An introduction to spin-orbit tracking

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- The problem:
  realistic simulation of spin-orbit motion for very large numbers of turns in a storage ring: bending magnets, quadrupoles, sextupoles, ...
- Why simulation?
  to assist design, to optimize performance, to lower costs (of machine time), diagnostics, analysis, avoid disasters, ...
- Tools:
  numerical solution of the EOMs for orbit and spin
- Challenges:
  speed (computing power), maintaining precision and symmetries (symplecticity, orthogonality).
- Various cases:
  for the orbit: large/small beam sizes, high/low curvature
  for spin: large/small beam sizes, high/low energies
- Including party-spoiling "extras":
  space charge, wake fields, ...

Literature

- M. Berz: "Modern Map Methods in Particle Beam Physics"
- A. Dragt: "Lie Methods for Nonlinear Dynamics with Applications to Accelerator Physics"
- É. Forest (for adventurers): "Beam Dynamics: a New Attitude and Framework"
- H. Goldstein (for nostalgics): "Classical Mechanics"
- G.H. Hoffstaetter: "High-Energy Polarized Proton Beams: a Modern View"
- G.V. José and E.J. Saletan: "Classical Dynamics: a Contemorary Approach"
- R. Talman: "Geometric Mechanics"
- M.Vogt, PhD thesis (2000): "Bounds on the Maximum Attainable Equilibrium Spin Polarisation of Protons at High Energy in HERA"

The starting points:

- The Lorentz force equation (LFE) describes the *orbital* motion of particles in magnetic and electric fields:

$$\frac{d\vec{p}}{dt} = e(\vec{E} + \vec{v} \times \vec{B})$$

- The Thomas-BMT equation for spin precession, including the effect of EDM, for the rest frame single-particle spin expectation value:

$$\frac{d\vec{S}}{dt} = \vec{\Omega} \times \vec{S}\,, \quad \vec{\Omega} = \vec{\Omega}_M + \vec{\Omega}_D$$

Magnetic dipole plus Thomas precession $(a = (g-2)/2)$:

$$\vec{\Omega}_M = -\frac{e}{m\gamma}\left[(a\gamma + 1)\,\vec{B} - a(\gamma - 1)(\hat{\beta}\cdot\vec{B})\hat{\beta} - \frac{\beta\gamma}{c}\left(a + \frac{1}{1+\gamma}\right)(\hat{\beta}\times\vec{E})\right]\,,$$

Electric dipole:

$$\vec{\Omega}_D = -\frac{e\eta}{2m}\left[\vec{E} - \frac{\gamma}{\gamma+1}\vec{\beta}(\vec{\beta}\cdot\vec{E}) + c\vec{\beta}\times\vec{B}\right]\,.$$

Part 1:
a short survey of relevant classical mechanics

Equations of particle motion (EOM)

Significant gains accrue by replacing the LFE by the equivalent Hamiltonian:

$$H = \sqrt{m^2c^4 + (\vec{p} - e\vec{A})^2c^2} + e\psi$$

Time is not the natural independent variable in accelerators: magnets are fixed, but flight times vary. So transform to a Hamiltonian wrt the curvilinear (natural) coords of the ring and distance s around the ring as the independent variable. In a frame with curvature κ in the horizontal plane,

$$H = -(1+\kappa x)\sqrt{(p_\tau - e\psi)^2/c^2 - m^2c^2 - (\vec{p}_\perp - e\vec{A}_\perp)^2} - e(1+\kappa x)A_s$$

The dynamical variables

$$u \equiv (q,p) \equiv (x, p_x,\ y, p_y,\ \tau = -t,\ p_\tau = m\gamma c^2)$$

EOM

$$\frac{dx}{ds} = \frac{\partial H}{\partial p_x}, \quad \frac{dp_x}{ds} = -\frac{\partial H}{\partial x}, \quad \text{etc.}$$

Poisson brackets:

$$\{f,g\} = \sum_{i=1\,..\,3}\left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\right)$$

Fundamental Poisson brackets:

$$\{x, p_x\} = 1 \quad \text{etc.}$$

EOM

$$\frac{du_a}{ds} = \{u_a, H\} = -\{H, u_a\} \equiv -:H: u_a$$

In general, for a dynamical function g,

$$\frac{dg}{ds} = \{g, H\} + \frac{\partial g}{\partial s} = -:H: g + \frac{\partial g}{\partial s}$$

Solutions of the EOM: maps

- The solutions of the EOM can be represented as maps:
$$(q^f, p^f) = \mathcal{M}(s^f, s^i; q^i, p^i)$$
- Composition of maps, e.g. from magnet to magnet
$$\mathcal{M} = \mathcal{M}_n \circ \cdots \mathcal{M}_2 \circ \mathcal{M}_1$$
One-turn map (OTM): transport from s_0 to $s_0 + C$. In general complicated functions.
- The dynamic variables are scaled to be small. So perhaps Taylor expansions will do. Perturbative methods and linearisation.
- The map $\mathcal{M}$ is a *canonical transformation!* (CT) i.e. the (q^f, p^f) preserve the fundamental Poisson brackets where we differentiate wrt either the original or the final (q, p). The Hamilton equations look the same, too.
- If known exactly, the OTM would tell us almost everything we need to know — but it's usually impossible to get a closed analytical expression!
- The Poincaré section — a stroboscopic view of (q, p) using the OTM — shows us the topology of phase space. It tells us about stability ....

A Poincaré section

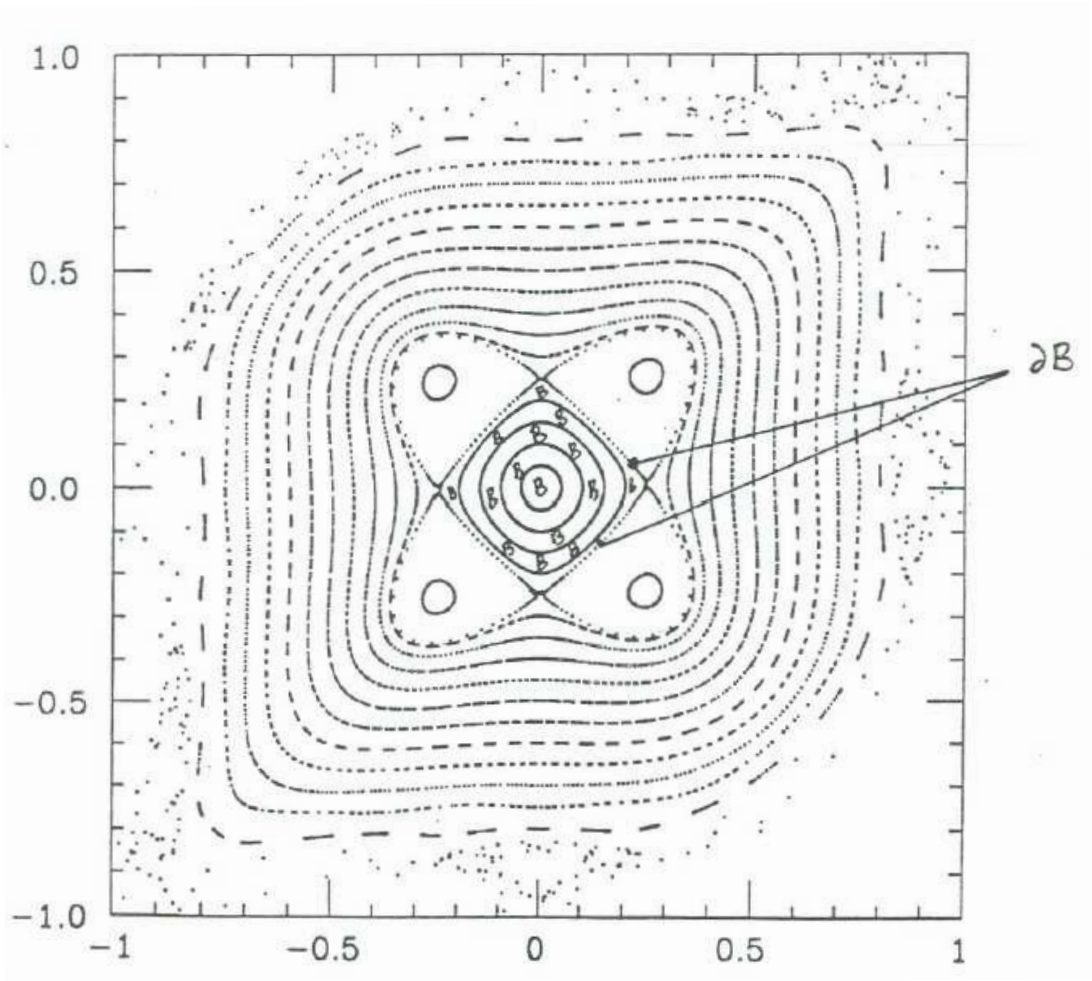


Figure 1: E. Forest, J. Irwin, LBL 28931, 1990. A Poincaré section for 1-dim motion of scaled (x, p_x)

Symmetries, symplectic geometry, conservation laws

- The Jacobian of a CT $u^i \to u^f$ is *symplectic* (Hermann Weyl: "The Classical Groups") i.e.

$$(Jac\,\mathcal{M})^T J\,(Jac\,\mathcal{M}) = J$$

$$J = \begin{pmatrix} J_2 & 0_2 & 0_2 \\ 0_2 & J_2 & 0_2 \\ 0_2 & 0_2 & J_2 \end{pmatrix}, \quad J_2 = \begin{pmatrix} 0 & +1 \\ -1 & 0 \end{pmatrix}, \quad 0_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

  Compositions of $\mathcal{M}$s are symplectic $\to$ CTs are representations of the *symplectic group*! Compare with SO(3): $(Jac\,\mathcal{M})^T(Jac\,\mathcal{M}) = I$.

- If the EOM are linearized: $du/ds = Au$ where A is a 6x6 matrix. If A is independent of s, then

$$u^f = \exp[(s^f - s^i)A]u^i \to u^f = M(s^f, s^i)u^i \text{ and } Jac(\mathcal{M}) = M(s^f, s^i)$$

  is symplectic. Note that

$$M(s_n, s_1) = M(s_n, s_{n-1}) \cdots M(s_2, s_1)$$

- Infinitesimal canonical trans: $M(s+\epsilon) = I + \epsilon \sum_{i=1}^{21} a_i G_i$ where the G_i are infinitesimal generators of the 21-dimensional Lie algebra sp(6) of the 6x6 symplectic matrix group. $\{G_i, G_j\} = c_{ijk} G_j$ with structure constants c_{ijk}

/Continued...

- We can write $M = \exp(JS_a)\exp(JS_c)$ where S_c, S_a commute/anti-commute with J. Compare with $\mathrm{SO}(3)$ later.
- Poincaré invariants: e.g. CTs preserve the volume of phase space. Liouville-like.
- Jacobi identity: for any functions a, b, c, $\{a,\{b,c\}\} + \{b,\{c,a\}\} + \{c,\{a,b\}\} = 0$
  $\Longrightarrow$ Poisson brackets form an infinite-dimensional Lie algebra on *functions*.
- Phase-space vectors have zero length: $u^T J u = 0$: symplectic geometry.
- Symplectic geometry + topology: a newish field. Implies strong constraints on outcomes of CTs: Mikhail Gromov's "*no squeezing theorem*" (Abel prize, 2009), the case of the symplectic camel! Connection to the Heisenberg Uncertainty Principle (M.A. de Gosson)?
- Modern differential-geometrical formulations: not here.

A symplectic camel

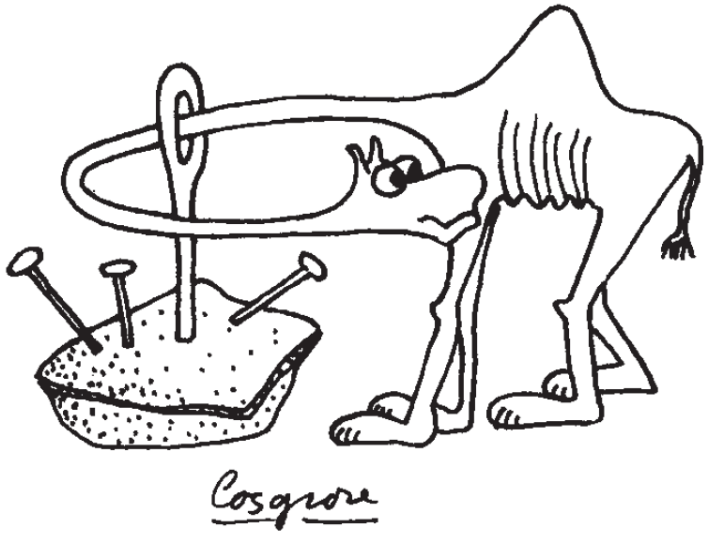


Figure 2: Ian Stewart, New Scientist 1989

For symplectic eggs see M.A. de Gosson: arXiv:1208.5969

Part 2:

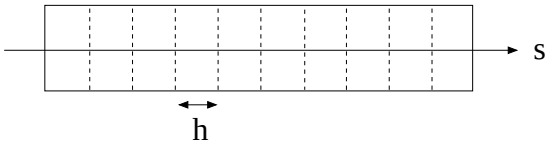
Calculating trajectories quickly over very many turns

The basic problem: $du/ds = F(u,s) = \{u, H\}$.

Best to use canonical variables associated with the Hamiltonian and symplectic integrators to ensure that the transport is canonical (symplectic): the volume of phase space is automatically conserved, so can distinguish between real and artificial particle loss! Control!

If we arrange for the canonical variables to be "small", then truncating a Taylor expansion is not too dangerous: perturbation theory.

Usually use step-by-step integration through magnetic elements.



Maintaining symplecticity, i.e. keeping the solutions on the right manifold, is an example of *geometric integration*. Large literature.

Possibilities:

- Runge-Kutta integrators can handle s-dependent F, but they're not necessarily symplectic. Small step size h and high order provide only approximate symplecticity.

  Symplectic Runge-Kutta integrators require solving implicit equations at each step. Potentially *very* slow!

- For autonomous cases, $F(u,s) \to F(u)$ (e.g. wrt the axis in a quadrupole):
  Taylor expansions using *Lie derivatives* $\mathcal{L}_F$:

$$\frac{du}{ds} = \mathcal{L}_F\, u = F(u) \cdot \nabla_u u$$

  For Hamiltonian systems, this becomes

$$\frac{du}{ds} = \{u, H\} = -:H:\, u$$

  where we define the *Lie operator* $:H: \equiv \{H, \ \ \}$ — a "Poisson bracket waiting to happen". Then

$$u^f = \exp[(s^f - s^i)\mathcal{L}_F]\, u^i = \sum_{j=0}^{\infty} \frac{(s^f - s^i)^j}{j!} (\mathcal{L}_F)^j\, u_i$$

  and

$$u_f = \exp\big[-(s^f - s^i)\, :H(u^i):\big]\, u^i$$

Poisson brackets form a Lie algebra. Then with the Baker-Campbell-Hausdorf (BCH) theorem and operators $:A:$ and $:B:$,

$$e^{h:A:}e^{h:B:} = e^{:C:}$$

where $:C:$ contains only $:A:$, $:B:$, and their multiple commutators.

$$C = h:A: + h:B: + \frac{h^2}{2}\{:A:, :B:\} + O(h^3)\ldots.$$

The full expansions are explicitly symplectic and provide extensive tools for concatenating maps of magnets: Dragt et al. Analysis!

But! we can handle only a finite number of terms in expansions.

Then symplecticity is lost and *restoration, symplectification* (= fabrication?) are needed to build a symplectic map which is close to the original one: moving the solutions back onto the required manifold.

E.g., from a slightly non-symplectic map, we can construct a mixed-variable generating function which gives a symplectic approximation to the original map.

E.g., construct products of simple (easy-to-compute) symplectic maps which reproduce the terms of a Taylor map correct through a given order. (But higher-order hopefully small.)

Restoration is usually equivalent to a *small modification of the Hamiltonian.*

CARE NEEDED to avoid self deception.

Or make approximate symplectic models from the start! instead of symplectifying an approximate map from the exact EOM: *splitting.*

Splitting:

Work with approximate maps which are exactly symplectic *from the start.*

Consider for example $H(q,p) = H_1(q) + H_2(p)$, e.g. $H(q,p) = V(q) + T(p)$

Make the subdivision into H_1 and H_2 and compute an approximate map in the *symmetric* form

$$e^{\frac{h}{2}:H_1:} e^{h:H_2:} e^{\frac{h}{2}:H_1:}$$

which can be evaluated exactly: the expansion cuts off or can be written using simple known functions.

Can show that

$$e^{\frac{h}{2}:H_1:} e^{h:H_2:} e^{\frac{h}{2}:H_1:} = e^{:hH_1+hH_2+O(h^3):}$$

The effective Hamiltonian differs from the real one by $O(h^3)$: a *2nd order symplectic integrator.*

Using Zassenhaus formulæ: the reverse of BCH formulæ.

For a quadrupole:

$$H = -\sqrt{p_\tau^2/c^2 - m^2c^2 - p_x^2 - p_y^2} \; - \; eg\frac{1}{2}(x^2 - y^2)$$

With $H_1(p) = T(p)$ and $H_2(q) = V(q)$, this is equivalent to DRIFT-KICK-DRIFT: a sharp change in p_x, p_y at the centre.

Or rearrange the terms in H : $H = H_M + H_K$ with $H_M \equiv$ pure linear quadrupole and $H_K \equiv$ a special drift which effectively shifts x and y at the centre: MATRIX-KICK-MATRIX which is good for spin.

- More complicated symmetric arrangements give 4th, 6th, 8th order symplectic integrators: Forest, Ruth, Neri, Yoshida, ...
- Can get negative lengths: some are uncomfortable with that.
- Care with phase advances. E.g. fit the parameters to the exact map before long term tracking.
- Fast! often called *Kick codes*.
- Energy ripples.: no guarentee of exact total energy conservation.
- CARE NEEDED to avoid self deception.

Can calibrate by comparing outcomes of the various approaches with the Poincaré section of a very high order Taylor map – but one should *not* do long-term tracking with Taylor maps!

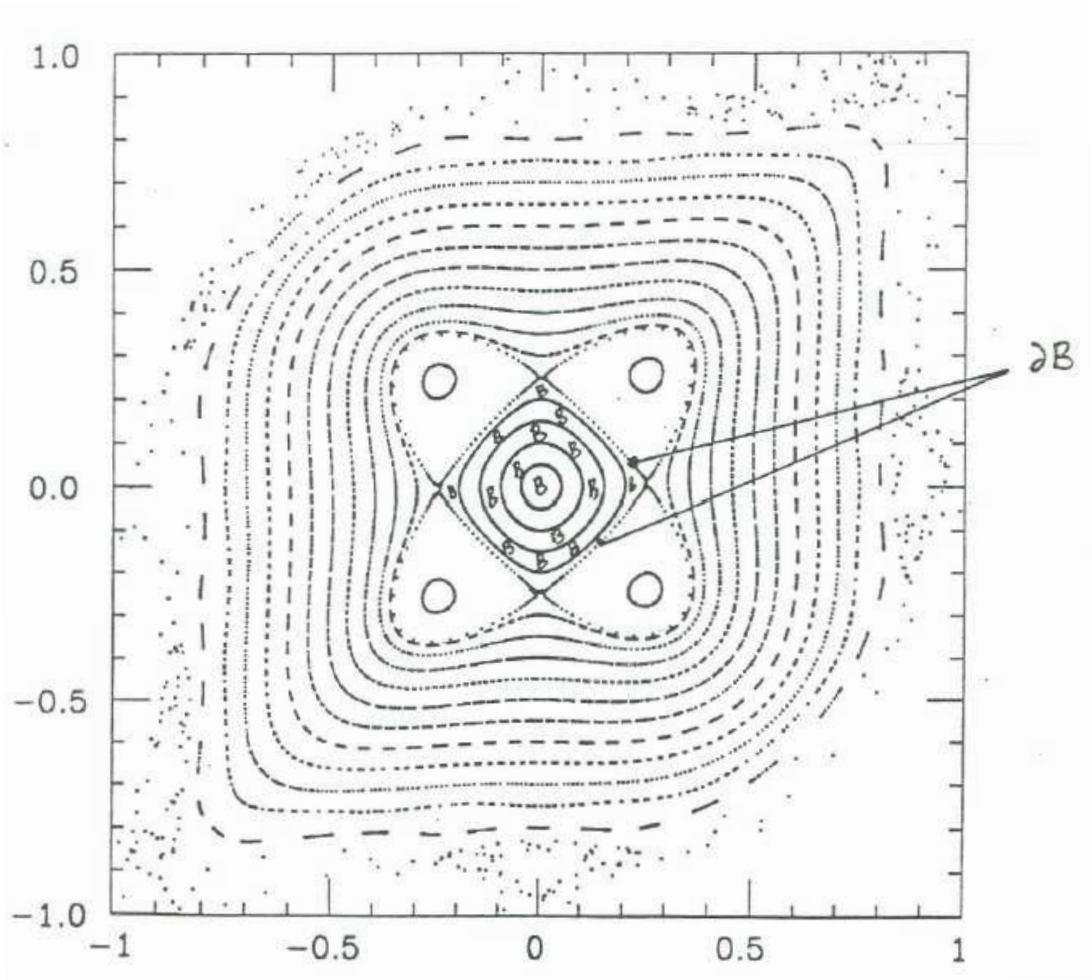


Figure 3: E. Forest, J. Irwin, LBL 28931, 1990. A Poincaré section for 1-dim motion of scaled x, p_x

TPSA and DA

- Evaluating sufficient terms and concatenating multidimensional Taylor maps of single elements needs a fast automatic system of handling power series.
- Recall vector multiplication, matrix multiplication etc: algebraic systems *designed* to deliver the required results when the algabraic rules are followed.
- Truncated power series algebra (TPSA): an algebraic structure to handle the concatenation of Taylor series and up to chosen orders.
- Differential algebra (DA), Berz et al.: extends TPSA to include operations of the calculus.
- Together: very powerful tools to evaluate (say) the $\exp[(s^f - s^i)\mathcal{L}_F]\, u^i$, to get Taylor series out of functions, to get Taylor series out of a splitting algorithm or a Runge-Kutta algorithm, to invert maps, to solve equations, ...

  The essential component for modern tracking and analysis!.

  The basis of code COSY-Infinity (M. Berz); used also in PTC/FPP (É. Forest), BMAD (D. Sagan), MaryLie (A.J. Dragt)

Part 3: bringing spin on board

Spins are passengers with no democratic rights (we are ignoring Stern-Gerlach).

$$\frac{d\vec{S}}{ds} = \vec{\Omega}(u,s) \times \vec{S}$$

$$\frac{d}{ds}\begin{pmatrix} S_x \\ S_y \\ S_s \end{pmatrix} = \begin{pmatrix} 0 & -\Omega_s & \Omega_y \\ \Omega_s & 0 & -\Omega_x \\ -\Omega_y & \Omega_x & 0 \end{pmatrix}\begin{pmatrix} S_x \\ S_y \\ S_s \end{pmatrix} = A_{3\times 3}\begin{pmatrix} S_x \\ S_y \\ S_s \end{pmatrix} = A_{3\times 3} S\,,$$

$A = \nu\,\hat{\boldsymbol{b}}\cdot\vec{\boldsymbol{L}} \equiv \vec{\boldsymbol{\Omega}}\cdot\vec{\boldsymbol{L}}$ where the L_i are infinitesimal generators in the LA $so(3)$.

$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad L_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad L_s = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

For s-independent $\vec{\Omega}$,

$$S^f = R_{3\times 3}(s^f, s^i)\, S^i \equiv e^{(s^f - s^i)A}\, S^i$$

$$R(s^f, s^i) = I + \hat{b}\cdot\vec{L}\sin\left[(s^f - s^i)\,\nu\right] + (\hat{b}\cdot\vec{L})^2\left(1 - \cos\left[(s^f - s^i)\,\nu\right]\right)$$

The exponential of an anti-symmetric matrix is orthogonal ($R^T R = I$): preserves lengths of spins. C.f., $SU(2)$: exponentiated anti-Hermitian matrices are unitary.

But even for autonomous orbital motion, the EOSM are **not** autonomous:

First thoughts:

- $$R_{3\times 3}(s^f, s^i;\, u^i) = \exp \int A(u(s), s) ds$$

  with s - ordering, i.e., a Dyson expansion

- $$R_{3\times 3}(s^f, s^i;\, u^i) = \exp\Big(\int A(u(s), s) ds + \int \{A(u(s_1), s_1), A(u(s_2), s_2)\}\, ds_1\, ds_2 + \cdots \Big)$$

  i.e., a Magnus expansion. Again have s - ordering but the commutators belong to $\mathrm{so}(3)$ and the exponent is always anti-symmetric, even if the series is cut off!

These are sensible only if A is small.

So write $\vec{\Omega}(u, s) = \vec{\Omega}_0(s) + \vec{\omega}(u, s)$ and transform to a rotating reference frame where $\vec{\Omega}_0$ is transformed away and only the small (?) $\vec{\omega}$ remains: a kind of *interaction picture*.

A is replaced be $\tilde{A}$, depending just on $\vec{\omega}$.

Orthogonality is essential! so it would be good to work with anti-symmetric exponents as in the Magnus expansion, but its just too messy beyond the 2nd commutator and double integral.

Analogy with splitting for the orbital motion: manipulate **exponents** to ensure symplecticity.

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Use the first integral in my SLICKTRACK and EpsSLICK but then with unit quaternions, $(r_0, \vec{r})$, to save time and with an intelligent choice of coordinate system for spin!!!!

$$\exp \frac{\theta}{2}\hat{b}\cdot\vec{\sigma} = I_{2\times 2}\cos(\theta/2) - i\vec{\sigma}\cdot\hat{b}\sin(\theta/2) \quad \equiv \quad I_{2\times 2}\, r_0 - i\vec{\sigma}\cdot\vec{r} \quad \text{with} \quad \sum_{i=0}^{3} r_i^2 = 1$$

Quaternion concatenation:

$$(a_0,\, \vec{a})\ (b_0,\, \vec{b}) = (a_0 b_0 - \vec{a}\cdot\vec{b},\, a_0\vec{b} + \vec{a}b_0 + \vec{a}\times\vec{b}) = (c_0,\, \vec{c})$$

$$R_{ij} = (2r_0^2 - 1)\delta_{ij} + 2r_i r_j + 2r_0\epsilon_{ijk}r_k$$

R is automatically orthogonal.

Capitulation!

- Brute force Runge-Kutta and, if necessary, renormalize the lengths of the spins on each turn.
- Develop Taylor series at high order for R and massage it to make it exactly orthogonal.
  Experience at DESY showed the Taylor expansions can be tricky for protons at very high $\nu_0 \approx \frac{g-2}{2}\gamma$
- Slot orthogonal spin matrices in at the centres of slices or between slices used for orbital tracking. For example use $R = \exp(hA)$ with A defined by the (u, s) at the centre or ends of a slice.
- For protons at high energy ($\nu_0 \approx 10^3$), naïve approaches employ very many slices (small stepsize h) to get precision: $\Rightarrow$ inefficient. For very low energy ν_0 is O(1). Then Taylor expansions should be fine.
- **Recent very careful work at the Tech-X corporation (D. Abell + D. Meiser)** for BNL with SPINK $\rightarrow$ TEASPINK, and porting to GPUs.
  Using quaternions to get R. MATRIX-KICK-MATRIX model in the quadrupoles, and exact integration in bends.
  Overcome the problem of many slices for spin integration by Richardson extrapolation (Romberg algorithm — special sampling and averaging) to reduce the number of slices by **orders of magnitude**. Huge increase in speed.
- PTC/FPP (É. Forest) now includes spin dynamics. It tracks both orbit and spin using geometric integration. PTC obtains spin maps about realistic closed orbits using polymorphism: $\Rightarrow$ analysis!

Further Remarks

- Balance speed and precision; and provide analysis capabilities (e.g. normal forms).
- Exploit GPUs.
- But for EDM simulations, we might need quadruple precision.
- EDGE fields!!! : C.f. the effect of dipole edge fields for deuteron spin flipping with RF dipoles.
- We need at least two codes for comparisons, and careful evaluation of results.
- Static electric fields are novel in the context of spin. S.R. Mane, *NIMA* (Sept. 2012).
- Static electric fields: conservation of total energy.
- We require much longer-term tracking than at (say) the LHC.
  Symplectic and orthogonal tracking is essential.
- Understand the single-particle orbital and spin motion before adding space charge, etc.
- The magnetic dipole effects must be very well simulated. Otherwise we cannot see the influence of an EDM.

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- Also **spin normal forms**: the invariant spin field (ISF), the amplitude dependent spin tune (ADST).
  The spread, over orbital amplitudes, of the ADST will determine the rate of decoherence of spins in the machine plane. Use standard modern tools to minimise the spread, thereby decreasing the rate of decoherence.
- A job for experienced people.

Thanks to Dan Abell, Jim Ellison, Étienne Forest, Klaus Heinemann, Georg Hoffstaetter, Mathias Vogt.