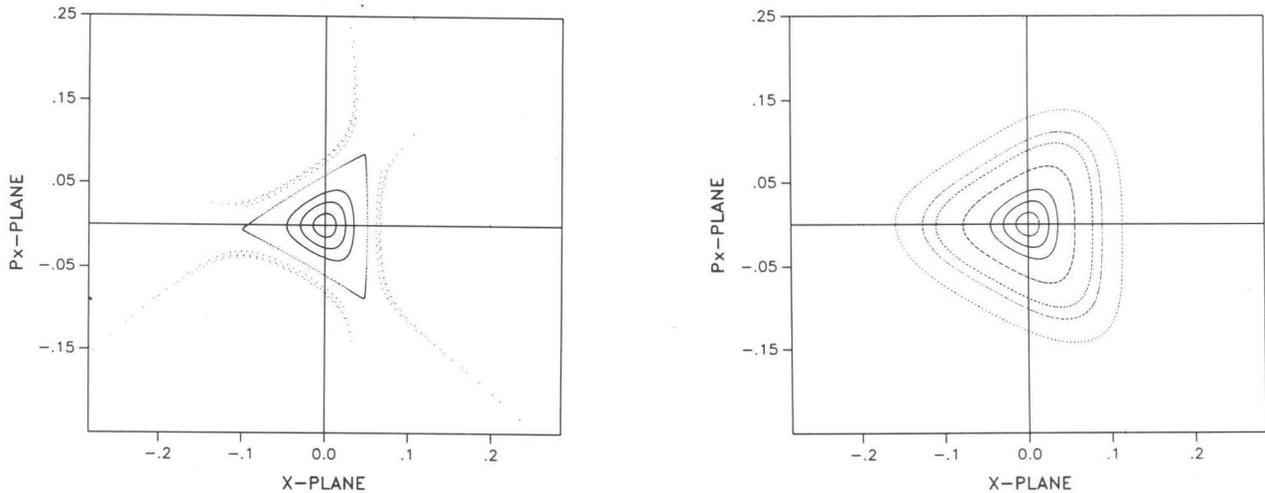


Figure 2. Phase-space plots for the “one-third integer” resonance where  $\nu_x = 1.014$  ( $\mu_x = 0.338(2\pi)$ ) for various values of the initial action,  $J_x$ . a) normalized sextupole strength  $S_x = -0.372$ , and octupole strength  $O_x = 0$ . b)  $S_x = -0.372$ , and  $O_x = -2.0$ .

high orders. Although cyclotrons are only quasi-periodic devices, *maps* still provide significant advantages over tracking in terms of speed, accuracy, and the ability to analyse many orbit-dynamical properties and in particular resonances. The analysis of resonances is accomplished very elegantly by the normal form transformations. Differential algebra is essential for the efficient computation of the maps and of the normal form transformation.

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