1. The leap-frog integrator

The leap frog integrator is a commonly used second order integrator. It operates on dynamical systems that can be written in terms of a Hamiltonian in the form $H(q,p) = T(p) + V(q)$. The kinetic term only depends upon momentum and the potential term only depends on the coordinate. We will take $T(p) = p^2/2$. The equations of motion are

$$
\begin{align*}
\dot{x} &= p \\
\dot{p} &= -\frac{\partial V(q)}{\partial x} 
\end{align*}
$$

A second order integrator for this system is the following

$$
\begin{align*}
q^{n+\frac{1}{2}} &= q^n + \frac{\tau}{2}p^n \\
p^{n+1} &= p^n - \tau \frac{\partial V(q^{n+\frac{1}{2}})}{\partial q} \\
q^{n+1} &= q^{n+\frac{1}{2}} + \frac{\tau}{2}p^{n+1}
\end{align*}
$$

First a half step is taken to update $q$. Then a full step is taken to update $p$. Then another half step is taken to update $q$. The indices refer to the time-step and are not powers and the time-step is $\tau$.

a) Show that the transformation

$$
q^n, p^n \rightarrow q^{n+1}, p^{n+1}
$$

is area preserving. You could compute the Jacobian matrix $J$ with

$$
J = \begin{pmatrix}
\frac{\partial q^{n+1}}{\partial q^n} & \frac{\partial q^{n+1}}{\partial p^n} \\
\frac{\partial p^{n+1}}{\partial q^n} & \frac{\partial p^{n+1}}{\partial p^n}
\end{pmatrix}
$$
and show that its determinant is 1. You could also divide the steps into three pieces

\[ q^n, p^n \rightarrow q^{n+\frac{1}{2}}, p^{n+1} \]
\[ q^{n+\frac{1}{2}}, p^{n+1} \rightarrow q^{n+1}, p^{n+1} \]
\[ q^{n+1}, p^{n+1} \rightarrow q^{n+1}, p^{n+1} \]

and show that the Jacobian for each piece has determinant of 1.

b) Show that the transformation

\[ q^n, p^n \rightarrow q^{n+1}, p^{n+1} \]

is a canonical transformation. This means that the Poisson bracket

\[ \{q^{n+1}, p^{n+1}\} = 1. \]

2. The leap frog integrator, continued

Code examples for a,b are available here [https://astro.pas.rochester.edu/~aquillen/phy411/lectures.html](https://astro.pas.rochester.edu/~aquillen/phy411/lectures.html)

a) Carry out a numerical integration of the harmonic oscillator using the leap frog integrator (which is second order).

b) Carry out a numerical integration of the same dynamical system with the same initial conditions but using a second order Runge-Kutta integrator.

c) Plot the energy error as a function of time. Show that the energy error for leap-frog integrator does not continue to grow with time, but the error in energy for the Runge-Kutta continues to grow.

d) Try choosing a slightly different duration for each timestep to see what happens with the error.

No matter how long you integrate with the leap-frog integrator, the numerically integrated orbit should not continue to diverge in energy from from the original value. The error in energy should oscillate but should not continually grow or shrink. This is because a type of energy is conserved, even if the actual energy is not conserved. This is a handy property of time reversible and symplectic integrators. Note that if you are varying the time step during the integration, you would lose this nice property of the integrator.
3. Two-forms

A two-form is a function of two vectors. When a two-form is applied to two vectors you get a function. The function depends on coordinates. At the point \( \mathbf{x} = (x_1, x_2, x_3) = (2, 0, 0) \) calculate the values of the two forms \( \omega_1, \omega_2, \omega_3 \) on the two vectors \( \xi, \eta \). Here are the two forms:

\[
\begin{align*}
\omega_1 &= dx_2 \wedge dx_3, \\
\omega_2 &= x_1 dx_3 \wedge dx_2 \\
\omega_3 &= dx_3 \wedge dr^2 
\end{align*}
\]

with \( r^2 = x_1^2 + x_2^2 + x_3^2 \). Here are the two vectors

\[
\xi = (1, 1, 1) \quad \text{and} \quad \eta = (1, 2, 3)
\]

Answer: \( \omega_1 \) gives 1, \( \omega_2 \) gives -2, \( \omega_3 \) gives -8. This problem is from Arnold’s book.

4. Cartan’s magic formula

The Lie derivative of a differential form \( \omega \) satisfies

\[
\mathcal{L}_X \omega = i_X d\omega + d(i_X \omega)
\]

This is known as Cartan’s magic formula. Here \( X \) is a vector, \( d \) is the exterior derivative and \( i_X \) gives a contraction. For example \( i_X \omega = \langle X, \omega \rangle = X^i \omega^i \) if \( \omega \) is a one-form and \( X \) a vector.

Show that

\[
d \mathcal{L}_X \omega = \mathcal{L}_X (d\omega)
\]

Hint: \( d^2 \) of anything is zero. Use Cartan’s formula on both sides of the equation.

5. Distance to resonance

Consider a pendulum-like Hamiltonian

\[
H(p, \phi) = \frac{1}{2}ap^2 + bp + \epsilon \cos \phi
\]

(a) Assuming that \( \phi \) is an angle, show that the coefficient \( b \) is a frequency. (This is a question of dimensional analysis).
(b) Find a canonical transformation and new coordinates that transform the Hamiltonian into the form
\[ K(p', \phi') = \frac{1}{2} b' p'^2 + \epsilon' \cos \phi' \]

**Remarks:** The coefficient \( b \) shifts the level curves vertically (in the \( p \) direction) on a plot of level curves of \( H(p, \phi) \). Only with \( b = 0 \) are the fixed points located along \( p = 0 \). If you subtract a constant from a Hamiltonian, Hamilton’s equations are unchanged.

We can consider \( ap^2 + bp \) as the expansion of an integrable system around a particular value of \( p \). The term \( \epsilon \cos \phi \) can be considered a perturbation. We sometimes refer to \( b \) as a frequency that sets the distance to resonance.

### 6. First order canonical transformations

(a) Consider a Hamiltonian with a time dependent perturbation
\[ H(I, \theta, t) = I \omega + \epsilon I^{1/2} \cos(\Omega_p t) \]

Find new variables \( J, \phi \) such that the Hamiltonian becomes
\[ K(J, \phi) = J \omega \]
and so is in action angle variables and is time independent.

Hint: Try a generating function in the form
\[ S_2(\theta, J) = \theta J + f(J) g(\Omega_p t) \]
with functions \( f() \) and \( g() \) to be determined.

(b) Show that the system (prior to canonical transformation) is equivalent to a time independent Hamiltonian system \( K(I, \theta, J, \alpha) \) in 4-dimensional phase space with new coordinate angle \( \alpha \) with \( \dot{\alpha} = \Omega_p \) and new momentum \( J \) that is conjugate to \( \alpha \).

### 7. Shearing Sheet

The shearing sheet approximation gives equations of motion near a circular orbit in an axisymmetric potential. An approximate Hamiltonian (in units of angular rotation rate and radius equal 1).

\[ H(x, y; p_x, p_y) \approx \frac{p_y^2}{2} + \frac{p_x^2}{2} - 2p_xy + \frac{\kappa^2 y^2}{2} \]  
(4)
With epicyclic frequency $\kappa = 1$ (for the Keplerian setting) we can recover Hill’s equations.

Show that $p_x$ is a conserved quantity.

As there is a fixed point at $x = 0, y = 0, p_x = 0, p_y = 0$ and the Hamiltonian is quadratic, this Hamiltonian can be written in the form

$$H = \frac{1}{2} x M x$$

with $M$ the Hessian matrix and $x = (x, y, p_x, p_y)$. Equations of motion are

$$\dot{x} = \omega M x$$

where $\omega$ is a symplectic type of identity matrix.

Find $M$.

Eigenvalues of $(\omega M)^2$ are the oscillation frequencies.

Find a set of canonical coordinates that give action angle variables. One way to do this is to use a generating function that looks like

$$F(y, \phi, p_x, X) = \frac{\kappa}{2} (y - ap_x)^2 \tan \phi + p_x X$$

and to look for a suitable value of $a$.

8. Complex notation and polynomial expansions

It is sometimes convenient to define

$$z = q + ip$$
$$\bar{z} = q - ip$$

Show that

$$\{z, \bar{z}\} = -2i$$

These are not canonical coordinates.

If $H(p, q)$ is written as $H(z, \bar{z})$ using Poisson brackets show that

$$\dot{z} = -i \frac{\partial H}{\partial \bar{z}}$$
$$\dot{\bar{z}} = i \frac{\partial H}{\partial z}$$
Define an operator
\[ D \equiv q \frac{\partial}{\partial p} - p \frac{\partial}{\partial q} \]

Show that
\[ D z^a \bar{z}^b = i(a - b) z^a \bar{z}^b \]
for integers \( a, b \). Define a pseudo inverse operator
\[ D^{-1} z^a \bar{z}^b \equiv \frac{1}{i(a - b)} z^a \bar{z}^b \]

\( D \) and \( D^{-1} \) do not change the order of a polynomial.

Compute \( D z^2 \bar{z} \) and \( D^{-1} z^2 \bar{z} \).

Let \( I(p, q) = \frac{1}{2}(p^2 + q^2) \). Show that \( D(I(p, q)^n) = 0 \) for any integer \( n > 0 \). Here \( n \) is the exponent of \( I \).

We look at a Hamiltonian that is a harmonic oscillator plus an additional higher order term
\[ H(p, q) = I(p, q) + H_3(p, q) \quad (5) \]
where \( H_3 \) is a polynomial in \( p, q \) that is degree three (contains terms like \( q^2 p \) and \( p^3 \) so that when you sum the exponents of \( p, q \) you get 3).

Choose a function \( w(p, q) = D^{-1} H_3 \). What is the degree of \( w \)?

We make a canonical transformation with generating function
\[ S(q, P) = qP + w(q, P) \]

Show that to second order in the polynomials of \( p, q \),
\[ p = P + \frac{\partial w}{\partial q} \]
\[ q = Q - \frac{\partial w}{\partial P} \]

Insert these into equation (5) and show that you can remove \( H_3 \) with the canonical transformation (to the next order).

Remarks. As long as there are no resonances this procedure can be used to transform a Hamiltonian expanded near a fixed point into action angle coordinates. The theory of Birkhoff normal forms is tersely introduced in Appendix 7 by Arnold in his book on Math Methods of Classical Mechanics.
9. On the small divisor problem with a single resonant perturbation

(a) Consider a Hamiltonian with a small perturbation term

\[ H(I, \theta) = g(I) + \epsilon h(I) \cos \theta \]

where \(\epsilon\) is small. Using a generating function in the form

\[ S_2(\theta, J) = \theta J + \epsilon f(\theta, J) \]

show that the Hamiltonian can be put via canonical transformation into a form \(K(J, \phi) = g(J) + O(\epsilon^2)\) that to first order only depends on action variables.

Hint: Assume that \(f(\theta, J)\) is separable and either proportional to \(\sin \theta\) or \(\cos \theta\).

(b) Consider the multidimensional Hamiltonian

\[ H(I, \theta) = g(I) + \epsilon \cos(k \cdot \theta) \]

where \(k\) is a vector of \(N\) integers. Momenta and angles \(I, \theta\) are \(N\) dimensional. The frequencies

\[ \omega(I) = \nabla g(I) \]

What condition on \(k\) and \(\omega\) allows the Hamiltonian to be put via canonical transformation into the form \(K(J, \phi) = f(J) + O(\epsilon^2)\) using the canonical transformation in the form of part a)?

Remark: As long as there is no commensurability (the angle \(\phi = k \cdot \theta\) is not slow), then it is possible to remove the perturbation term to first order from the Hamiltonian with a first order canonical transformation. Near the commensurability or resonance, to first order, the new coordinates diverge.

(c) Consider the possibility that \(\phi\) is a slow angle. We can transfer to a new canonical coordinate system with new angle \(\phi = k \cdot \theta\). Use the generating function of old angles \((\theta)\) and new momenta \((J_1, J_2, J_3, \ldots J_N)\)

\[ F_2 = J_1(k \cdot \theta) + \sum_{i=2}^{N} J_i \theta_i \]

to show that this Hamiltonian has \(N\) conserved quantities and so is integrable.

Hints: Energy can be a conserved quantity. If the Hamiltonian lacks a coordinate then the momentum conjugate to the coordinate is conserved.

Remark: In this coordinate system there are no divergences.
(d) Are there fixed points in the Hamiltonian that you find in part c)?

(e) Consider initial values for the momenta $I_0$ and $k = (2, 5)$ so that $\phi = 2\theta_1 + 5\theta_2$ and frequencies such that

$$k \cdot \omega(I_0) = 0$$

The system has initial angles $\theta_0$ where $\theta$ is the vector of angles. Denote the frequency vector as $\omega(I_0) = (\omega_1, \omega_2)$. Assume that $\epsilon$ is extremely small (like zero).

In terms of period $P = \frac{2\pi}{\omega_1}$ how long does it take the system to return to the initial values of all its angles $\theta_0$?

Remark: In this setting a fixed point in the transformed Hamiltonian is equivalent to a periodic orbit in the original Hamiltonian.

10. Canonical Transformation to a frame in a Rotating Coordinate System

Consider the following Hamiltonian that has been used to represent a fourth order epicyclic approximation near a Lindblad resonance with a spiral or bar pattern in a galaxy disk that is moving with pattern speed $\Omega_p$

$$H(I_1, \theta_1; I_2, \theta_2; t) = \Omega I_2 + \kappa I_1 + aI_1^2 + bI_2^2 + cI_1I_2 + \epsilon I_1^{1/2} \cos(\theta_1 - m(\theta_2 - \Omega_p t))$$

where $m$ is an integer. Here $\Omega$ and $\kappa$ are the angular rotation rate and epicyclic frequency and both are approximately functions of orbital radius. Coefficients $a, b, c$ are also approximately functions of radius in the galaxy. Here $I_2$ is related to the angular momentum of the orbit and $I_1$ the epicyclic amplitude. The parameter $\epsilon$ depends on the bar or spiral perturbation strength.

Consider the following generating function

$$F_2(\theta_1, \theta_2; J_1, J_2) = [\theta_1 - m(\theta_2 - \Omega_p t)]J_1 + \theta_2J_2$$

that is a function of old coordinates and new momenta.

(a) Following a canonical transformation find the form of the Hamiltonian in new coordinates and show that $I_2 + mI_1$ is a conserved quantity. Is energy in the new coordinate system conserved?

(b) In what way is $[(c - 2bm)(I_2 + mI_1) + \kappa - m(\Omega - \Omega_p)]$ the distance to the resonance?

Hint: After transformation, the system is only a function of a single momentum and coordinate (as the other momentum is conserved). It may be
possible to group terms so that the Hamiltonian resembles a lower dimensional one, in the form
\[ H(p, \phi) = ap^2 + bp + f(p) \cos \phi, \]
with constants \(a, b\).

(c) Is there a small divisor problem with this coordinate transformation?

11. On Constraints – Variational equations

Consider the Lagrangian
\[ L(x, y, z, \dot{x}, \dot{y}) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - mgz \]
with constraint
\[ y\dot{x} - x\dot{y} = 0 \quad (6) \]

The problem seems to conserve angular momentum about the origin in \(z\) while being under the influence of gravity.

(a) Is the constraint holonomic or non-holonomic?

(b) Using the Lagrange-d’Alembert equations of motion, find the equations of motion. These assume that an action is minimized only over paths that satisfy the constraint. You don’t need to solve for \(x, y, z\) as a function of time.

Writing the constraint in the form \(a_x\dot{x} + a_y\dot{y} = 0\), the Lagrange-d’Alembert equations of motion are
\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x} + \lambda a_x \]
\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{y}} = \frac{\partial L}{\partial y} + \lambda a_y \]

(c) Use the Lagrangian with Lagrange multipliers
\[ \tilde{L}(x, \dot{x}, \lambda) = L(x, \dot{x}) + \lambda(y\dot{x} - x\dot{y}) \]
to find the equations of motion. These are known as the variational non-holonomic or vakonomic equations of motion.

(d) Are these two equations of motion the same?

Consider the Lagrangian
\[ L(x, y, z, \dot{x}, \dot{y}, \dot{z}) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) \]
with constraint

\[ \dot{z} - y\dot{x} = 0 \]

These problems are from the book by A. M. Block. The second problem is by Rosenberg 1977.

(e) Again find the two sets of equations of motion and compare them.

Notes: I find it hard to work with the vaganomic constraints as \( \lambda(t) \) making the solutions depend on \( \lambda \) and \( \dot{\lambda} \). Seems like there is a variety of solutions.

12. Propose and work on your own problem!