# Hamiltonian Dynamics Lecture 2

David Kelliher

ISIS/Rutherford Appleton Laboratory November 13<sup>th</sup>, 2024

#### Deriving the Hamiltonian for an accelerator

- Goal: build a Hamiltonian map to represent entire ring.
- Starting point the Hamiltonian for a relativistic particle in an electromagnetic field H(q,P,t).

$$H(q, P, t) = c\sqrt{m^2c^2 + (\mathbf{P} - e\mathbf{A})^2} + e\phi$$

- Apply following steps
  - 1. Transform into convenient coordinates (Frenet-Serret).
  - 2. Change the independent variable from time to longitudinal coordinate "s".
  - 3. Convert to small dynamic variables with respect to reference momentum (allows us to expand the square root).
  - 4. Introduce convenient longitudinal coordinates.

#### Particle in a general electromagnetic field

• The Lagrangian for a free particle in a general EM field  $U(x, \dot{x}, t) = e(\phi - \mathbf{v} \cdot \mathbf{A})$  is given

$$L(x, \dot{x}, t) = -mc^2\sqrt{1-\beta^2} - e\phi + e\mathbf{v} \cdot \mathbf{A}$$

• Calculate the conjugate momentum as usual. Note the vector potential contributes to the momentum!

$$P_i = \frac{\partial L}{\partial \dot{x}_i} = \frac{m \dot{x}_i}{\sqrt{1 - \beta^2}} + eA_i$$

• The Hamiltonian is given by

$$H(q, P, t) = \sum_{i} P_i \dot{q}_i - L = \frac{mc^2}{\sqrt{1 - \beta^2}} + e\phi.$$

which can be written (using  $\frac{mc^2}{\sqrt{1-\beta^2}} = \gamma mc^2 = c\sqrt{m^2c^2 + \mathbf{p}^2}$  )

$$H(q, P, t) = c\sqrt{m^2c^2 + (\mathbf{P} - e\mathbf{A})^2} + e\phi$$

#### Step 1: Change coordinate system



Along a reference orbit  $r_0$ , define set of orthogonal unit vectors  $\hat{s}$ ,  $\hat{x}$ , $\hat{z}$ . These vectors form the basis of the Frenet-Serret curvilinear coordinate system.

$$\mathbf{\hat{s}}(s) = \frac{d\mathbf{r_0}(s)}{ds}, \quad \mathbf{\hat{x}}(s) = -\rho(s)\frac{d\mathbf{s}(s)}{ds}, \quad \mathbf{\hat{z}}(s) = \mathbf{\hat{x}}(s) \times \mathbf{\hat{s}}(s)$$

where  $\rho(s)$  is the local curvature.

In order to express the conjugate momentum **P** and vector potential **A** in these coordinates perform a canonical transformation. It can be shown that the resulting Hamiltonian is

$$H(s, x, z, p_s, p_x, p_z, t) = c \sqrt{m_o^2 c^2 + \frac{(p_s - eA_s)^2}{\left(1 + \frac{x}{\rho}\right)^2} + (p_x - eA_x)^2 + (p_z - eA_z)^2} + e\phi$$

#### Step 2: Change of independent variable

- It is convenient to change the independent variable from time t to location around the ring ("s").
- To do this, rearrange equation so that  $-p_s$  is on the LHS. Define this the new Hamiltonian  $H_{1.}$

$$H_1 = -p_s = -eA_s - \left(1 + \frac{x}{\rho}\right)\sqrt{\frac{1}{c^2}(H - e\phi)^2 - m^2c^2 - (p_x - eA_x)^2 - (p_z - eA_z)^2}$$

• Now the old Hamiltonian is one of the canonical variables which are now

$$(x, p_x), (y, p_y), (-t, H)$$

• Since the independent coordinate is now in units of distance rather than time, the equations of motion are written

$$t' = \frac{\partial p_s}{\partial H}, \quad x' = -\frac{\partial p_s}{\partial p_x} \quad z' = -\frac{\partial p_s}{\partial p_z}$$
 $H' = -\frac{\partial p_s}{\partial t}, \quad p'_x = \frac{\partial p_s}{\partial x} \quad p'_z = \frac{\partial p_s}{\partial z}$ 

#### Step 3: Introduce reference momentum

 Normalise variables with respect to reference momentum P<sub>0</sub>. Usually, we can assume small deviations from the reference momentum.

$$p_i \to \tilde{p_i} = \frac{p_i}{P_0}, \ H_1 \to \tilde{H} = \frac{H_1}{P_0}, \ A_i \to \mathbf{a} = e\frac{A_i}{P_0}, \ e_i \to \frac{E}{P_0}, \ \varphi = \frac{q_0}{P_0 c}\phi$$

• Updated Hamiltonian (where  $h = 1/\rho$ )

$$ilde{H} = -(1+hx)\left(\sqrt{\left(rac{e}{c} - arphi
ight)^2 - rac{1}{eta_0^2\gamma_0^2} - ( ilde{p_x} - a_x)^2 - ( ilde{p_y} - a_y)^2} + a_s
ight)$$

• Note – in the following slides the tilde is omitted.

#### Step 4: Change longitudinal coordinates

• Beam has a time and energy spread around a reference particle. Introduce scaled time deviation  $\tau$  and energy deviation  $p_{\tau}$ . Note: here we follow the nomenclature of the Xsuite Physics guide (page 9)\*

$$au = rac{s}{eta_0} - ct, \, \, p_ au = rac{1}{eta_0} rac{E - E_0}{E_0}$$

• The Hamiltonian for a general accelerator element  $H(x, p_x, y, p_y, \tau, p_\tau)$  is given by

$$H = \frac{p_{\tau}}{\beta_0} - (1 + hx) \left( \sqrt{\left( p_{\tau} + \frac{1}{\beta_0} - \varphi \right)^2 - \frac{1}{\beta_0^2 \gamma_0^2} - (p_x - a_x)^2 - (p_y - a_y)^2} + a_s \right)$$

• When  $\varphi$  is zero (e.g. in magnets) the Hamiltonian simplifies to ( $\delta = dp/p$ )

$$H = \frac{p_{\tau}}{\beta_0} - (1 + hx) \left( \sqrt{(1 + \delta)^2 - (p_x - a_x)^2 - (p_y - a_y)^2} + a_s \right)$$

• The Hamiltonian for each magnet can be found by substituting the corresponding vector potential

#### \* https://xsuite.readthedocs.io/en/latest/index.html

#### Multipole magnets



FIG. 4. Normal and skew 2*n*-pole magnets in Cartesian coordinates. Each figure shows magnetic (electric) field streamlines and poles' shape in transverse cross section. North (positive electrostatic potential) and south (negative electrostatic potential) poles are shown in red and blue and are given by  $(\mathcal{B}, \mathcal{A})_n = \mp R_p^n$  respectively, where  $R_p$  is the distance to the pole's tip.

• The ideal magnetic field for a straight multipole magnet with axial symmetry is

$$B_x + iB_y = -\frac{\partial A_s}{\partial x} + i\frac{\partial A_s}{\partial y} = \mathcal{R}\sum_{n=1}^{\infty} (b_n + ia_n)\frac{(x+iy)^{n-1}}{r_0}$$

#### Dipole magnet (sector) – vector potential



Normal dipole

$$B_x = 0, \quad B_y = B_y$$

• Aim to have a constant vertical field only along the design orbit. Note that in general the curl in curvilinear coordinates is given by

$$B_x = [\nabla \times A]_x = \frac{\partial A_s}{\partial y} - \frac{1}{1+hx} \frac{\partial A_y}{\partial s}$$
$$B_y = [\nabla \times A]_y = \frac{1}{1+hx} \frac{\partial A_x}{\partial s} - \frac{h}{1+hx} A_s - \frac{\partial A_s}{\partial x}$$
$$B_s = [\nabla \times A]_s = \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}$$

• The following vector potential results in desired dipole field

$$A_x = 0, \quad A_y = 0, \quad A_s = -B_y \left( x - \frac{hx^2}{2(1+hx)} \right)$$



#### Dipole magnet – Hamiltonian

• Substitute the vector potential for a sector dipole to obtain the exact Hamiltonian

$$H = rac{p_{ au}}{eta_0} - (1+hx)\sqrt{\left(1+\delta
ight)^2 - p_x^2 - p_y^2} + k_0\left(x+rac{hx^2}{2}
ight)$$

where the normaliszed dipole strength  $k_0$  is defined as  $k_0 = eB_y/p$ 

Assuming small dynamics variables , series expand the square root term to first order (Xsuite manual Eqn. 1.53).

$$H \approx \frac{p_{\tau}}{\beta_0} + \frac{1}{2} \frac{p_x^2 + p_y^2}{1 + \delta} - (1 + hx)(1 + \delta) + k_0 \left(x + \frac{hx^2}{2}\right)$$

• This approximation makes the equation of motion more tractable. The higher order terms that are ignored are known as *kinematic terms*.

#### Dipole magnet – Hamiltonian observations

$$H \approx \frac{p_{\tau}}{\beta_0} + \frac{1}{2} \frac{p_x^2 + p_y^2}{1 + \delta} - (1 + hx)(1 + \delta) + k_0 \left(x + \frac{hx^2}{2}\right)$$

• Applying the equations of motion, the  $(k_0 - h)x$  term leads to a change in momentum.

$$p'_x = \frac{\partial H}{\partial x} = k_0 - h$$

This is zero so long as  $k0 = h = 1/\rho$ , i.e. the  $p_x$  is unchanged if the magnet strength matches the design orbit!

- Next, look at the term  $hk_0x^2/2$ . This is the potential energy term of a harmonic oscillator. Even in a uniform magnetic field, particles tend to oscillate around the design trajectory. This is known as *weak focusing* and only appears in the horizontal plane.
- Finally, the term -hxδ represents dispersion, i.e. particles with different momentum from the design will be deflected by different amounts by the magnet.

#### Dipole magnet – equations of motion (weak focusing)

• Apply Hamilton's equations (assume k<sub>0</sub> = h)

$$\begin{aligned} x' &= \frac{dx}{ds} = \frac{\partial H}{\partial p_x} = p_x \\ p'_x &= \frac{dp_x}{ds} = -\frac{\partial H}{\partial x} = -hk_0x + h\delta \end{aligned}$$

$$y' = \frac{dy}{ds} = \frac{\partial H}{\partial p_y} = p_y$$
$$p'_y = \frac{dp_y}{ds} = -\frac{\partial H}{\partial y} = 0$$

• In the case  $\delta$ =0, it follows

where  $\omega = \sqrt{hk_0}$ 

#### Dipole magnet – transfer matrix

• It is convenient to express the map of a dipole magnet of length L in the form of a transfer matrix

$$M_{dip} = \begin{pmatrix} \cos\omega L & \frac{\sin\omega L}{\omega} & 0 & 0 & 0 & \frac{1-\cos\omega L}{\omega\beta_0} \\ -\omega\sin\omega L & \cos\omega L & 0 & 0 & 0 & \frac{\sin\omega L}{\beta_0} \\ 0 & 0 & 1 & L & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -\frac{\sin\omega L}{\beta_0} & -\frac{1-\cos\omega L}{\omega\beta_0} & 0 & 0 & 1 & \frac{L}{\beta_0^2\gamma_0^2} - \frac{\omega L-\sin\omega L}{\omega\beta_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

• M will multiply the phase space vector  $z = (x, p_x, y, p_y, \tau, p_\tau)$ 

$$z_1 = M z_0$$

#### Quadrupole magnet (Hamiltonian)

Starting with vector potential for a quadrupole

$$A_x = 0, \quad A_y = 0, \quad A_s = -\frac{g}{1+hx} \left(\frac{x^2}{2} - \frac{y^2}{2}\right) \qquad \text{ where } \quad g = \frac{\partial B}{\partial x} = -\frac{\partial B}{\partial y}$$

Use curl equations to find field equations

$$B_x = gy, \quad B_y = gx, \quad B_s = 0$$

The vector potential leads to the following Hamiltonian (the norm. quadrupole strength  $k_1 = eg/p$ ).

$$H = \frac{p_{\tau}}{\beta_0} - (1 + hx)\sqrt{(1 + \delta)^2 - p_x^2 - p_y^2} + \frac{1}{2}k_1\left(x^2 - y^2\right)$$



Assuming a straight quadrupole, h=0, the expanded Hamiltonian can be written

$$H pprox rac{p_x^2 + p_y^2}{2} + k_1 rac{x^2 - y^2}{2} + rac{1}{2eta_0^2 \gamma_0^2} p_ au^2$$

#### Quadrupole magnet (transfer matrix)

• The "focusing" quadrupole transfer matrix  $(k_1 > 0)$  is

$$M_{quad} = \begin{pmatrix} \cos \omega L & \frac{\sin \omega L}{\omega} & 0 & 0 & 0 & 0\\ -\omega \sin \omega L & \cos \omega L & 0 & 0 & \frac{\sin \omega L}{\beta_0} \\ 0 & 0 & \cosh \omega L & \frac{\sinh \omega L}{\omega} & 0 & 0\\ 0 & 0 & \omega \sinh \omega L & \cosh \omega L & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & \frac{L}{\beta_0^2 \gamma_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

where  $\omega = \sqrt{k_1}$ 

#### Symplectic integration of a Harmonic Oscillator (1)

• The Hamiltonian for a harmonic oscillator in one dimension is

$$H = H_{true} = \frac{1}{2} \left( p^2 + q^2 \right)$$

where the potential energy is  $U(q) = q^2/2$ . The equations of motion follow

$$\dot{q} = rac{\partial H}{\partial p} = p$$
  
 $\dot{p} = -rac{\partial H}{\partial q} = -q$ 

The exact evolution is given by

$$\begin{pmatrix} q(\tau) \\ p(\tau) \end{pmatrix} = M \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} = \begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}$$

### Symplectic integration of a Harmonic Oscillator (2)

• Note the symplectic condition is met (M $\Omega$ M =  $\Omega$ )

$$\begin{pmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \cos\tau & -\sin\tau \\ \sin\tau & \cos\tau \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

This condition must be satisfied to preserve phase space volume under evolution (Liouville). Next, expand cosine and sine terms to first order (cos τ ~ 1, sin τ ~ τ).

$$\left(\begin{array}{c}q(\tau)\\p(\tau)\end{array}\right) = \left(\begin{array}{cc}1&\tau\\-\tau&1\end{array}\right) \left(\begin{array}{c}q(0)\\p(0)\end{array}\right)$$

• The symplectic condition is not satisfied in this case and furthermore

$$\left| det \left( \begin{array}{cc} 1 & \tau \\ -\tau & 1 \end{array} \right) \right| = 1 + \tau^2$$

### Symplectic integration of a Harmonic Oscillator (3)

• The energy after one timestep

$$H_{integrated} = \frac{1}{2} \left( p(\tau)^2 + q(\tau)^2 \right) = \frac{1}{2} (1 + \tau^2) \left( p^2 + q^2 \right)$$

• The increase in energy will cause the trajectory to spiral outwards. A *symplectic integration* (one that preserves phase space volume) can be created as follows

$$\left(\begin{array}{c}q(\tau)\\p(\tau)\end{array}\right) = \left(\begin{array}{cc}1&\tau\\-\tau&1-\tau^2\end{array}\right) \left(\begin{array}{c}q(0)\\p(0)\end{array}\right)$$

• Although the symplectic condition is now met, the effective Hamiltonian becomes

$$H_{integrated} = \frac{1}{2} \left( p^2 + q^2 \right) + \frac{\tau}{2} p q$$

Since H<sub>integrated</sub> is conserved in this case, the difference between it and H<sub>true</sub> is a constant and the motion remains bounded.

#### Symplectic integrator – splitting the Hamiltonian (1)

• In general, a symplectic integrator is constructed by splitting the Hamiltonian into R and K that depend on momentum and coordinates only, respectively. In 1D we can write

$$H = \frac{p_x^2}{2} + V(x) = R(p_x) + K(x)$$

• The Lie operator for R and for K become

$$: R: x = \frac{\partial R}{\partial x} \frac{\partial x}{\partial p_x} - \frac{\partial R}{\partial p_x} \frac{\partial x}{\partial x} = -\frac{\partial R}{\partial p_x} \qquad : K: x = \frac{\partial K}{\partial x} \frac{\partial x}{\partial p_x} - \frac{\partial K}{\partial p_x} \frac{\partial x}{\partial x} = 0$$
$$: R: p_x = \frac{\partial R}{\partial x} \frac{\partial p_x}{\partial p_x} - \frac{\partial R}{\partial p_x} \frac{\partial p_x}{\partial x} = 0 \qquad : K: p_x = \frac{\partial K}{\partial x} \frac{\partial p_x}{\partial p_x} - \frac{\partial K}{\partial p_x} \frac{\partial p_x}{\partial x} = \frac{\partial K}{\partial x}$$

#### Symplectic integrator – splitting the Hamiltonian (2)

• Applying the Lie transform, it is clear that the Hamiltonian K (the "kick") updates the momentum only

$$e^{:K:}x = x + :K:x = x$$
  
 $e^{:K:}p_x = p_x + :K:p_x = p_x + \frac{\partial K}{\partial x}$ 

while the Hamiltonian R (the "drift") updates the position alone

$$e^{:R:}x = x - rac{\partial R}{\partial p_x}$$
 $e^{:R:}p_x = p_x$ 

#### First order integrator – symplectic Euler

To first order we can write

$$e^{-t:R(p_x)+K(x)} = e^{-t:R(p_x)}e^{-t:K(x)}$$

• This is the symplectic Euler method. Dividing the interval into steps of length h

$$p_{n+1} = p_n - h \frac{dK}{dx} (q_n)$$
$$q_{n+1} = q_n + h \frac{dR}{dp_x} (p_{n+1})$$

 Note, the standard ("explicit") Euler method is non-symplectic as in the lower equation the derivative of R is evaluated at p<sub>n</sub> rather than p<sub>n+1</sub>.



#### M. Leok - "Introduction to geometrical numerical integration", link to Youtube video

#### Second order integrator – drift-kick-drift



Figure: One step of a symplectic Euler integrator (left) and second order leapfrog (right). [S. Baturin]

If the Hamiltonian is split as follows

$$H = \frac{1}{2}R(p_x) + K(x) + \frac{1}{2}R(p_x)$$

then to second order

$$e^{-t:\frac{1}{2}R(p_x)+K(x)+\frac{1}{2}R(p_x)} = e^{-t:\frac{1}{2}R(p_x)}e^{-t:K(x)}e^{t:\frac{1}{2}R(p_x)}$$

This is known as the *drift-kick-drift* integrator (also known as leapfrog or Störmer-Verlet integrator)

### Second order integrator – kick-drift-kick

• In simplified terms, the kick-drift-kick integrator is given by

$$p_{n+1/2} = p_n + rac{h}{2} rac{\partial K}{\partial q} (q_n)$$
  
 $x_{n+1} = x_n + hp_{n+1/2},$   
 $p_n = p_{n+1/2} + rac{h}{2} rac{\partial K}{\partial q} (q_{n+1})$ 



#### Fourth order integrator – Yoshida



Figure: One step of the fourth order Yoshida integrator. [S. Baturin]

Yoshida found that a set of integrators at order 2n can be found by building on the second order integrator S<sub>2</sub>  $S_4 = S_2(\gamma t) \circ S_2(\kappa t) \circ S_2(\gamma t)$ where  $\gamma = 1/(2 - 2^{1/3})$ ,  $\kappa = 1/[2^{1/3}(2 - 2^{1/3})]$ 

H. Yoshida, "Construction of higher order symplectic integrators", Physics Letters A, vol. 150, no. 5, pp. 262 – 268, 1990.

# Integrability

• The ideal linear Hamiltonian

$$H = Q_x J_x + Q_y J_y$$

has two invariants of motion, the transverse actions  $J_x$ ,  $J_y$ . This ensure the system is integrable.

- However, the addition of nonlinearities may compromise this integrability and lead to a reduction in the dynamic aperture.
- Nonlinear magnets may be added intentionally, for example sextupole magnets to correct chromaticity, or arise from magnet imperfections or other sources

### A non-integrable Hamiltonian – the Hénon-Heiles system



• The Hénon-Heiles potential may be written

$$V(x,y) = \frac{1}{2} \left( x^2 + y^2 \right) + x^2 y - \frac{1}{3} y^3$$

with Hamiltonian

$$H = \frac{1}{2} \left( p_x^2 + p_y^2 + x^2 + y^2 \right) + x^2 y - \frac{1}{3} y^3 = E$$

- This is a time-independent Hamiltonian. It is integrable only for limited number of initial conditions.
- The potential can be realised by adding a sextupole to a linear lattice in such a way that the Hamiltonian is time independent.\*
- \*S.A. Antipov and S. Nagaitsev, "Hénon-Heiles Single particle Dynamics at IOTA", Proc. IPAC2017 WEOAB1

# Hénon-Heiles phase space



- The figure shows Poincare section in the Henon-Heiles cases for increasing values of E.
- The motion tends to be integrable for low values of E but becomes increasingly chaotic as E approaches the escape value E = 1/6.



Figure 6: The dynamic aperture of the accelerator (light blue line) is about 70% of that of the ideal 2D system (black dashed line). Color denotes the FMA amplitude. Sextupole strength  $\alpha = 800 \text{ m}^{-1/2}$ . The aperture is calculated using the particle tracking for  $10^5$  turns; FMA –  $2^{13}$  turns.

## Hamiltonian with nonlinear multipoles

• Multipoles of any order in the Hamiltonian we may written as follows

$$H = \frac{p_x^2 + p_y^2}{2} - \frac{x^2}{2\rho^2} + Re\sum_{n=1}^M \frac{k_n + ij_n}{(n+1)!} (x + iy)^{n+1}$$

• The Hamiltonian may be split into a linear part  $H_0$  and nonlinear part V.

$$H_0 = rac{p_x^2 + p_y^2}{2} - rac{x^2}{2
ho^2} + k_1 rac{x^2 - y^2}{2}$$

$$V = Re \sum_{n \ge 2} \frac{k_n + ij_n}{(n+1)!} (x + iy)^{n+1} = \sum_{n \ge 3} V_{mn} x^m y^m$$

• The V<sub>mn</sub> terms are coefficients for different orders of x and y.

# **Resonance driving terms**

• In action-angle coordinates

$$\begin{split} H(\bar{J},\bar{\phi};s) &= \frac{Q_x J_x + Q_y J_y}{\underset{m_y}{R}} + V(\bar{J},\bar{\phi};s) \\ V(\bar{J},\bar{\phi};s) &= \frac{\epsilon}{R} \sum_{\substack{j=0\\J+k=m_x}}^{m_x} \sum_{\substack{l=0\\J+k=m_y}}^{m_y} J_x^{\frac{j+k}{2}} J_y^{\frac{l+m}{2}} h_{jklm} e^{i[(j-k)\phi_x + (l-m)\phi_y]} \end{split}$$

where  $\varepsilon$  indicates the nonlinear part is a small perturbation. The **h**<sub>jklm</sub> terms are known as *resonance driving* terms.

$$h_{jklm} = \frac{1}{2^{\frac{j+k+l+m}{2}}} \begin{pmatrix} j+k\\ j \end{pmatrix} \binom{l+m}{l} \int_{s_0}^{s_0+2\pi R} V_{j+k,l+m}(s) \beta_x^{\frac{j+k}{2}}(s) \beta_y^{\frac{l+m}{2}}(s) e^{i[(j-k)\phi_x(s)+(l-m)\phi_y(s)]} ds$$

- Each multipole drives a set of resonance driving terms.
- Note terms with j=k, l=m has no angular dependence. This terms result instead result in tune shift with amplitude (e.g. the octupole drives detuning terms h<sub>2200</sub>, h<sub>1111</sub>, h<sub>0022</sub>)

#### Credit: H. Bartosik

#### Resonance driving term examples



Sextupole driven resonance

Octupole driven resonance

Credit: H. Bartosik