SYMPLECTIC INTERPOLATION*

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Abstract

It is important to have symplectic maps for the various electromagnetic elements in an accelerator ring. For some tracking problems we must consider elements which evolve during a ramp. Rather than performing a computationally intensive numerical integration for every turn, it should be possible to integrate the trajectory for a few sets of parameters, and then interpolate the transport map as a function of one or more parameters, such as energy. We present two methods for interpolation of symplectic matrices as a function of parameters: one method is based on the calculation of a representation in terms of a basis of group generators[2, 3] and the other is based on the related but simpler symplectification method of Healy[1]. Both algorithms guarantee a symplectic result.

METHOD I: GROUP GENERATORS

As a starting point, consider a relativistic Hamiltonian[5, 6, 7] written in terms of conjugate coordinates and momenta:

$$\begin{aligned} H &= -P_z = H(x, P_x, y, Py, ct, -U; s) \qquad (1)\\ &= -qA_s - \left(1+\frac{x}{\rho}\right)\\ &\times\sqrt{\left(\frac{U-q\phi}{c}\right)^2 - (mc)^2 - (P_x - qA_x)^2 - (P_y - qA_y)^2}. \end{aligned}$$

This Hamiltonian may be expanded about the design trajectory in a Taylor series:

$$\begin{aligned} H =& H_0 + \sum_{j=1}^{6} B_j X_j + \sum_{j=1}^{6}\sum_{k=1}^{6}(1-\tfrac{1}{2}\delta_{jk})C_{jk}X_jX_k\\ &+ \mathcal{O}(X^3), \quad \text{with} \qquad (2)\\ \mathbf{X}^{\mathrm{T}} =& (\Delta x, \Delta P_x, \Delta y, \Delta P_y, \Delta z, -\Delta U). \qquad (3) \end{aligned}$$

Note that the second derivatives from the quadratic terms form a symmetric matrix with $C_{jk} = C_{kj}$.

Hamilton's equations may be written in the form[7]

$$\frac{dX_j}{dt} = -\sum_k S_{jk}\frac{\partial H}{\partial X_k} \qquad (4)$$

with the group metric chosen to be the usual

$$\mathbf{S} = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & -1\\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \qquad (5)$$

Converting Hamilton's equations into a set of infinitesimal difference equations yields

$$\mathbf{X}_{n+1} = [\mathbf{I} - \mathbf{SC}\Delta t]\mathbf{X}_n, \quad \text{where} \qquad (6)$$

$$C_{jk} = \frac{\partial H}{\partial X_j \partial X_k} = C_{jk}. \qquad (7)$$

Eq. 4 becomes

$$\frac{d\mathbf{X}}{dt} = \mathbf{GX} \quad \text{where} \quad G_{ik} = -\sum_{j=1}^{6} S_{ij}\frac{\partial H}{\partial X_j \partial X_k}. \qquad (8)$$

Here we have expanded about an actual trajectory rather than the design orbit, so the linear B_j terms drop out. Because of the symmetry of $\mathbf{C}$, the matrix $\mathbf{G}$ still only has 21 free parameters for a 6×6 symplectic matrix. It is also worth noting that the trace of $\mathbf{G}$ is zero as expected for any Lie group, and additionally that the three traces of the 2×2-blocks along the diagonal are also each independently zero.

For the case of static magnetic fields with no rf fields we may take

$$\phi = 0 \qquad \text{and} \qquad \frac{\partial \vec{A}}{\partial t} = 0. \qquad (9)$$

Then the eleven elements (six free parameters) with fives in the subscripts of C_{ij} are identically zero, and we are left with only fifteen free parameters. An infinitesimal difference equation for the trajectory in terms of the linear matrix $\mathbf{G}$ is formed by

$$\mathbf{X}_(s_0 + \Delta s) = [\mathbf{I} + \mathbf{G}(s_0)\Delta s]\mathbf{X}(s_0). \qquad (10)$$

If $\mathbf{G}$ is constant over some range $s \in [s_0, s_1]$, then the trajectory may be easily integrated as

$$\mathbf{X}(s) = \lim_{n\to\infty}\left(\mathbf{I} + \mathbf{G}\tfrac{s-s_0}{n}\right)^n = e^{\mathbf{G}(s-s_0)}. \qquad (11)$$

Conversely, any symplectic matrix $\mathbf{M}$ in this representation may be written in the form

$$\mathbf{M} = e^{\mathbf{G}} = e^{-\mathbf{SC}}, \qquad (12)$$

where $\mathbf{C}$ is a symmetric matrix as above.

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By taking the logarithm of the matrices[8] to be interpolated, we end up with only 15 independent parameters (21 for the general 6×6-case) which must be interpolated. So a series of 6×6 transport matrices $\mathbf{M}_i(\vec{v}_i)$ may be interpolated as a function of the parameters $\vec{v}$ by first calculating the set matrices

$$\mathbf{L}_i = -\mathbf{S}\log[\mathbf{M}_i(\vec{v}_i)], \tag{13}$$

to obtain the $C_{jk}(\vec{v}_i)$. The 15 (or 21) functions $C_{jk}(\vec{v}_i)$ are then interpolated to the desired value $\hat{v}$. For example a fit to some appropriate functions (polynomials for example) may be made. Finally the desired transport matrix is then calculated via exponentiation[9]:

$$\mathbf{M}(\hat{v}) = e^{-\mathbf{SC}(\hat{v})}. \tag{14}$$

METHOD II: HEALY'S ALGORITHM

Provided that the transport matrices $\mathbf{M}_i(\vec{v}_i)$ do not have any eigenvalues which are equal to -1 (See Ref. 5.), then a symmetric matrix may be calculated from the symplectic transport matrices:

$$\mathbf{V}_i(\vec{v}_i) = \mathbf{S}[\mathbf{I}-\mathbf{M}_i(\vec{v}_i)][\mathbf{I}+\mathbf{M}_i(\vec{v}_i)]^{-1}. \tag{15}$$

For this new symmetric 6×6 matrix, there are again 21 independent elements; however another six are identically zero as before for static magnetic fields. These elements V_{jk} may be interpolated as for the C_{jk}, and then the desired $\mathbf{M}(\hat{v})$ may be found by the inversion formula

$$\mathbf{M}(\hat{v}) = [\mathbf{I}+\mathbf{SV}(\hat{v})][\mathbf{I}-\mathbf{SV}(\hat{v})]^{-1}. \tag{16}$$

The symmetric matrices $\mathbf{V}$ and $\mathbf{C}$ of the two methods are related by the equation

$$\mathbf{V} = \mathbf{S}\tanh(\mathbf{SC}). \tag{17}$$

FORM OF MATRICES WITHOUT TIME-DEPENDENT FIELDS OR ELECTRIC POTENTIAL

For the case with $\phi = 0$ and $\partial\vec{A}/\partial t = 0$ (i. e. static magnets), the general linear transport matrix obtained from a Hamiltonian of the form of Eq. 1 is

$$\mathbf{M} = \begin{pmatrix} X & X & X & X & 0 & X \\ X & X & X & X & 0 & X \\ X & X & X & X & 0 & X \\ X & X & X & X & 0 & X \\ X & X & X & X & 1 & X \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{18}$$

where the X's are place holders for unknown values. It is clear that the product of two matrices with this form yields another matrix of the same form. In other words, the symplectic matrices with zeros and ones as given in Eq. 4 form a subgroup of the symplectic group Sp(6,r). The $\mathbf{G}$ of Eq. 2 will be similar with all 11 of the elements in the fifth column and last row being zero. (The matrix $\mathbf{M}-\mathbf{I}$ has zeros in the same row and column.)

Since a general transformation from s_0 to s_1 may be obtained as a restricted canonical transformation (see § 3.4 of Ref. [7]), a general transport matrix should have the same form as for an infinitesimal step. It also follows that from the Hamilton's equation:

$$\frac{d(-U)}{d(ct)} = -\frac{\partial H}{\partial(ct)} = 0 \tag{19}$$

at each step along the beam line, all eleven of the C_{ij} with a 5 for either of the indices will be zero. The integration along the finite beam line is then of the form

$$\mathbf{M} = [\mathbf{I}-\mathbf{SC}(s_0)\,ds][\mathbf{I}-\mathbf{SC}(s_0+ds)\,ds]\cdots \tag{20}$$
$$\times\,[\mathbf{I}-\mathbf{SC}(s_1-ds)\,ds,] \tag{21}$$

where in general the $\mathbf{C}(s)$ will evolve along the beam line but still always have the same general form with zeros in the fifth row and column. The resulting transport matrix will be the sum of the identity matrix plus products of the various $\mathbf{SC}(s)$ products which always have zeros in the fifth column and last row. If we then take the logarithm of this transport matrix then the resulting $\mathbf{G}$ will also have zeros in the fifth column and last row.

In the case of the symmetric $\mathbf{V}$ of Method II, since $\mathbf{V}$ is related to the $\mathbf{C}$ by Eq. 3 and the hyperbolic tangent may be expanded in a Taylor series, we find that the fifth column and last row of $\mathbf{V}$ must also contain zeros.

Because a numerical calculation of the second partial derivatives for $\mathbf{M}$ from integration of trajectories through a magnet may yield errors in some elements in the fifth column and last row, one might be tempted to set these elements to the correct zero and one values given in Eq. 4. A better correction might be to first calculate either of the symmetric matrices $\mathbf{C}$ or $\mathbf{V}$ and then to set the fifth column and last row elements identically to zero before inverting the corrected symmetric matrix via the appropriate method to reconstruct the new symplectified transport matrix.

INTERPOLATION OF MATRICES

While the Cayley-Hamilton Theorem[10] could be applied with the characteristic equation for each 6×6 matrix to find a closed solution requiring only multiples of the matrix up to the 5^{th} power in evaluating the logarithm or exponential of the matrix, for this numerical example, it is much simpler to use the brute force expansions:

$$\log\mathbf{M} = \log[\mathbf{I}+(\mathbf{M}-\mathbf{I})] = \sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}(\mathbf{M}-\mathbf{I})^n, \tag{22}$$

$$\mathbf{M} = e^{\mathbf{G}} = \mathbf{I}+\sum_{n=1}^{\infty}\frac{1}{n!}\mathbf{G}^n. \tag{23}$$

It should be noted in particular that the expansion for the logarithm is not absolutely convergent; however for the typical matrices such as those from integration through helical dipoles of snake magnets, these series do converge quickly with a fast computer. To test the algorithms we used a set of matrices calculated for different energies by tracking particles through a model of a helical partial Siberian snake magnet[11] in the AGS. A solenoid was added inside the central region of the helix to minimize the coupling along the trajectory near the spin intrinsic resonance at $G\gamma = Q_v$. For the logarithm, we summed over the first 99 terms of the series (gross overkill), and for the exponential series only the first 19 terms were calculated. Clearly a more careful algorithm could be devised to test for the desired convergence thus minimizing the multiplication of matrices, however this was unnecessary for the present study. If this method were used inside a tracking code to interpolate matrices, then a careful optimization of the code should be performed. However, method II using Healy's algorithm is simpler to calculate and gives essentially the same results as method I with the group generators.

It should be noted that in a helical snake the diagonal blocks for x and y,

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} M_{33} & M_{34} \\ M_{43} & M_{44} \end{pmatrix} \tag{24}$$

respectively, scale reasonably well with $(\beta\gamma)^{-2}$ as expected from a simple consideration of the transverse magnetic field components. The off-diagonal blocks (coupling terms) and dispersion terms, however show a considerable deviation from this simple scaling as would be expected with the extra solenoid superimposed inside the middle of the helical dipole. The amount of the coupling in the resultant matrices were estimated by the determinant $|\mathbf{m} + \mathbf{Sn}^{\mathrm{T}}\mathbf{S}^{\mathrm{T}}|$ in terms of the x-y off-diagonal 2×2-blocks[12, 13, 4]

$$\mathbf{n} = \begin{pmatrix} M_{13} & M_{14} \\ M_{23} & M_{24} \end{pmatrix}, \quad \text{and} \quad \mathbf{m} = \begin{pmatrix} M_{31} & M_{32} \\ M_{41} & M_{42} \end{pmatrix}. \tag{25}$$

Curves for both $\mathbf{V}$ and $\mathbf{C}$ components were fit to polynomials up to 8^{th}-order: The polynomials used for fitting were

$$C_{ij}(\zeta) = \sum_{n=0}^{8} C_{ij,n}\zeta^n, \quad \text{and} \quad V_{ij}(\zeta) = \sum_{n=0}^{8} V_{ij,n}\zeta^n, \tag{26}$$

where

$$\zeta = (\beta\gamma)^{-2a_{ij}}. \tag{27}$$

The a_{ij} was set to 1 for most coefficients, but was set to 0.7 for some elements to improve the fitting to 8^{th} order polynomials by decreasing the slope of the data at low values of $(\beta\gamma)^{-2}$, otherwise a higher order polynomial would have been necessary.

SUMMARY

Both these methods work quite well, although the second method is simpler in that it only requires matrix inversion rather than exponentiation and taking the logarithm of matrices. It should be noted that the matrix logarithms are only required to determine the constants of the interpolations formulae for the $C_{jk}(v_i)$; then only exponentiation of $\mathbf{SC}$ would be required for tracking. Since both methods reduce the symplectic matrix to a symmetric matrix, the same number of interpolation formulae are required for each method. Both these methods automatically guarantee symplectic results without any additional pass through a symplectification algorithm.

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REFERENCES

[1] L. M. Healy, *Lie Algebraic Methods for Treating Lattice Parameter Errors in Particle Accelerators*, Doctoral thesis, University of Maryland, unpublished (1986).

[2] Robert Gilmore, *Lie Groups, Lie Algebras, and Some of Their Applications*, John Wiley and Sons, New York (1974).

[3] A. J. Dragt, "Lectures on Nonlinear Orbit Dynamics", *Physics of High Energy Accelerators'* (Fermilab Summer School, 1981), AIP. Conf. Proc. 87, R. A. Carrigan, F. R. Huson, and M. Month, editors (1982).

[4] W. W. MacKay, "Comment on Healy's Symplectification Algorithm", These Proceedings.

[5] E. D. Courant and H. S. Snyder, "Theory of the Alternating-Gradient Synchrotron", *Ann. Phys.*, **3**, 1 (1958).

[6] R. Ruth, "Single Particle Dynamics and Nonlinear Resonances in Circular Accelerators", SLAC-PUB-3836 (1985).

[7] Mario Conte and William W. MacKay, *An Introduction to the Physics of Particle Accelerators*, World Sci., (1991).

[8] Sheung Hun Cheng et al., "Approximating the Logarithm of a Matrix to Specified Accuracy", SIAM J. Matrix Anal, Appl., **22**, 1112 (2001).

[9] Cleve Moler and Charles van Loan, "Nineteen Dubious Ways to Compute the Exponential of a Matrix", SIAM Rev. **20**, 801 (1978).

[10] Roger A. Horn and Charles R. Johnson, *Matrix Analysis*, Cambridge University Press, Cambridge (1985).

[11] A. U. Luccio, et al., "Cold AGS Snake Optimization by Modeling", C-A/AP/128 (2003).

[12] L. C. Teng, "Concerning n-Dimensional Coupled Motions", FN-229 0100, National Accelerator Laboratory, Batavia, IL (1971).

[13] D. A. Edwards and L. C. Teng, *IEEE Trans. on Nucl. Sci.*, NS-20, no. 3, 885 (1973).